

ForceBalance Developer API Guide version 1.3

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Contents

1 Project Roadmap	2
1.1 Most Recently Implemented (version 1.3.0):	2
1.2 Current Development Goals, for version 1.3.1:	2
1.3 Longterm Development Ideas	2
2 Todo List	3
3 Namespace Index	4
3.1 Packages	4
4 Hierarchical Index	6
4.1 Class Hierarchy	6
5 Class Index	9
5.1 Class List	9
6 File Index	13
6.1 File List	13
7 Namespace Documentation	14
7.1 forcebalance Namespace Reference	14
7.1.1 Variable Documentation	15
7.2 forcebalance.abinitio Namespace Reference	16
7.2.1 Detailed Description	16
7.2.2 Function Documentation	16
7.2.3 Variable Documentation	16
7.3 forcebalance.abinitio_internal Namespace Reference	16
7.3.1 Detailed Description	17
7.4 forcebalance.amberio Namespace Reference	17
7.4.1 Detailed Description	17
7.4.2 Function Documentation	18
7.4.3 Variable Documentation	18
7.5 forcebalance.binding Namespace Reference	18
7.5.1 Detailed Description	19
7.5.2 Function Documentation	19
7.5.3 Variable Documentation	19
7.6 forcebalance.chemistry Namespace Reference	19
7.6.1 Function Documentation	20
7.6.2 Variable Documentation	20
7.7 forcebalance.contact Namespace Reference	21
7.7.1 Function Documentation	21
7.8 forcebalance.counterpoise Namespace Reference	22
7.8.1 Detailed Description	22
7.8.2 Variable Documentation	22
7.9 forcebalance.custom_io Namespace Reference	23
7.9.1 Detailed Description	23
7.9.2 Variable Documentation	23
7.10 forcebalance.engine Namespace Reference	24
7.10.1 Variable Documentation	24
7.11 forcebalance.finite_difference Namespace Reference	24
7.11.1 Function Documentation	25
7.11.2 Variable Documentation	27
7.12 forcebalance.forcefield Namespace Reference	27

7.12.1	Detailed Description	27
7.12.2	Function Documentation	28
7.12.3	Variable Documentation	29
7.13	forcebalance.gmxio Namespace Reference	29
7.13.1	Detailed Description	30
7.13.2	Function Documentation	31
7.13.3	Variable Documentation	32
7.14	forcebalance.interaction Namespace Reference	33
7.14.1	Detailed Description	34
7.14.2	Variable Documentation	34
7.15	forcebalance.leastsq Namespace Reference	34
7.15.1	Function Documentation	34
7.15.2	Variable Documentation	34
7.16	forcebalance.lipid Namespace Reference	34
7.16.1	Detailed Description	35
7.16.2	Function Documentation	35
7.16.3	Variable Documentation	35
7.17	forcebalance.liquid Namespace Reference	35
7.17.1	Detailed Description	35
7.17.2	Function Documentation	35
7.17.3	Variable Documentation	35
7.18	forcebalance.Mol2 Namespace Reference	36
7.18.1	Variable Documentation	36
7.19	forcebalance.mol2io Namespace Reference	36
7.19.1	Detailed Description	36
7.19.2	Variable Documentation	36
7.20	forcebalance.molecule Namespace Reference	37
7.20.1	Function Documentation	38
7.20.2	Variable Documentation	42
7.21	forcebalance.moments Namespace Reference	44
7.21.1	Detailed Description	44
7.21.2	Variable Documentation	44
7.22	forcebalance.nifty Namespace Reference	44
7.22.1	Detailed Description	46
7.22.2	Function Documentation	47
7.22.3	Variable Documentation	56
7.23	forcebalance.objective Namespace Reference	57
7.23.1	Detailed Description	57
7.23.2	Variable Documentation	57
7.24	forcebalance.openmmio Namespace Reference	58
7.24.1	Detailed Description	59
7.24.2	Function Documentation	59
7.24.3	Variable Documentation	61
7.25	forcebalance.optimizer Namespace Reference	62
7.25.1	Detailed Description	62
7.25.2	Function Documentation	62
7.25.3	Variable Documentation	63
7.26	forcebalance.output Namespace Reference	63
7.27	forcebalance.parser Namespace Reference	63
7.27.1	Detailed Description	64
7.27.2	Function Documentation	65
7.27.3	Variable Documentation	66
7.28	forcebalance.psi4io Namespace Reference	67
7.28.1	Detailed Description	67

7.28.2	Variable Documentation	68
7.29	forcebalance.PT Namespace Reference	68
7.29.1	Variable Documentation	68
7.30	forcebalance.qchemio Namespace Reference	68
7.30.1	Detailed Description	69
7.30.2	Function Documentation	69
7.30.3	Variable Documentation	69
7.31	forcebalance.quantity Namespace Reference	70
7.31.1	Function Documentation	70
7.31.2	Variable Documentation	71
7.32	forcebalance.target Namespace Reference	71
7.32.1	Variable Documentation	71
7.33	forcebalance.thermo Namespace Reference	71
7.33.1	Variable Documentation	71
7.34	forcebalance.tinkerio Namespace Reference	71
7.34.1	Detailed Description	72
7.34.2	Function Documentation	72
7.34.3	Variable Documentation	73
7.35	forcebalance.vibration Namespace Reference	74
7.35.1	Detailed Description	74
7.35.2	Function Documentation	74
7.35.3	Variable Documentation	74
8	Class Documentation	75
8.1	forcebalance.abinitio.AblInitio Class Reference	75
8.1.1	Detailed Description	79
8.1.2	Constructor & Destructor Documentation	79
8.1.3	Member Function Documentation	79
8.1.4	Member Data Documentation	92
8.2	forcebalance.amberio.AblInitio_AMBER Class Reference	96
8.2.1	Detailed Description	101
8.2.2	Constructor & Destructor Documentation	102
8.2.3	Member Function Documentation	102
8.2.4	Member Data Documentation	114
8.3	forcebalance.gmxio.AblInitio_GMX Class Reference	118
8.3.1	Detailed Description	123
8.3.2	Constructor & Destructor Documentation	124
8.3.3	Member Function Documentation	124
8.3.4	Member Data Documentation	136
8.4	forcebalance.abinitio_internal.AblInitio_Internal Class Reference	140
8.4.1	Detailed Description	145
8.4.2	Constructor & Destructor Documentation	146
8.4.3	Member Function Documentation	146
8.4.4	Member Data Documentation	158
8.5	forcebalance.openmmio.AblInitio_OpenMM Class Reference	162
8.5.1	Detailed Description	167
8.5.2	Constructor & Destructor Documentation	168
8.5.3	Member Function Documentation	168
8.5.4	Member Data Documentation	180
8.6	forcebalance.tinkerio.AblInitio_TINKER Class Reference	184
8.6.1	Detailed Description	189
8.6.2	Constructor & Destructor Documentation	190
8.6.3	Member Function Documentation	190
8.6.4	Member Data Documentation	202

8.7	forcebalance.forcefield.BackedUpDict Class Reference	206
8.7.1	Detailed Description	207
8.7.2	Constructor & Destructor Documentation	207
8.7.3	Member Function Documentation	207
8.7.4	Member Data Documentation	207
8.8	forcebalance.BaseClass Class Reference	207
8.8.1	Detailed Description	209
8.8.2	Constructor & Destructor Documentation	209
8.8.3	Member Function Documentation	209
8.8.4	Member Data Documentation	209
8.9	forcebalance.BaseReader Class Reference	209
8.9.1	Detailed Description	211
8.9.2	Constructor & Destructor Documentation	211
8.9.3	Member Function Documentation	211
8.9.4	Member Data Documentation	212
8.10	forcebalance.binding.BindingEnergy Class Reference	212
8.10.1	Detailed Description	215
8.10.2	Constructor & Destructor Documentation	215
8.10.3	Member Function Documentation	215
8.10.4	Member Data Documentation	225
8.11	forcebalance.gmxio.BindingEnergy_GMX Class Reference	226
8.11.1	Detailed Description	230
8.11.2	Constructor & Destructor Documentation	230
8.11.3	Member Function Documentation	230
8.11.4	Member Data Documentation	240
8.12	forcebalance.openmmio.BindingEnergy_OpenMM Class Reference	241
8.12.1	Detailed Description	245
8.12.2	Constructor & Destructor Documentation	245
8.12.3	Member Function Documentation	245
8.12.4	Member Data Documentation	255
8.13	forcebalance.tinkerio.BindingEnergy_TINKER Class Reference	256
8.13.1	Detailed Description	260
8.13.2	Constructor & Destructor Documentation	260
8.13.3	Member Function Documentation	260
8.13.4	Member Data Documentation	270
8.14	forcebalance.output.CleanFileHandler Class Reference	271
8.14.1	Detailed Description	272
8.14.2	Member Function Documentation	272
8.15	forcebalance.output.CleanStreamHandler Class Reference	273
8.15.1	Detailed Description	273
8.15.2	Constructor & Destructor Documentation	273
8.15.3	Member Function Documentation	274
8.16	forcebalance.counterpoise.Counterpoise Class Reference	274
8.16.1	Detailed Description	277
8.16.2	Constructor & Destructor Documentation	277
8.16.3	Member Function Documentation	277
8.16.4	Member Data Documentation	289
8.17	forcebalance.engine.Engine Class Reference	290
8.17.1	Detailed Description	291
8.17.2	Constructor & Destructor Documentation	292
8.17.3	Member Function Documentation	292
8.17.4	Member Data Documentation	292
8.18	forcebalance.forcefield.FF Class Reference	293
8.18.1	Detailed Description	295

8.18.2	Constructor & Destructor Documentation	295
8.18.3	Member Function Documentation	296
8.18.4	Member Data Documentation	304
8.19	forcebalance.output.ForceBalanceLogger Class Reference	306
8.19.1	Detailed Description	307
8.19.2	Constructor & Destructor Documentation	307
8.19.3	Member Function Documentation	307
8.19.4	Member Data Documentation	307
8.20	forcebalance.amberio.FrcMod_Reader Class Reference	307
8.20.1	Detailed Description	309
8.20.2	Constructor & Destructor Documentation	309
8.20.3	Member Function Documentation	309
8.20.4	Member Data Documentation	310
8.21	forcebalance.psi4io.GBS_Reader Class Reference	310
8.21.1	Detailed Description	312
8.21.2	Constructor & Destructor Documentation	312
8.21.3	Member Function Documentation	312
8.21.4	Member Data Documentation	313
8.22	forcebalance.custom_io.Gen_Reader Class Reference	314
8.22.1	Detailed Description	315
8.22.2	Constructor & Destructor Documentation	315
8.22.3	Member Function Documentation	315
8.22.4	Member Data Documentation	316
8.23	forcebalance.gmxio.GMX Class Reference	316
8.23.1	Detailed Description	319
8.23.2	Constructor & Destructor Documentation	319
8.23.3	Member Function Documentation	319
8.23.4	Member Data Documentation	325
8.24	forcebalance.psi4io.Grid_Reader Class Reference	327
8.24.1	Detailed Description	329
8.24.2	Constructor & Destructor Documentation	329
8.24.3	Member Function Documentation	329
8.24.4	Member Data Documentation	329
8.25	forcebalance.interaction.Interaction Class Reference	330
8.25.1	Detailed Description	333
8.25.2	Constructor & Destructor Documentation	333
8.25.3	Member Function Documentation	333
8.25.4	Member Data Documentation	343
8.26	forcebalance.gmxio.Interaction_GMX Class Reference	345
8.26.1	Detailed Description	348
8.26.2	Constructor & Destructor Documentation	348
8.26.3	Member Function Documentation	349
8.26.4	Member Data Documentation	358
8.27	forcebalance.openmmio.Interaction_OpenMM Class Reference	360
8.27.1	Detailed Description	363
8.27.2	Constructor & Destructor Documentation	363
8.27.3	Member Function Documentation	364
8.27.4	Member Data Documentation	373
8.28	forcebalance.tinkerio.Interaction_TINKER Class Reference	375
8.28.1	Detailed Description	378
8.28.2	Constructor & Destructor Documentation	378
8.28.3	Member Function Documentation	379
8.28.4	Member Data Documentation	388
8.29	forcebalance.gmxio.ITP_Reader Class Reference	390

8.29.1	Detailed Description	392
8.29.2	Constructor & Destructor Documentation	392
8.29.3	Member Function Documentation	392
8.29.4	Member Data Documentation	393
8.30	forcebalance.leastsq.LeastSquares Class Reference	394
8.30.1	Detailed Description	397
8.30.2	Constructor & Destructor Documentation	397
8.30.3	Member Function Documentation	397
8.30.4	Member Data Documentation	407
8.31	forcebalance.nifty.LineChunker Class Reference	408
8.31.1	Detailed Description	409
8.31.2	Constructor & Destructor Documentation	409
8.31.3	Member Function Documentation	409
8.31.4	Member Data Documentation	410
8.32	forcebalance.lipid.Lipid Class Reference	410
8.32.1	Detailed Description	414
8.32.2	Constructor & Destructor Documentation	414
8.32.3	Member Function Documentation	415
8.32.4	Member Data Documentation	426
8.33	forcebalance.gmxio.Lipid_GMX Class Reference	429
8.33.1	Detailed Description	432
8.33.2	Constructor & Destructor Documentation	433
8.33.3	Member Function Documentation	433
8.33.4	Member Data Documentation	444
8.34	forcebalance.liquid.Liquid Class Reference	447
8.34.1	Detailed Description	449
8.34.2	Constructor & Destructor Documentation	450
8.34.3	Member Function Documentation	450
8.34.4	Member Data Documentation	462
8.35	forcebalance.gmxio.Liquid_GMX Class Reference	464
8.35.1	Detailed Description	467
8.35.2	Constructor & Destructor Documentation	468
8.35.3	Member Function Documentation	468
8.35.4	Member Data Documentation	481
8.36	forcebalance.openmmio.Liquid_OpenMM Class Reference	483
8.36.1	Detailed Description	487
8.36.2	Constructor & Destructor Documentation	488
8.36.3	Member Function Documentation	488
8.36.4	Member Data Documentation	500
8.37	forcebalance.tinkerio.Liquid_TINKER Class Reference	502
8.37.1	Detailed Description	506
8.37.2	Constructor & Destructor Documentation	507
8.37.3	Member Function Documentation	507
8.37.4	Member Data Documentation	520
8.38	forcebalance.output.ModLogger Class Reference	522
8.38.1	Detailed Description	523
8.38.2	Member Function Documentation	523
8.39	forcebalance.Mol2.mol2 Class Reference	523
8.39.1	Detailed Description	524
8.39.2	Constructor & Destructor Documentation	524
8.39.3	Member Function Documentation	524
8.39.4	Member Data Documentation	527
8.40	forcebalance.Mol2.mol2.atom Class Reference	527
8.40.1	Detailed Description	528

8.40.2	Constructor & Destructor Documentation	528
8.40.3	Member Function Documentation	528
8.40.4	Member Data Documentation	530
8.41	forcebalance.Mol2.mol2.bond Class Reference	530
8.41.1	Detailed Description	531
8.41.2	Constructor & Destructor Documentation	531
8.41.3	Member Function Documentation	531
8.41.4	Member Data Documentation	532
8.42	forcebalance.mol2io.Mol2_Reader Class Reference	533
8.42.1	Detailed Description	534
8.42.2	Constructor & Destructor Documentation	534
8.42.3	Member Function Documentation	534
8.42.4	Member Data Documentation	534
8.43	forcebalance.amberio.Mol2_Reader Class Reference	535
8.43.1	Detailed Description	537
8.43.2	Constructor & Destructor Documentation	537
8.43.3	Member Function Documentation	537
8.43.4	Member Data Documentation	537
8.44	forcebalance.Mol2.mol2.set Class Reference	538
8.44.1	Detailed Description	538
8.44.2	Constructor & Destructor Documentation	538
8.44.3	Member Function Documentation	538
8.44.4	Member Data Documentation	538
8.45	forcebalance.molecule.Molecule Class Reference	539
8.45.1	Detailed Description	542
8.45.2	Constructor & Destructor Documentation	543
8.45.3	Member Function Documentation	543
8.45.4	Member Data Documentation	558
8.46	forcebalance.molecule.MolfileTimestep Class Reference	559
8.46.1	Detailed Description	560
8.47	forcebalance.moments.Moments Class Reference	560
8.47.1	Detailed Description	563
8.47.2	Constructor & Destructor Documentation	563
8.47.3	Member Function Documentation	563
8.47.4	Member Data Documentation	573
8.48	forcebalance.gmxio.Moments_GMX Class Reference	574
8.48.1	Detailed Description	578
8.48.2	Constructor & Destructor Documentation	578
8.48.3	Member Function Documentation	578
8.48.4	Member Data Documentation	588
8.49	forcebalance.openmmio.Moments_OpenMM Class Reference	589
8.49.1	Detailed Description	593
8.49.2	Constructor & Destructor Documentation	593
8.49.3	Member Function Documentation	593
8.49.4	Member Data Documentation	603
8.50	forcebalance.tinkerio.Moments_TINKER Class Reference	604
8.50.1	Detailed Description	608
8.50.2	Constructor & Destructor Documentation	608
8.50.3	Member Function Documentation	608
8.50.4	Member Data Documentation	618
8.51	forcebalance.molecule.MyG Class Reference	620
8.51.1	Detailed Description	621
8.51.2	Constructor & Destructor Documentation	621
8.51.3	Member Function Documentation	621

8.51.4 Member Data Documentation	622
8.52 forcebalance.objective.Objective Class Reference	622
8.52.1 Detailed Description	624
8.52.2 Constructor & Destructor Documentation	624
8.52.3 Member Function Documentation	624
8.52.4 Member Data Documentation	625
8.53 forcebalance.openmmio.OpenMM Class Reference	626
8.53.1 Detailed Description	629
8.53.2 Constructor & Destructor Documentation	629
8.53.3 Member Function Documentation	629
8.53.4 Member Data Documentation	635
8.54 forcebalance.openmmio.OpenMM_Reader Class Reference	637
8.54.1 Detailed Description	638
8.54.2 Constructor & Destructor Documentation	638
8.54.3 Member Function Documentation	638
8.54.4 Member Data Documentation	639
8.55 forcebalance.optimizer.Optimizer Class Reference	639
8.55.1 Detailed Description	642
8.55.2 Constructor & Destructor Documentation	642
8.55.3 Member Function Documentation	642
8.55.4 Member Data Documentation	651
8.56 forcebalance.objective.Penalty Class Reference	653
8.56.1 Detailed Description	654
8.56.2 Constructor & Destructor Documentation	654
8.56.3 Member Function Documentation	654
8.56.4 Member Data Documentation	656
8.57 forcebalance.nifty.Pickler_LP Class Reference	656
8.57.1 Detailed Description	657
8.57.2 Constructor & Destructor Documentation	657
8.58 forcebalance.thermo.Point Class Reference	658
8.58.1 Detailed Description	659
8.58.2 Constructor & Destructor Documentation	659
8.58.3 Member Function Documentation	659
8.58.4 Member Data Documentation	659
8.59 forcebalance.qchemio.QCIn_Reader Class Reference	659
8.59.1 Detailed Description	661
8.59.2 Constructor & Destructor Documentation	661
8.59.3 Member Function Documentation	661
8.59.4 Member Data Documentation	662
8.60 forcebalance.quantity.Quantity Class Reference	662
8.60.1 Detailed Description	664
8.60.2 Constructor & Destructor Documentation	664
8.60.3 Member Function Documentation	664
8.60.4 Member Data Documentation	664
8.61 forcebalance.quantity.Quantity_Density Class Reference	665
8.61.1 Detailed Description	666
8.61.2 Constructor & Destructor Documentation	666
8.61.3 Member Function Documentation	666
8.61.4 Member Data Documentation	666
8.62 forcebalance.quantity.Quantity_H_vap Class Reference	667
8.62.1 Detailed Description	668
8.62.2 Constructor & Destructor Documentation	668
8.62.3 Member Function Documentation	668
8.62.4 Member Data Documentation	668

8.63	forcebalance.output.RawFileHandler Class Reference	669
8.63.1	Detailed Description	669
8.63.2	Member Function Documentation	669
8.64	forcebalance.output.RawStreamHandler Class Reference	670
8.64.1	Detailed Description	670
8.64.2	Constructor & Destructor Documentation	670
8.64.3	Member Function Documentation	671
8.65	forcebalance.psi4io.RDVR3_Psi4 Class Reference	671
8.65.1	Detailed Description	674
8.65.2	Constructor & Destructor Documentation	674
8.65.3	Member Function Documentation	674
8.65.4	Member Data Documentation	685
8.66	forcebalance.target.RemoteTarget Class Reference	687
8.66.1	Detailed Description	689
8.66.2	Constructor & Destructor Documentation	690
8.66.3	Member Function Documentation	690
8.66.4	Member Data Documentation	699
8.67	forcebalance.target.Target Class Reference	700
8.67.1	Detailed Description	704
8.67.2	Constructor & Destructor Documentation	704
8.67.3	Member Function Documentation	704
8.67.4	Member Data Documentation	714
8.68	forcebalance.psi4io.THCDF_Psi4 Class Reference	715
8.68.1	Detailed Description	718
8.68.2	Constructor & Destructor Documentation	718
8.68.3	Member Function Documentation	718
8.68.4	Member Data Documentation	730
8.69	forcebalance.thermo.Thermo Class Reference	732
8.69.1	Detailed Description	735
8.69.2	Constructor & Destructor Documentation	735
8.69.3	Member Function Documentation	735
8.69.4	Member Data Documentation	745
8.70	forcebalance.gmxio.Thermo_GMX Class Reference	747
8.70.1	Detailed Description	751
8.70.2	Constructor & Destructor Documentation	751
8.70.3	Member Function Documentation	751
8.70.4	Member Data Documentation	762
8.71	forcebalance.tinkerio.TINKER Class Reference	764
8.71.1	Detailed Description	767
8.71.2	Constructor & Destructor Documentation	767
8.71.3	Member Function Documentation	767
8.71.4	Member Data Documentation	772
8.72	forcebalance.tinkerio.Tinker_Reader Class Reference	773
8.72.1	Detailed Description	775
8.72.2	Constructor & Destructor Documentation	775
8.72.3	Member Function Documentation	775
8.72.4	Member Data Documentation	776
8.73	forcebalance.nifty.Unpickler_LP Class Reference	776
8.73.1	Detailed Description	777
8.73.2	Constructor & Destructor Documentation	777
8.74	forcebalance.vibration.Vibration Class Reference	777
8.74.1	Detailed Description	780
8.74.2	Constructor & Destructor Documentation	781
8.74.3	Member Function Documentation	781

8.74.4 Member Data Documentation	790
8.75 forcebalance.gmxio.Vibration_GMX Class Reference	792
8.75.1 Detailed Description	795
8.75.2 Constructor & Destructor Documentation	795
8.75.3 Member Function Documentation	795
8.75.4 Member Data Documentation	805
8.76 forcebalance.tinkerio.Vibration_TINKER Class Reference	807
8.76.1 Detailed Description	810
8.76.2 Constructor & Destructor Documentation	810
8.76.3 Member Function Documentation	810
8.76.4 Member Data Documentation	820
9 File Documentation	822
9.1 __init__.py File Reference	822
9.2 abinitio.py File Reference	822
9.3 abinitio_Internal.py File Reference	823
9.4 amberio.py File Reference	823
9.5 api.dox File Reference	823
9.6 binding.py File Reference	823
9.7 chemistry.py File Reference	824
9.8 contact.py File Reference	824
9.9 counterpoise.py File Reference	825
9.10 custom_io.py File Reference	825
9.11 engine.py File Reference	825
9.12 finite_difference.py File Reference	826
9.13 forcefield.py File Reference	826
9.14 gmxio.py File Reference	827
9.15 interaction.py File Reference	828
9.16 leastsq.py File Reference	828
9.17 lipid.py File Reference	829
9.18 liquid.py File Reference	829
9.19 Mol2.py File Reference	829
9.20 mol2io.py File Reference	830
9.21 molecule.py File Reference	830
9.22 moments.py File Reference	832
9.23 nifty.py File Reference	832
9.24 objective.py File Reference	834
9.25 openmmio.py File Reference	835
9.26 optimizer.py File Reference	836
9.27 output.py File Reference	837
9.28 parser.py File Reference	837
9.29 psi4io.py File Reference	838
9.30 PT.py File Reference	838
9.31 qchemio.py File Reference	838
9.32 quantity.py File Reference	839
9.33 target.py File Reference	839
9.34 thermo.py File Reference	840
9.35 tinkerio.py File Reference	840
9.36 vibration.py File Reference	841
Index	842

1 Project Roadmap

ForceBalance is a work in progress and is continually being improved and expanded! Here are some current and future project development ideas.

Some notes on updating the version:

The formalism for the version number goes something like this:

v1.2.1[ab][1-9]

where:

- 1.2.1 stands for major release (may break compatibility), medium-sized release (important features), minor release (improvements)
- a or b, if present, stands for alpha or beta release, with numbers standing for the n-th alpha or beta release

To manually specify a release, create a tag and push it to the remote repository: git tag -a v1.2.1 -m "version 1.2.1" git push --tags

The version number should then be automatically generated by "git describe" which is run by setup.py at installation.

Finally, remember to update the version number in the documentation generation scripts!

1.1 Most Recently Implemented (version 1.3.0):

- Engine class is a unified interface to MD simulation codes.
- Added Gromacs, OpenMM, and TINKER engines.
- Thermo target; simple support for general thermodynamic properties. (Erik)
- Lipid target; lipid bilayer properties. (Keri)
- ForceBalance –continue option continues an aborted run and loads as much data as possible from the latest iteration.
- Parameter filtering allows targets to skip over parameters that are known to be irrelevant, for efficiency of finite difference derivatives.
- (Optimizer / Liquid / Lipid) Increase simulation length as we get closer to convergence.
- (Gromacs) Now supports binding energies, interaction energies, multipole moments and vibrational frequencies.
- (OpenMM) Now supports binding energies, interaction energies, and multipole moments.
- ([nifty.py](#)) exec_() reads from stdout and stderr asynchronously, allowing us to split the streams and tail -f the output at the same time.

1.2 Current Development Goals, for version 1.3.1:

- More comprehensive tutorial to walk users through the initial process of setting up targets and preparing for a successful ForceBalance run

1.3 Longterm Development Ideas

- Visualization of running calculations

2 Todo List

Member [forcebalance.abinitio.AblInitio.__init__](#)

Obtain the number of true atoms (or the particle -> atom mapping) from the force field.

Member [forcebalance.abinitio.AblInitio.get_energy_force](#)

Parallelization over snapshots is not implemented yet

Member [forcebalance.abinitio.AblInitio.read_reference_data](#)

Add an option for picking any slice out of qdata.txt, helpful for cross-validation

Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Member [forcebalance.counterpoise.Counterpoise.loadxyz](#)

I should probably put this into a more general library for reading coordinates.

Member [forcebalance.forcefield.FF.mktransmat](#)

Only project out changes in total charge of a molecule, and perhaps generalize to fragments of molecules or other types of parameters.

The AMOEBA selection of charge depends not only on the atom type, but what that atom is bonded to.

Member [forcebalance.forcefield.FF.rsmake](#)

Pass in rsfactors through the input file

Namespace [forcebalance.gmxio](#)

Even more stuff from [forcefield.py](#) needs to go into here.

Class [forcebalance.gmxio.ITP_Reader](#)

Note that I can also create the opposite virtual site position by changing the atom labeling, woo!

Member [forcebalance.openmmio.OpenMM.Reader.build_pid](#)

Add a link here

Member [forcebalance.optimizer.Optimizer.GeneticAlgorithm](#)

Massive parallelization hasn't been implemented yet

Member [forcebalance.optimizer.Optimizer.Scan_Values](#)

Maybe a multidimensional grid can be done.

Parameters

in	<i>MathPhys</i>	Switch to use mathematical (True) or physical (False) parameters.
----	-----------------	---

Member [forcebalance.tinkerio.Tinker_Reader.feed](#)

Put the rescaling factors for TINKER parameters in here. Currently we're using the initial value to determine the rescaling factor which is not very good.

Member [forcebalance::gmxio.pdict](#)

This needs to become more flexible because the parameter isn't always in the same field. Still need to figure out how to do this.

How about making the PDIHS less ugly?

Member [forcebalance::nifty.floatornan](#)

I could use suggestions for making this better.

Member [forcebalance::parser.parse_inputs](#)

Implement internal coordinates.

Implement sampling correction.

Implement charge groups.

3 Namespace Index

3.1 Packages

Here are the packages with brief descriptions (if available):

forcebalance	14
forcebalance.abinitio	
Ab-initio fitting module (energies, forces, resp)	16
forcebalance.abinitio_internal	
Internal implementation of energy matching (for TIP3P water only)	16
forcebalance.amberio	
AMBER force field input/output	17
forcebalance.binding	
Binding energy fitting module	18
forcebalance.chemistry	19
forcebalance.contact	21
forcebalance.counterpoise	
Match an empirical potential to the counterpoise correction for basis set superposition error (BS-SE)	22

forcebalance.custom_io	
Custom force field parser	23
forcebalance.engine	24
forcebalance.finite_difference	24
forcebalance.forcefield	
Force field module	27
forcebalance.gmxio	
GROMACS input/output	29
forcebalance.interaction	
Interaction energy fitting module	33
forcebalance.leastsq	34
forcebalance.lipid	
Matching of lipid bulk properties	34
forcebalance.liquid	
Matching of liquid bulk properties	35
forcebalance.Mol2	36
forcebalance.mol2io	
Mol2 I/O	36
forcebalance.molecule	37
forcebalance.moments	
Multipole moment fitting module	44
forcebalance.nifty	
Nifty functions, intended to be imported by any module within ForceBalance	44
forcebalance.objective	
ForceBalance objective function	57
forcebalance.openmmio	
OpenMM input/output	58
forcebalance.optimizer	
Optimization algorithms	62
forcebalance.output	63
forcebalance.parser	
Input file parser for ForceBalance jobs	63
forcebalance.psi4io	
PSI4 force field input/output	67
forcebalance.PT	68

forcebalance.qchemio	
Q-Chem input file parser	68
forcebalance.quantity	70
forcebalance.target	71
forcebalance.thermo	71
forcebalance.tinkerio	
TINKER input/output	71
forcebalance.vibration	
Vibrational mode fitting module	74

4 Hierarchical Index

4.1 Class Hierarchy

This inheritance list is sorted roughly, but not completely, alphabetically:

dict	
forcebalance.forcefield.BackedUpDict	206
FileHandler	
forcebalance.output.CleanFileHandler	271
Graph	
forcebalance.molecule.MyG	620
Logger	
forcebalance.output.ForceBalanceLogger	306
forcebalance.output.ModLogger	522
forcebalance.Mol2.mol2	523
forcebalance.Mol2.mol2_atom	527
forcebalance.Mol2.mol2_bond	530
forcebalance.Mol2.mol2_set	538
object	
forcebalance.BaseClass	207
forcebalance.engine.Engine	290
forcebalance.gmxio.GMX	316
forcebalance.openmmio.OpenMM	626
forcebalance.tinkerio.TINKER	764
forcebalance.forcefield.FF	293

forcebalance.objective.Objective	622
forcebalance.optimizer.Optimizer	639
forcebalance.target.Target	700
forcebalance.abinitio.ABInitio	75
forcebalance.abinitio_internal.ABInitio_Internal	140
forcebalance.amberio.ABInitio_AMBER	96
forcebalance.gmxio.ABInitio_GMX	118
forcebalance.openmmio.ABInitio_OpenMM	162
forcebalance.tinkerio.ABInitio_TINKER	184
forcebalance.binding.BindingEnergy	212
forcebalance.gmxio.BindingEnergy_GMX	226
forcebalance.openmmio.BindingEnergy_OpenMM	241
forcebalance.tinkerio.BindingEnergy_TINKER	256
forcebalance.counterpoise.Counterpoise	274
forcebalance.interaction.Interaction	330
forcebalance.gmxio.Interaction_GMX	345
forcebalance.openmmio.Interaction_OpenMM	360
forcebalance.tinkerio.Interaction_TINKER	375
forcebalance.leastsq.LeastSquares	394
forcebalance.psi4io.THCDF_Psi4	715
forcebalance.lipid.Lipid	410
forcebalance.gmxio.Lipid_GMX	429
forcebalance.liquid.Liquid	447
forcebalance.gmxio.Liquid_GMX	464
forcebalance.openmmio.Liquid_OpenMM	483
forcebalance.tinkerio.Liquid_TINKER	502
forcebalance.moments.Moments	560
forcebalance.gmxio.Moments_GMX	574
forcebalance.openmmio.Moments_OpenMM	589
forcebalance.tinkerio.Moments_TINKER	604

forcebalance.psi4io.RDVR3_Psi4	671
forcebalance.target.RemoteTarget	687
forcebalance.thermo.Thermo	732
forcebalance.gmxio.Thermo_GMX	747
forcebalance.vibration.Vibration	777
forcebalance.gmxio.Vibration_GMX	792
forcebalance.tinkerio.Vibration_TINKER	807
forcebalance.BaseReader	209
forcebalance.amberio.FrcMod_Reader	307
forcebalance.amberio.Mol2_Reader	535
forcebalance.custom_io.Gen_Reader	314
forcebalance.gmxio.ITP_Reader	390
forcebalance.mol2io.Mol2_Reader	533
forcebalance.openmmio.OpenMM_Reader	637
forcebalance.psi4io.GBS_Reader	310
forcebalance.psi4io.Grid_Reader	327
forcebalance.qchemio.QCIn_Reader	659
forcebalance.tinkerio.Tinker_Reader	773
forcebalance.molecule.Molecule	539
forcebalance.nifty.LineChunker	408
forcebalance.quantity.Quantity	662
forcebalance.quantity.Quantity_Density	665
forcebalance.quantity.Quantity_H_vap	667
forcebalance.thermo.Point	658
forcebalance.objective.Penalty	653
Pickler	
forcebalance.nifty.Pickler_LP	656
StreamHandler	
forcebalance.output.CleanStreamHandler	273
forcebalance.output.RawStreamHandler	670
Structure	

forcebalance.molecule.MolfileTimestep	559
Unpickler	
forcebalance.nifty.Unpickler_LP	776

5 Class Index

5.1 Class List

Here are the classes, structs, unions and interfaces with brief descriptions:

forcebalance.abinitio.AbInitio Subclass of Target for fitting force fields to ab initio data	75
forcebalance.amberio.AbInitio_AMBER Subclass of Target for force and energy matching using AMBER	96
forcebalance.gmxio.AbInitio_GMX Subclass of AbInitio for force and energy matching using GROMACS	118
forcebalance.abinitio_internal.AbInitio_Internal Subclass of Target for force and energy matching using an internal implementation	140
forcebalance.openmmio.AbInitio_OpenMM Force and energy matching using OpenMM	162
forcebalance.tinkerio.AbInitio_TINKER Subclass of Target for force and energy matching using TINKER	184
forcebalance.forcefield.BackedUpDict	206
forcebalance.BaseClass Provides some nifty functions that are common to all ForceBalance classes	207
forcebalance.BaseReader The 'reader' class	209
forcebalance.binding.BindingEnergy Improved subclass of Target for fitting force fields to binding energies	212
forcebalance.gmxio.BindingEnergy_GMX Binding energy matching using Gromacs	226
forcebalance.openmmio.BindingEnergy_OpenMM Binding energy matching using OpenMM	241
forcebalance.tinkerio.BindingEnergy_TINKER Binding energy matching using TINKER	256
forcebalance.output.CleanFileHandler File handler that does not write terminal escape codes and carriage returns to files	271
forcebalance.output.CleanStreamHandler Similar to RawStreamHandler except it does not write terminal escape codes	273

forcebalance.counterpoise.Counterpoise		
Target subclass for matching the counterpoise correction		274
forcebalance.engine.Engine		
Base class for all engines		290
forcebalance.forcefield.FF		
Force field class		293
forcebalance.output.ForceBalanceLogger		
This logger starts out with a default handler that writes to stdout addHandler removes this default the first time another handler is added		306
forcebalance.amberio.FrcMod_Reader		
Finite state machine for parsing FrcMod force field file		307
forcebalance.psi4io.GBS_Reader		
Interaction type -> Parameter Dictionary		310
forcebalance.custom_io.Gen_Reader		
Finite state machine for parsing custom GROMACS force field files		314
forcebalance.gmxio.GMX		
Derived from Engine object for carrying out general purpose GROMACS calculations		316
forcebalance.psi4io.Grid_Reader		
Finite state machine for parsing DVR grid files		327
forcebalance.interaction.Interaction		
Subclass of Target for fitting force fields to interaction energies		330
forcebalance.gmxio.Interaction_GMX		
Interaction energy matching using GROMACS		345
forcebalance.openmmio.Interaction_OpenMM		
Interaction matching using OpenMM		360
forcebalance.tinkerio.Interaction_TINKER		
Subclass of Target for interaction matching using TINKER		375
forcebalance.gmxio.ITP_Reader		
Finite state machine for parsing GROMACS force field files		390
forcebalance.leastsq.LeastSquares		
Subclass of Target for general least squares fitting		394
forcebalance.nifty.LineChunker		
forcebalance.lipid.Lipid		
Subclass of Target for lipid property matching		410
forcebalance.gmxio.Lipid_GMX		
forcebalance.liquid.Liquid		
Subclass of Target for liquid property matching		447
forcebalance.gmxio.Liquid_GMX		

forcebalance.openmmio.Liquid_OpenMM		
Condensed phase property matching using OpenMM		483
forcebalance.tinkerio.Liquid_TINKER		
Condensed phase property matching using TINKER		502
forcebalance.output.ModLogger		522
forcebalance.Mol2.mol2		
This is to manage one mol2 series of lines on the form:		523
forcebalance.Mol2.mol2_atom		
This is to manage mol2 atomic lines on the form: 1 C1 5.4790 42.2880 49.5910 C.ar 1 <1> 0.0424		527
forcebalance.Mol2.mol2_bond		
This is to manage mol2 bond lines on the form: 1 1 2 ar		530
forcebalance.mol2io.Mol2_Reader		
Finite state machine for parsing Mol2 force field file		533
forcebalance.amberio.Mol2_Reader		
Finite state machine for parsing Mol2 force field file		535
forcebalance.Mol2.mol2_set		538
forcebalance.molecule.Molecule		
Lee-Ping's general file format conversion class		539
forcebalance.molecule.MolfileTimestep		
Wrapper for the timestep C structure used in molfile plugins		559
forcebalance.moments.Moments		
Subclass of Target for fitting force fields to multipole moments (from experiment or theory)		560
forcebalance.gmxio.Moments_GMX		
Multipole moment matching using GROMACS		574
forcebalance.openmmio.Moments_OpenMM		
Multipole moment matching using OpenMM		589
forcebalance.tinkerio.Moments_TINKER		
Subclass of Target for multipole moment matching using TINKER		604
forcebalance.molecule.MyG		620
forcebalance.objective.Objective		
Objective function		622
forcebalance.openmmio.OpenMM		
Derived from Engine object for carrying out general purpose OpenMM calculations		626
forcebalance.openmmio.OpenMM_Reader		
Class for parsing OpenMM force field files		637
forcebalance.optimizer.Optimizer		
Optimizer class		639

forcebalance.objective.Penalty	Penalty functions for regularizing the force field optimizer	653
forcebalance.nifty.Pickler_LP	A subclass of the python Pickler that implements pickling of <code>ElementTree</code> types	656
forcebalance.thermo.Point		658
forcebalance.qchemio.QCIn.Reader	Finite state machine for parsing Q-Chem input files	659
forcebalance.quantity.Quantity	Base class for thermodynamical quantity used for fitting	662
forcebalance.quantity.Quantity_Density		665
forcebalance.quantity.Quantity_H_vap		667
forcebalance.output.RawFileHandler	Exactly like <code>output.FileHandler</code> except it does no extra formatting before sending logging messages to the file	669
forcebalance.output.RawStreamHandler	Exactly like <code>output.StreamHandler</code> except it does no extra formatting before sending logging messages to the stream	670
forcebalance.psi4io.RDVR3_Psi4	Subclass of Target for R-DVR3 grid fitting	671
forcebalance.target.RemoteTarget		687
forcebalance.target.Target	Base class for all fitting targets	700
forcebalance.psi4io.THCDF_Psi4		715
forcebalance.thermo.Thermo	A target for fitting general experimental data sets	732
forcebalance.gmxio.Thermo_GMX	Thermodynamical property matching using GROMACS	747
forcebalance.tinkerio.TINKER	Engine for carrying out general purpose <code>TINKER</code> calculations	764
forcebalance.tinkerio.Tinker.Reader	Finite state machine for parsing <code>TINKER</code> force field files	773
forcebalance.nifty.Unpickler_LP	A subclass of the python Unpickler that implements unpickling of <code>ElementTree</code> types	776
forcebalance.vibration.Vibration	Subclass of Target for fitting force fields to vibrational spectra (from experiment or theory)	777
forcebalance.gmxio.Vibration_GMX	Vibrational frequency matching using GROMACS	792

6 File Index

6.1 File List

Here is a list of all files with brief descriptions:

<code>__init__.py</code>	822
<code>abinitio.py</code>	822
<code>abinitio_internal.py</code>	823
<code>amberio.py</code>	823
<code>binding.py</code>	823
<code>chemistry.py</code>	824
<code>contact.py</code>	824
<code>counterpoise.py</code>	825
<code>custom_io.py</code>	825
<code>engine.py</code>	825
<code>finite_difference.py</code>	826
<code>forcefield.py</code>	826
<code>gmxio.py</code>	827
<code>interaction.py</code>	828
<code>leastsq.py</code>	828
<code>lipid.py</code>	829
<code>liquid.py</code>	829
<code>Mol2.py</code>	829
<code>mol2io.py</code>	830
<code>molecule.py</code>	830
<code>moments.py</code>	832
<code>nifty.py</code>	832
<code>objective.py</code>	834
<code>openmmio.py</code>	835

optimizer.py	836
output.py	837
parser.py	837
psi4io.py	838
PT.py	838
qchemio.py	838
quantity.py	839
target.py	839
thermo.py	840
tinkerio.py	840
vibration.py	841

7 Namespace Documentation

7.1 forcebalance Namespace Reference

Namespaces

- [abinitio](#)
Ab-initio fitting module (energies, forces, resp).
- [abinitio_internal](#)
Internal implementation of energy matching (for TIP3P water only)
- [amberio](#)
AMBER force field input/output.
- [binding](#)
Binding energy fitting module.
- [chemistry](#)
- [contact](#)
- [counterpoise](#)
Match an empirical potential to the counterpoise correction for basis set superposition error (BSSE).
- [custom_io](#)
Custom force field parser.
- [engine](#)
- [finite_difference](#)
- [forcefield](#)
Force field module.
- [gmxio](#)
GROMACS input/output.
- [interaction](#)
Interaction energy fitting module.
- [leastsq](#)
- [lipid](#)

- **liquid**
Matching of lipid bulk properties.
- **Mol2**
Matching of liquid bulk properties.
- **mol2io**
Mol2 I/O.
- **molecule**
- **moments**
Multipole moment fitting module.
- **nifty**
Nifty functions, intended to be imported by any module within ForceBalance.
- **objective**
ForceBalance objective function.
- **openmmio**
OpenMM input/output.
- **optimizer**
Optimization algorithms.
- **output**
- **parser**
Input file parser for ForceBalance jobs.
- **psi4io**
PSI4 force field input/output.
- **PT**
- **qchemio**
Q-Chem input file parser.
- **quantity**
- **target**
- **thermo**
- **tinkerio**
TINKER input/output.
- **vibration**
Vibrational mode fitting module.

Classes

- class **BaseClass**
Provides some nifty functions that are common to all ForceBalance classes.
- class **BaseReader**
The 'reader' class.

Variables

- tuple **__version__** = pkg_resources.get_distribution("forcebalance")

7.1.1 Variable Documentation

string forcebalance.__version__ = pkg_resources.get_distribution("forcebalance") Definition at line 17 of file __init__.py.

7.2 forcebalance.abinitio Namespace Reference

Ab-initio fitting module (energies, forces, resp).

Classes

- class [AbInitio](#)

Subclass of Target for fitting force fields to ab initio data.

Functions

- def [weighted_variance](#)

A more generalized version of build_objective which is callable for derivatives, but the covariance is not there anymore.

- def [weighted_variance2](#)

A bit of a hack, since we have to subtract out two mean quantities to get Hessian elements.

- def [build_objective](#)

This function builds an objective function (number) from the complicated polytensor and covariance matrices.

Variables

- tuple [logger](#) = getLogger(__name__)

7.2.1 Detailed Description

Ab-initio fitting module (energies, forces, resp).

Author

Lee-Ping Wang

Date

05/2012

7.2.2 Function Documentation

def forcebalance.abinitio.build_objective (*SPiXi*, *WCiW*, *Z*, *Q0*, *M0*, *NCP1*, *subtract_mean = True*)

This function builds an objective function (number) from the complicated polytensor and covariance matrices.

Definition at line 1208 of file abinitio.py.

def forcebalance.abinitio.weighted_variance (*SPiXi*, *WCiW*, *Z*, *L*, *R*, *NCP1*, *subtract_mean = True*) A more generalized version of build_objective which is callable for derivatives, but the covariance is not there anymore.

Definition at line 1178 of file abinitio.py.

def forcebalance.abinitio.weighted_variance2 (*SPiXi*, *WCiW*, *Z*, *L*, *R*, *L2*, *R2*, *NCP1*, *subtract_mean = True*) A bit of a hack, since we have to subtract out two mean quantities to get Hessian elements.

Definition at line 1192 of file abinitio.py.

7.2.3 Variable Documentation

tuple forcebalance.abinitio.logger = getLogger(__name__) Definition at line 24 of file abinitio.py.

7.3 forcebalance.abinitio_internal Namespace Reference

Internal implementation of energy matching (for TIP3P water only)

Classes

- class [AbInitio_Internal](#)

Subclass of Target for force and energy matching using an internal implementation.

7.3.1 Detailed Description

Internal implementation of energy matching (for TIP3P water only)

Author

Lee-Ping Wang

Date

04/2012

7.4 forcebalance.amberio Namespace Reference

AMBER force field input/output.

Classes

- class [Mol2_Reader](#)
Finite state machine for parsing Mol2 force field file.
- class [FrcMod_Reader](#)
Finite state machine for parsing FrcMod force field file.
- class [AbInitio_AMBER](#)
Subclass of Target for force and energy matching using AMBER.

Functions

- def [is_mol2_atom](#)

Variables

- tuple [logger](#) = getLogger(__name__)
- dictionary [mol2_pdct](#) = {'COUL': {'Atom': [1], 8: ''}}
- dictionary [frcmod_pdct](#)

7.4.1 Detailed Description

AMBER force field input/output. This serves as a good template for writing future force matching I/O modules for other programs because it's so simple.

Author

Lee-Ping Wang

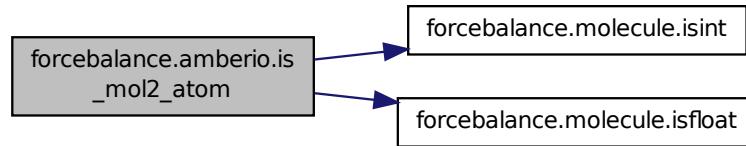
Date

01/2012

7.4.2 Function Documentation

def forcebalance.amberio.is_mol2_atom (*line*) Definition at line 35 of file amberio.py.

Here is the call graph for this function:



7.4.3 Variable Documentation

dictionary forcebalance.amberio.frcmod_pdct Initial value:

```
1 = {'BONDS': {'Atom':[0], 1:'K', 2:'B'},  
2      'ANGLES': {'Atom':[0], 1:'K', 2:'B'},  
3      'PDIHS1': {'Atom':[0], 2:'K', 3:'B'},  
4      'PDIHS2': {'Atom':[0], 2:'K', 3:'B'},  
5      'PDIHS3': {'Atom':[0], 2:'K', 3:'B'},  
6      'PDIHS4': {'Atom':[0], 2:'K', 3:'B'},  
7      'PDIHS5': {'Atom':[0], 2:'K', 3:'B'},  
8      'PDIHS6': {'Atom':[0], 2:'K', 3:'B'},  
9      'IDIHS': {'Atom':[0], 1:'K', 3:'B'},  
10     'VDW': {'Atom':[0], 1:'S', 2:'T'}  
11 }
```

Definition at line 23 of file amberio.py.

tuple forcebalance.amberio.logger = getLogger(*_name_*) Definition at line 19 of file amberio.py.

dictionary forcebalance.amberio.mol2_pdct = {'COUL': {'Atom': [1], 8: ''}} Definition at line 21 of file amberio.py.

7.5 forcebalance.binding Namespace Reference

Binding energy fitting module.

Classes

- class [BindingEnergy](#)

Improved subclass of Target for fitting force fields to binding energies.

Functions

- def [parse_interactions](#)

Parse through the interactions input file.

Variables

- tuple [logger = getLogger\(*_name_*\)](#)

7.5.1 Detailed Description

Binding energy fitting module.

Author

Lee-Ping Wang

Date

05/2012

7.5.2 Function Documentation

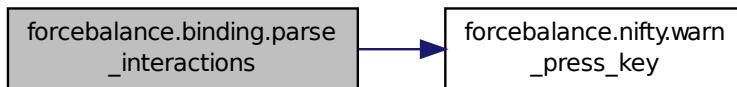
def forcebalance.binding.parse.interactions (*input_file*) Parse through the interactions input file.

Parameters

in	<i>input_file</i>	The name of the input file.
----	-------------------	-----------------------------

Definition at line 30 of file binding.py.

Here is the call graph for this function:



7.5.3 Variable Documentation

tuple forcebalance.binding.logger = getLogger(__name__) Definition at line 22 of file binding.py.

7.6 forcebalance.chemistry Namespace Reference

Functions

- def [LookupByMass](#)
- def [BondStrengthByLength](#)

Variables

- tuple [BondEnergies](#) = defaultdict(lambda:defaultdict(dict))
- list [Radii](#)

Covalent radii from Cordero et al.
- tuple [PeriodicTable](#)
- list [Elements](#)
- list [BondChars](#) = ['-','=','3']
- string [data_from_web](#)
- tuple [line](#) = line.expandtabs()
- tuple [BE](#) = float(line.split()[1])
- tuple [L](#) = float(line.split()[2])
- tuple [atoms](#) = re.split('[-=3]', line.split()[0])

- list **A** = atoms[0]
- list **B** = atoms[1]
- tuple **bo** = BondChars.index(re.findall('[-=3]', line.split()[0])[0])

7.6.1 Function Documentation

def forcebalance.chemistry.BondStrengthByLength (A, B, length, artol = 0.33, bias = 0.0) Definition at line 164 of file chemistry.py.

def forcebalance.chemistry.LookupByMass (mass) Definition at line 155 of file chemistry.py.

7.6.2 Variable Documentation

list forcebalance.chemistry.A = atoms[0] Definition at line 149 of file chemistry.py.

tuple forcebalance.chemistry.atoms = re.split('[-=3]', line.split()[0]) Definition at line 148 of file chemistry.py.

list forcebalance.chemistry.B = atoms[1] Definition at line 150 of file chemistry.py.

tuple forcebalance.chemistry.BE = float(line.split()[1]) Definition at line 146 of file chemistry.py.

tuple forcebalance.chemistry.bo = BondChars.index(re.findall('[-=3]', line.split()[0])[0]) Definition at line 151 of file chemistry.py.

list forcebalance.chemistry.BondChars = [-,=,3] Definition at line 49 of file chemistry.py.

tuple forcebalance.chemistry.BondEnergies = defaultdict(lambda:defaultdict(dict)) Definition at line 7 of file chemistry.py.

string forcebalance.chemistry.data_from_web Definition at line 51 of file chemistry.py.

list forcebalance.chemistry.Elements Initial value:

```
1 = ["None",'H','He',
2           'Li','Be','B','C','N','O','F','Ne',
3           'Na','Mg','Al','Si','P','S','Cl','Ar',
4           'K','Ca','Sc','Ti','V','Cr','Mn','Fe','Co','Ni','Cu','Zn','Ga','Ge','As','Se','Br','Kr',
5           'Rb','Sr','Y','Zr','Nb','Mo','Tc','Ru','Rh','Pd','Ag','Cd','In','Sn','Sb','Te','I','Xe',
6           'Cs','Ba','La','Ce','Pr','Nd','Pm','Sm','Eu','Gd','Tb','Dy','Ho','Er','Tm','Yb',
7           'Lu','Hf','Ta','W','Re','Os','Ir','Pt','Au','Hg','Tl','Pb','Bi','Po','At','Rn',
8           'Fr','Ra','Ac','Th','Pa','U','Np','Pu','Am','Cm','Bk','Cf','Es','Fm','Md','No','Lr','Rf','Db',
     Sg,'Bh','Hs','Mt']
```

Definition at line 40 of file chemistry.py.

tuple forcebalance.chemistry.L = float(line.split()[2]) Definition at line 147 of file chemistry.py.

tuple forcebalance.chemistry.line = line.expandtabs() Definition at line 145 of file chemistry.py.

tuple forcebalance.chemistry.PeriodicTable Initial value:

```
1 = OrderedDict([( ('H', 1.0079), ('He', 4.0026),
2                 ('Li', 6.941), ('Be', 9.0122), ('B', 10.811), ('C', 12.0107), ('N', 14.0067), ('O', 15.99
3                 94), ('F', 18.9984), ('Ne', 20.1797),
4                 ('Na', 22.9897), ('Mg', 24.305), ('Al', 26.9815), ('Si', 28.0855), ('P', 30.9738), ('S',
5                 32.065), ('Cl', 35.453), ('Ar', 39.948),
6                 ('K', 39.0983), ('Ca', 40.078), ('Sc', 44.9559), ('Ti', 47.867), ('V', 50.9415), ('Cr', 5
7                 1.9961), ('Mn', 54.938), ('Fe', 55.845), ('Co', 58.9332),
8                 ('Ni', 58.6934), ('Cu', 63.546), ('Zn', 65.39), ('Ga', 69.723), ('Ge', 72.64), ('As', 74.
9                 9216), ('Se', 78.96), ('Br', 79.904), ('Kr', 83.8),
10                ('Rb', 85.4678), ('Sr', 87.62), ('Y', 88.9059), ('Zr', 91.224), ('Nb', 92.9064), ('Mo', 9
11                5.94), ('Tc', 98), ('Ru', 101.07), ('Rh', 102.9055),
12                ('Pd', 106.42), ('Ag', 107.8682), ('Cd', 112.411), ('In', 114.818), ('Sn', 118.71), ('Sb
13                ', 121.76), ('Te', 127.6), ('I', 126.9045), ('Xe', 131.293),
14                ('Cs', 132.9055), ('Ba', 137.327), ('La', 138.9055), ('Ce', 140.116), ('Pr', 140.9077),
('Nd', 144.24), ('Pm', 145), ('Sm', 150.36),
('Eu', 151.964), ('Gd', 157.25), ('Tb', 158.9253), ('Dy', 162.5), ('Ho', 164.9303), ('Er
167.259), ('Tm', 168.9342), ('Yb', 173.04),
('Lu', 174.967), ('Hf', 178.49), ('Ta', 180.9479), ('W', 183.84), ('Re', 186.207), ('Os
190.23), ('Ir', 192.217), ('Pt', 195.078),
('Au', 196.9665), ('Hg', 200.59), ('Tl', 204.3833), ('Pb', 207.2), ('Bi', 208.9804), ('Po
209), ('At', 210), ('Rn', 222),
('Fr', 223), ('Ra', 226), ('Ac', 227), ('Th', 232.0381), ('Pa', 231.0359), ('U
238.0289), ('Np', 237), ('Pu', 244),
('Am', 243), ('Cm', 247), ('Bk', 247), ('Cf', 251), ('Es', 252), ('Fm', 257), ('Md', 258),
('No', 259),
('Lr', 262), ('Rf', 261), ('Db', 262), ('Sg', 266), ('Bh', 264), ('Hs', 277), ('Mt', 268)])
```

Definition at line 25 of file chemistry.py.

list forcebalance.chemistry.Radii Initial value:

```
1 = [0.31, 0.28, # H and He
2     1.28, 0.96, 0.84, 0.76, 0.71, 0.66, 0.57, 0.58, # First row elements
3     1.66, 1.41, 1.21, 1.11, 1.07, 1.05, 1.02, 1.06, # Second row elements
4     2.03, 1.76, 1.70, 1.60, 1.53, 1.39, 1.61, 1.52, 1.50,
5     1.24, 1.32, 1.22, 1.20, 1.19, 1.20, 1.20, 1.16, # Third row elements, K through Kr
6     2.20, 1.95, 1.90, 1.75, 1.64, 1.54, 1.47, 1.46, 1.42,
7     1.39, 1.45, 1.44, 1.42, 1.39, 1.39, 1.38, 1.39, 1.40, # Fourth row elements, Rb through Xe
8     2.44, 2.15, 2.07, 2.04, 2.03, 2.01, 1.99, 1.98,
9     1.98, 1.96, 1.94, 1.92, 1.92, 1.89, 1.90, 1.87, # Fifth row elements, s and f blocks
10    1.87, 1.75, 1.70, 1.62, 1.51, 1.44, 1.41, 1.36,
11    1.36, 1.32, 1.45, 1.46, 1.48, 1.40, 1.50, 1.50, # Fifth row elements, d and p blocks
12    2.60, 2.21, 2.15, 2.06, 2.00, 1.96, 1.90, 1.87, 1.80, 1.69]
```

Covalent radii from Cordero et al.

'Covalent radii revisited' Dalton Transactions 2008, 2832-2838.

Definition at line 10 of file chemistry.py.

7.7 forcebalance.contact Namespace Reference

Functions

- def `atom_distances`

For each frame in xyzlist, compute the (euclidean) distance between pairs of atoms whos indices are given in contacts.

- def `residue_distances`

For each frame in xyzlist, and for each pair of residues in the array contact, compute the distance between the closest pair of atoms such that one of them belongs to each residue.

7.7.1 Function Documentation

`def forcebalance.contact.atom_distances(xyzlist, atom_contacts, box = None)` For each frame in xyzlist, compute the (euclidean) distance between pairs of atoms whos indices are given in contacts.

xyzlist should be a traj_length x num_atoms x num_dims array of type float32

contacts should be a num_contacts x 2 array where each row gives the indices of 2 atoms whos distance you care to monitor.

box should be a 3-element array containing the a, b, and c lattice lengths.

Returns: traj_length x num_contacts array of euclidean distances

Note: For nice wrappers around this, see the prepare_trajectory method of various metrics in metrics.py

Definition at line 29 of file contact.py.

def forcebalance.contact.residue_distances (xyzlist, residue_membership, residue_contacts) For each frame in xyzlist, and for each pair of residues in the array contact, compute the distance between the closest pair of atoms such that one of them belongs to each residue.

xyzlist should be a traj_length x num_atoms x num_dims array of type float32

residue_membership should be a list of lists where residue_membership[i] gives the list of atomindices that belong to residue i. residue_membership should NOT be a numpy 2D array unless you really mean that all of the residues have the same number of atoms

residue_contacts should be a 2D numpy array of shape num_contacts x 2 where each row gives the indices of the two RESIDUES who you are interested in monitoring for a contact.

Returns: a 2D array of traj_length x num_contacts where out[i,j] contains the distance between the pair of atoms, one from residue_membership[residue_contacts[j,0]] and one from residue_membership[residue_contacts[j,1]] that are closest.

Definition at line 99 of file contact.py.

7.8 forcebalance.counterpoise Namespace Reference

Match an empirical potential to the counterpoise correction for basis set superposition error (BSSE).

Classes

- class [Counterpoise](#)

Target subclass for matching the counterpoise correction.

Variables

- tuple [logger](#) = getLogger(__name__)

7.8.1 Detailed Description

Match an empirical potential to the counterpoise correction for basis set superposition error (BSSE). Here we test two different functional forms: a three-parameter Gaussian repulsive potential and a four-parameter Gaussian which goes smoothly to an exponential. The latter can be written in two different ways - one which gives us control over the exponential, the switching distance and the Gaussian decay constant, and another which gives us control over the Gaussian and the switching distance. They are called 'CPGAUSS', 'CPEXPG', and 'CPGEXP'. I think the third option is the best although our early tests have indicated that none of the force fields perform particularly well for the water dimer.

This subclass of Target implements the 'get' method.

Author

Lee-Ping Wang

Date

12/2011

7.8.2 Variable Documentation

tuple forcebalance.counterpoise.logger = getLogger(__name__) Definition at line 30 of file counterpoise.py.

7.9 forcebalance.custom.io Namespace Reference

Custom force field parser.

Classes

- class [Gen_Reader](#)

Finite state machine for parsing custom GROMACS force field files.

Variables

- list [cptypes](#) = [None, 'CPGAUSS', 'CPEXPG', 'CPGEXP']

Types of counterpoise correction.

- list [ndtypes](#) = [None]

Types of NDDO correction.

- dictionary [fdict](#)

Section -> Interaction type dictionary.

- dictionary [pdict](#)

Interaction type -> Parameter Dictionary.

7.9.1 Detailed Description

Custom force field parser. We take advantage of the sections in GROMACS and the 'interaction type' concept, but these interactions are not supported in GROMACS; rather, they are computed within our program.

Author

Lee-Ping Wang

Date

12/2011

7.9.2 Variable Documentation

list forcebalance.custom.io.cptypes = [None, 'CPGAUSS', 'CPEXPG', 'CPGEXP'] Types of counterpoise correction.

Definition at line 16 of file custom.io.py.

dictionary forcebalance.custom.io.fdict Initial value:

```
1 = {
2     'counterpoise' : cptypes }
```

Section -> Interaction type dictionary.

Definition at line 21 of file custom.io.py.

list forcebalance.custom.io.ndtypes = [None] Types of NDDO correction.

Definition at line 18 of file custom.io.py.

dictionary forcebalance.custom.io.pdict Initial value:

```
1 = {'CPGAUSS':{3:'A', 4:'B', 5:'C'},
2      'CPGEXP':{3:'A', 4:'B', 5:'G', 6:'X'},
3      'CPEXPG':{3:'A1', 4:'B', 5:'X0', 6:'A2'}
4 }
```

Interaction type -> Parameter Dictionary.

Definition at line 25 of file custom.io.py.

7.10 forcebalance.engine Namespace Reference

Classes

- class [Engine](#)

Base class for all engines.

Variables

- tuple [logger](#) = getLogger(__name__)

7.10.1 Variable Documentation

tuple forcebalance.engine.logger = getLogger(__name__) Definition at line 17 of file engine.py.

7.11 forcebalance.finite_difference Namespace Reference

Functions

- def [f1d2p](#)

A two-point finite difference stencil.

- def [f1d5p](#)

A highly accurate five-point finite difference stencil for computing derivatives of a function.

- def [f1d7p](#)

A highly accurate seven-point finite difference stencil for computing derivatives of a function.

- def [f12d7p](#)

- def [f12d3p](#)

A three-point finite difference stencil.

- def [f2var](#)

A finite difference stencil for a function of two variables.

- def [in_fd](#)

Invoking this function from anywhere will tell us whether we're being called by a finite-difference function.

- def [in_fd_srch](#)

Invoking this function from anywhere will tell us whether we're being called by a finite-difference function.

- def [fdwrap](#)

A function wrapper for finite difference designed for differentiating 'get'-type functions.

- def [fdwrap_G](#)

A driver to fdwrap for gradients (see documentation for fdwrap) Inputs: tgt = The Target containing the objective function that we want to differentiate mvals0 = The 'central' values of the mathematical parameters - i.e.

- def [fdwrap_H](#)

A driver to fdwrap for Hessians (see documentation for fdwrap) Inputs: tgt = The Target containing the objective function that we want to differentiate mvals0 = The 'central' values of the mathematical parameters - i.e.

Variables

- tuple [logger](#) = getLogger(__name__)

7.11.1 Function Documentation

def forcebalance.finite_difference.f12d3p (f, h, f0 = None) A three-point finite difference stencil.

This function does either two computations or three, depending on whether the 'center' value is supplied. This is done in order to avoid recomputing the center value many times.

The first derivative is evaluated using central difference. One advantage of using central difference (as opposed to forward difference) is that we get zero at the bottom of a parabola.

Using this formula we also get an approximate second derivative, which can then be inserted into the diagonal of the Hessian. This is very useful for optimizations like BFGS where the diagonal determines how far we step in the parameter space.

How to use: use fdwrap or something similar to generate a one-variable function from the (usually) much more complicated function that we wish to differentiate. Then pass it to this function.

Inputs: f = The one-variable function f(x) that we're differentiating h = The finite difference step size, usually a small number

Outputs: fp = The finite difference derivative of the function f(x) around x=0.

Definition at line 109 of file finite_difference.py.

def forcebalance.finite_difference.f12d7p (f, h) Definition at line 75 of file finite_difference.py.

def forcebalance.finite_difference.f1d2p (f, h, f0 = None) A two-point finite difference stencil.

This function does either two computations or one, depending on whether the 'center' value is supplied. This is done in order to avoid recomputing the center value many times when we repeat this function for each index of the gradient.

How to use: use fdwrap or something similar to generate a one-variable function from the (usually) much more complicated function that we wish to differentiate. Then pass it to this function.

Inputs: f = The one-variable function f(x) that we're differentiating h = The finite difference step size, usually a small number

Outputs: fp = The finite difference derivative of the function f(x) around x=0.

Definition at line 29 of file finite_difference.py.

def forcebalance.finite_difference.f1d5p (f, h) A highly accurate five-point finite difference stencil for computing derivatives of a function.

It works on both scalar and vector functions (i.e. functions that return arrays). Since the function does four computations, it's costly but recommended if we really need an accurate reference value.

The function is evaluated at points -2h, -h, +h and +2h and these values are combined to make the derivative according to: <http://www.holoborodko.com/pavel/numerical-methods/numerical-derivative/central-difference-formulas/>

How to use: use fdwrap or something similar to generate a one-variable function from the (usually) much more complicated function that we wish to differentiate. Then pass it to this function.

Inputs: f = The one-variable function f(x) that we're differentiating h = The finite difference step size, usually a small number

Outputs: fp = The finite difference derivative of the function f(x) around x=0.

Definition at line 60 of file finite_difference.py.

def forcebalance.finite_difference.f1d7p (f, h) A highly accurate seven-point finite difference stencil for computing derivatives of a function.

Definition at line 70 of file finite_difference.py.

def forcebalance.finite_difference.f2var (f, h) A finite difference stencil for a function of two variables.

Definition at line 120 of file finite_difference.py.

```
def forcebalance.finite.difference.fdwrap ( func, mvals0, pidx, key = None, kwargs )
```

A function wrapper for finite difference designed for differentiating 'get'-type functions.

Since our finite difference stencils take single-variable functions and differentiate them around zero, and our objective function is quite a complicated function, we need a wrapper to serve as a middleman. The alternative would be to copy the finite difference formula to wherever we're taking the derivative, and that is prone to mistakes.

Inputs: func = Either get_X or get_G; these functions return dictionaries. ['X'] = 1.23, ['G'] = [0.12, 3, 45, ...] mvals0 = The 'central' values of the mathematical parameters - i.e. the wrapped function's origin is here. pidx = The index of the parameter that we're differentiating key = either 'G' or 'X', the value we wish to take out of the dictionary kwargs = Anything else we want to pass to the objective function (for instance, Project.Objective takes Order as an argument)

Outputs: func1 = Wrapped version of func, which takes a single float argument.

Definition at line 160 of file finite_difference.py.

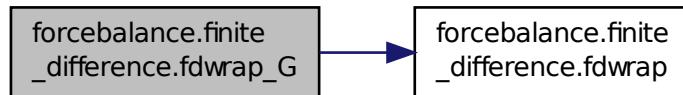
```
def forcebalance.finite.difference.fdwrap_G ( tgt, mvals0, pidx )
```

A driver to fdwrap for gradients (see documentation for fdwrap) Inputs: tgt = The Target containing the objective function that we want to differentiate mvals0 = The 'central' values of the mathematical parameters - i.e.

the wrapped function's origin is here. pidx = The index of the parameter that we're differentiating

Definition at line 179 of file finite_difference.py.

Here is the call graph for this function:



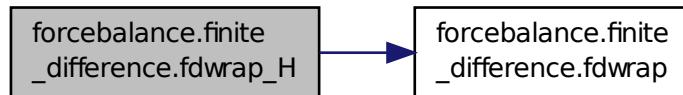
```
def forcebalance.finite.difference.fdwrap_H ( tgt, mvals0, pidx )
```

A driver to fdwrap for Hessians (see documentation for fdwrap) Inputs: tgt = The Target containing the objective function that we want to differentiate mvals0 = The 'central' values of the mathematical parameters - i.e.

the wrapped function's origin is here. pidx = The index of the parameter that we're differentiating

Definition at line 190 of file finite_difference.py.

Here is the call graph for this function:



```
def forcebalance.finite.difference.in_fd ( )
```

Invoking this function from anywhere will tell us whether we're being called by a finite-difference function.

This is mainly useful for deciding when to update the 'qualitative indicators' and when not to.
Definition at line 127 of file finite_difference.py.

def forcebalance.finite_difference.in_fd_srch () Invoking this function from anywhere will tell us whether we're being called by a finite-difference function.

This is mainly useful for deciding when to update the 'qualitative indicators' and when not to.
Definition at line 134 of file finite_difference.py.

7.11.2 Variable Documentation

tuple forcebalance.finite_difference.logger = getLogger(__name__) Definition at line 7 of file finite_difference.py.

7.12 forcebalance.forcefield Namespace Reference

Force field module.

Classes

- class [BackedUpDict](#)
- class [FF](#)

Force field class.

Functions

- def [determine_fftype](#)
Determine the type of a force field file.
- def [rs_override](#)
This function takes in a dictionary (rsfactors) and a string (termtype).

Variables

- tuple [logger = getLogger\(__name__\)](#)
- dictionary [FF_Extensions](#)
- dictionary [FF_IOModules](#)

7.12.1 Detailed Description

Force field module. In ForceBalance a 'force field' is built from a set of files containing physical parameters. These files can be anything that enter into any computation - our original program was quite dependent on the GROMACS force field format, but this program is set up to allow very general input formats.

We introduce several important concepts:

1) Adjustable parameters are allocated into a vector.

To cast the force field optimization as a math problem, we treat all of the parameters on equal footing and write them as indices in a parameter vector.

2) A mapping from interaction type to parameter number.

Each element in the parameter vector corresponds to one or more interaction types. Whenever we change the parameter vector and recompute the objective function, this amounts to changing the physical parameters in the simulations, so we print out new force field files for external programs. In addition, when these programs are computing the objective function we are often in low-level subroutines that compute terms in the energy and force. If we need an analytic derivative of the objective function, then these subroutines need to know which index of the parameter vector needs to be modified.

This is done by way of a hash table: for example, when we are computing a Coulomb interaction between atom 4 and atom 5, we can build the words 'COUL4' and 'COUL5' and look it up in the parameter map; this gives us two

numbers (say, 10 and 11) corresponding to the eleventh and twelfth element of the parameter vector. Then we can compute the derivatives of the energy w.r.t. these parameters (in this case, COUL5/rij and COUL4/rij) and increment these values in the objective function gradient.

In custom-implemented force fields (see counterpoisematch.py) the hash table can also be used to look up parameter values for computation of interactions. This is probably not the fastest way to do things, however.

3) Distinction between physical and mathematical parameters.

The optimization algorithm works in a space that is related to, but not exactly the same as the physical parameter space. The reasons for why we do this are:

a) Each parameter has its own physical units. On the one hand it's not right to treat different physical units all on the same footing, so nondimensionalization is desirable. To make matters worse, the force field parameters can be small as 1e-8 or as large as 1e+6 depending on the parameter type. This means the elements of the objective function gradient / Hessian have elements that differ from each other in size by 10+ orders of magnitude, leading to mathematical instabilities in the optimizer.

b) The parameter space can be constrained, most notably for atomic partial charges where we don't want to change the overall charge on a molecule. Thus we wish to project out certain movements in the mathematical parameters such that they don't change the physical parameters.

c) We wish to regularize our optimization so as to avoid changing our parameters in very insensitive directions (linear dependencies). However, the sensitivity of the objective function to changes in the force field depends on the physical units!

For all of these reasons, we introduce a 'transformation matrix' which maps mathematical parameters onto physical parameters. The diagonal elements in this matrix are rescaling factors; they take the mathematical parameter and magnify it by this constant factor. The off-diagonal elements correspond to rotations and other linear transformations, and currently I just use them to project out the 'increase the net charge' direction in the physical parameter space.

Note that with regularization, these rescaling factors are equivalent to the widths of prior distributions in a maximum likelihood framework. Because there is such a correspondence between rescaling factors and choosing a prior, they need to be chosen carefully. This is work in progress. Another possibility is to sample the width of the priors from a noninformative distribution – the hyperprior (we can choose the Jeffreys prior or something). This is work in progress.

Right now only GROMACS parameters are supported, but this class is extensible, we need more modules!

Author

Lee-Ping Wang

Date

04/2012

7.12.2 Function Documentation

```
def forcebalance.forcefield.determine_fftype( ffname, verbose = False )
```

Determine the type of a force field file.

It is possible to specify the file type explicitly in the input file using the syntax 'force_field.ext:type'. Otherwise this function will try to determine the force field type by extension.

Definition at line 146 of file forcefield.py.

```
def forcebalance.forcefield.rs_override( rsfactors, termtype, Temperature = 298.15 )
```

This function takes in a dictionary (rsfactors) and a string (termtype).

If termtype matches any of the strings below, rsfactors[termtype] is assigned to one of the numbers below.

This is LPW's attempt to simplify the rescaling factors.

Parameters

<code>out</code>	<code>rsfactors</code>	The computed rescaling factor.
<code>in</code>	<code>termtyp</code>	The interaction type (corresponding to a physical unit)
<code>in</code>	<code>Temperature</code>	The temperature for computing the kT energy scale

Definition at line 1212 of file forcefield.py.

7.12.3 Variable Documentation

dictionary `forcebalance.forcefield.FF_Extensions` Initial value:

```

1 = {"itp" : "gmx",
2          "top" : "gmx",
3          "in" : "qchem",
4          "prm" : "tinker",
5          "gen" : "custom",
6          "xml" : "openmm",
7          "frcmod" : "frcmod",
8          "mol2" : "mol2",
9          "gbs" : "gbs",
10         "grid" : "grid"
11        }

```

Definition at line 117 of file forcefield.py.

dictionary `forcebalance.forcefield.FF_IOModules` Initial value:

```

1 = {"gmx": gmxio.ITP_Reader ,
2      "qchem": qchemio.QCIn.Reader ,
3      "tinker": tinkerio.Tinker.Reader ,
4      "custom": customio.Gen.Reader ,
5      "openmm": openmmio.OpenMM.Reader,
6      "frcmod": amberio.FrcMod.Reader,
7      "mol2": amberio.Mol2.Reader,
8      "gbs": psi4io.GBS.Reader,
9      "grid": psi4io.Grid.Reader
10     }

```

Definition at line 130 of file forcefield.py.

tuple `forcebalance.forcefield.logger = getLogger(__name__)` Definition at line 115 of file forcefield.py.

7.13 forcebalance.gmxio Namespace Reference

GROMACS input/output.

Classes

- class [ITP_Reader](#)
Finite state machine for parsing GROMACS force field files.
- class [GMX](#)
Derived from Engine object for carrying out general purpose GROMACS calculations.
- class [Liquid_GMX](#)
- class [Lipid_GMX](#)
- class [AbInitio_GMX](#)
Subclass of AbInitio for force and energy matching using GROMACS.
- class [BindingEnergy_GMX](#)
Binding energy matching using Gromacs.
- class [Interaction_GMX](#)
Interaction energy matching using GROMACS.
- class [Moments_GMX](#)

Multipole moment matching using GROMACS.

- class `Vibration_GMX`

Vibrational frequency matching using GROMACS.

- class `Thermo_GMX`

Thermodynamical property matching using GROMACS.

Functions

- def `write_mdp`

Create or edit a Gromacs MDP file.

- def `write_ndx`

Create or edit a Gromacs ndx file.

- def `parse_atomtype_line`

Parses the 'atomtype' line.

- def `rm_gmx_baks`

Variables

- tuple `logger` = getLogger(__name__)
- list `nftypes` = [None, 'VDW', 'VDW_BHAM']

VdW interaction function types.

- list `pftypes` = [None, 'VPAIR', 'VPAIR_BHAM']

Pairwise interaction function types.

- list `bftypes` = [None, 'BONDS', 'G96BONDS', 'MORSE']

Bonded interaction function types.

- list `aftypes`

Angle interaction function types.

- list `dftypes` = [None, 'PDIHS', 'IDIHS', 'RBDIHS', 'PIMPDIHS', 'FOURDIHS', None, None, 'TABDIHS', 'PDIHMLS']

Dihedral interaction function types.

- dictionary `fdict`

Section -> Interaction type dictionary.

- dictionary `pdict`

Interaction type -> Parameter Dictionary.

7.13.1 Detailed Description

GROMACS input/output.

Todo Even more stuff from `forcefield.py` needs to go into here.

Author

Lee-Ping Wang

Date

12/2011

7.13.2 Function Documentation

```
def forcebalance.gmxio.parse_atomtype_line( line ) Parses the 'atomtype' line.  
Parses lines like this:  
opls_135 CT 6 12.0107 0.0000 A 3.5000e-01 2.7614e-01  
C 12.0107 0.0000 A 3.7500e-01 4.3932e-01  
Na 11 22.9897 0.0000 A 6.068128070229e+03 2.662662556402e+01 0.0000e+00 ;  
PRM 5 6
```

Look at all the variety!

Parameters

in	<i>line</i>	Input line.
----	-------------	-------------

Returns

answer Dictionary containing:
atom type
bonded atom type (if any)
atomic number (if any)
atomic mass
charge
particle type
force field parameters
number of optional fields

Definition at line 234 of file gmxio.py.

Here is the call graph for this function:



```
def forcebalance.gmxio.rm_gmx_baks( dir ) Definition at line 481 of file gmxio.py.
```

```
def forcebalance.gmxio.write_mdp( fout, options, fin = None, defaults = {}, verbose = False ) Create or edit a Gromacs MDP file.
```

The MDP file contains GROMACS run parameters.

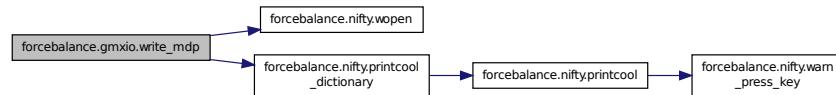
Parameters

in	<i>fout</i>	Output file name, can be the same as input file name.
in	<i>options</i>	Dictionary containing mdp options. Existing options are replaced, new options are added at the end.

in	<i>fin</i>	Input file name.
in	<i>defaults</i>	Default options to add to the mdp only if they don't already exist.
in	<i>verbose</i>	Print out all modifications to the file.

Definition at line 46 of file gmxio.py.

Here is the call graph for this function:

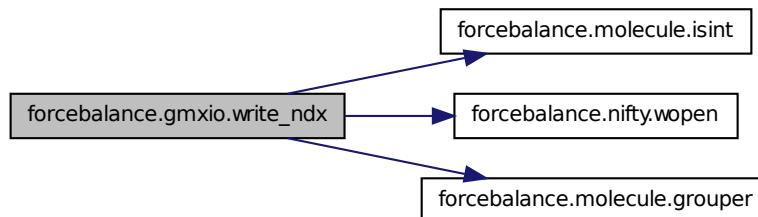


def forcebalance.gmxio.write_ndx (*fout*, *grps*, *fin = None*) Create or edit a Gromacs ndx file.
Parameters

in	<i>fout</i>	Output file name, can be the same as input file name.
in	<i>grps</i>	Dictionary containing key : atom selections.
in	<i>fin</i>	Input file name.

Definition at line 116 of file gmxio.py.

Here is the call graph for this function:



7.13.3 Variable Documentation

list forcebalance.gmxio.aftypes Initial value:

```

1 = [None, 'ANGLES', 'G96ANGLES', 'CROSS_BOND_BOND',
2      'CROSS_BOND_ANGLE', 'UREY_BRADLEY', 'QANGLES']
  
```

Angle interaction function types.

Definition at line 144 of file gmxio.py.

list forcebalance.gmxio.bftypes = [None, 'BONDS', 'G96BONDS', 'MORSE'] Bonded interaction function types.
Definition at line 142 of file gmxio.py.

list forcebalance.gmxio.dftypes = [None, 'PDIHS', 'IDIHS', 'RBDIHS', 'PIMPDIHS', 'FOURDIHS', None, None, 'T-ABDIHS', 'PDIHMULS'] Dihedral interaction function types.

Definition at line 147 of file gmxio.py.

dictionary forcebalance.gmxio.fdict Initial value:

```
1 = {
2     'atomtypes'      : nftypes,
3     'nonbond_params': pftypes,
4     'bonds'          : bftypes,
5     'bondtypes'      : bftypes,
6     'angles'          : aftytypes,
7     'angletypes'      : aftytypes,
8     'dihedrals'       : dftytypes,
9     'dihedraltypes'   : dftytypes,
10    'virtual_sites2': ['NONE','VSITE2'],
11    'virtual_sites3': ['NONE','VSITE3','VSITE3FD','VSITE3FAD','VSITE3OUT'],
12    'virtual_sites4': ['NONE','VSITE4FD','VSITE4FDN']
13 }
```

Section -> Interaction type dictionary.

Based on the section you're in and the integer given on the current line, this looks up the 'interaction type' - for example, within bonded interactions there are four interaction types: harmonic, G96, Morse, and quartic interactions.

Definition at line 155 of file gmxio.py.

tuple forcebalance.gmxio.logger = getLogger(__name__) Definition at line 35 of file gmxio.py.

list forcebalance.gmxio.nftypes = [None, 'VDW', 'VDW_BHAM'] VdW interaction function types.

Definition at line 138 of file gmxio.py.

dictionary forcebalance.gmxio.pdict Interaction type -> Parameter Dictionary.

A list of supported GROMACS interaction types in force matching. The keys in this dictionary (e.g. 'BONDS';'ANGLES') are values in the interaction type dictionary. As the program loops through the force field file, it first looks up the interaction types in 'fdict' and then goes here to do the parameter lookup by field.

Todo This needs to become more flexible because the parameter isn't always in the same field. Still need to figure out how to do this.

How about making the PDIHS less ugly?

Definition at line 178 of file gmxio.py.

list forcebalance.gmxio.pftypes = [None, 'VPAIR', 'VPAIR_BHAM'] Pairwise interaction function types.

Definition at line 140 of file gmxio.py.

7.14 forcebalance.interaction Namespace Reference

[Interaction](#) energy fitting module.

Classes

- class [Interaction](#)

Subclass of Target for fitting force fields to interaction energies.

Variables

- tuple [logger](#) = getLogger(__name__)

7.14.1 Detailed Description

[Interaction](#) energy fitting module.

Author

Lee-Ping Wang

Date

05/2012

7.14.2 Variable Documentation

tuple forcebalance.interaction.logger = getLogger(__name__) Definition at line 21 of file interaction.py.

7.15 forcebalance.leastsq Namespace Reference

Classes

- class [LeastSquares](#)

Subclass of Target for general least squares fitting.

Functions

- def [CheckBasis](#)
- def [LastMvals](#)

Variables

- tuple [logger](#) = getLogger(__name__)
- [CHECK_BASIS](#) = False
- [LAST_MVALS](#) = None

7.15.1 Function Documentation

def forcebalance.leastsq.CheckBasis () Definition at line 24 of file leastsq.py.

def forcebalance.leastsq.LastMvals () Definition at line 29 of file leastsq.py.

7.15.2 Variable Documentation

forcebalance.leastsq.CHECK_BASIS = False Definition at line 23 of file leastsq.py.

forcebalance.leastsq.LAST_MVALS = None Definition at line 28 of file leastsq.py.

tuple forcebalance.leastsq.logger = getLogger(__name__) Definition at line 21 of file leastsq.py.

7.16 forcebalance.lipid Namespace Reference

Matching of lipid bulk properties.

Classes

- class [Lipid](#)

Subclass of Target for lipid property matching.

Functions

- def [weight_info](#)

Variables

- tuple [logger](#) = getLogger(__name__)

7.16.1 Detailed Description

Matching of lipid bulk properties. Under development.

author Lee-Ping Wang

Date

04/2012

7.16.2 Function Documentation

def forcebalance.lipid.weight_info (W, PT, N_k, verbose = True) Definition at line 32 of file [lipid.py](#).

7.16.3 Variable Documentation

tuple forcebalance.lipid.logger = getLogger(__name__) Definition at line 30 of file [lipid.py](#).

7.17 forcebalance.liquid Namespace Reference

Matching of liquid bulk properties.

Classes

- class [Liquid](#)

Subclass of Target for liquid property matching.

Functions

- def [weight_info](#)

Variables

- tuple [logger](#) = getLogger(__name__)

7.17.1 Detailed Description

Matching of liquid bulk properties. Under development.

author Lee-Ping Wang

Date

04/2012

7.17.2 Function Documentation

def forcebalance.liquid.weight_info (W, PT, N_k, verbose = True) Definition at line 32 of file [liquid.py](#).

7.17.3 Variable Documentation

tuple forcebalance.liquid.logger = getLogger(__name__) Definition at line 30 of file [liquid.py](#).

7.18 forcebalance.Mol2 Namespace Reference

Classes

- class `mol2_atom`
This is to manage mol2 atomic lines on the form: 1 C1 5.4790 42.2880 49.5910 C.ar 1 <1> 0.0424.
- class `mol2_bond`
This is to manage mol2 bond lines on the form: 1 1 2 ar.
- class `mol2`
This is to manage one mol2 series of lines on the form:
- class `mol2_set`

Variables

- tuple `data = mol2_set(sys.argv[1], subset=["RNase.xray.inh8.1QHC"])`

7.18.1 Variable Documentation

`tuple forcebalance.Mol2.data = mol2_set(sys.argv[1], subset=["RNase.xray.inh8.1QHC"])` Definition at line 651 of file Mol2.py.

7.19 forcebalance.mol2io Namespace Reference

Mol2 I/O.

Classes

- class `Mol2_Reader`
Finite state machine for parsing Mol2 force field file.

Variables

- dictionary `mol2_pdct = {'COUL': {'Atom': [1], 6: ''}}`

7.19.1 Detailed Description

Mol2 I/O. This serves as a good template for writing future force matching I/O modules for other programs because it's so simple.

Author

Lee-Ping Wang

Date

05/2012

7.19.2 Variable Documentation

`dictionary forcebalance.mol2io.mol2_pdct = {'COUL': {'Atom': [1], 6: ''}}` Definition at line 18 of file mol2io.py.

7.20 forcebalance.molecule Namespace Reference

Classes

- class [MyG](#)
- class [MolfileTimestep](#)

Wrapper for the timestep C structure used in molfile plugins.

- class [Molecule](#)

Lee-Ping's general file format conversion class.

Functions

- def [getElement](#)

- def [elem_from_atomname](#)

Given an atom name, attempt to get the element in most cases.

- def [nodematch](#)

- def [isint](#)

ONLY matches integers! If you have a decimal point? None shall pass!

- def [isfloat](#)

Matches ANY number; it can be a decimal, scientific notation, integer, or what have you.

- def [CubicLattice](#)

This function takes in three lattice lengths and three lattice angles, and tries to return a complete box specification.

- def [BuildLatticeFromLengthsAngles](#)

This function takes in three lattice lengths and three lattice angles, and tries to return a complete box specification.

- def [BuildLatticeFromVectors](#)

This function takes in three lattice vectors and tries to return a complete box specification.

- def [format_xyz_coord](#)

Print a line consisting of (element, x, y, z) in accordance with .xyz file format.

- def [format_gro_coord](#)

Print a line in accordance with .gro file format, with six decimal points of precision.

- def [format_xyzgen_coord](#)

Print a line consisting of (element, p, q, r, s, t, ...) where (p, q, r) are arbitrary atom-wise data (this might happen, for instance, with atomic charges)

- def [format_gro_box](#)

Print a line corresponding to the box vector in accordance with .gro file format.

- def [is_gro_coord](#)

Determines whether a line contains GROMACS data or not.

- def [is_charmm_coord](#)

Determines whether a line contains CHARMM data or not.

- def [is_gro_box](#)

Determines whether a line contains a GROMACS box vector or not.

- def [add_strip_to_mat](#)

- def [pvec](#)

- def [grouper](#)

Groups a big long iterable into groups of ten or what have you.

- def [even_list](#)

Creates a list of number sequences divided as evenly as possible.

- def [both](#)

- def [diff](#)

- def `either`
- def `EulerMatrix`
Constructs an Euler matrix from three Euler angles.
- def `ComputeOverlap`
Computes an 'overlap' between two molecules based on some fictitious density.
- def `AlignToDensity`
Computes a "overlap density" from two frames.
- def `AlignToMoments`
Pre-aligns molecules to 'moment of inertia'.
- def `get_rotate_translate`
- def `cartesian_product2`
Form a Cartesian product of two NumPy arrays.
- def `main`

Variables

- tuple `FrameVariableNames`
- tuple `AtomVariableNames` = set(['elem', 'partial_charge', 'atomname', 'atomtype', 'tinkersuf', 'resid', 'resname', 'qcsuf', 'qm_ghost', 'chain', 'altloc', 'icode'])
- tuple `MetaVariableNames` = set(['fnm', 'ftype', 'qcrems', 'qctemplate', 'qcerr', 'charge', 'mult', 'bonds'])
- tuple `QuantumVariableNames` = set(['qcrems', 'qctemplate', 'charge', 'mult', 'qcsuf', 'qm_ghost'])
- `AllVariableNames` = `QuantumVariableNames|AtomVariableNames|MetaVariableNames|FrameVariableNames`
- list `Radii`
- list `Elements`
- tuple `PeriodicTable`
- float `bohrang` = 0.529177249
One bohr equals this many angstroms.
- tuple `splitter` = re.compile(r'(\s+|\S+)')
- tuple `Box` = namedtuple('Box',[‘a’,‘b’,‘c’,‘alpha’,‘beta’,‘gamma’,‘A’,‘B’,‘C’,‘V’])
- int `radian` = 180
- int `have_contact` = 0

7.20.1 Function Documentation

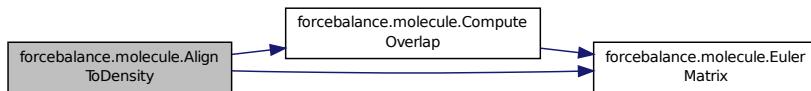
`def forcebalance.molecule.add_strip_to_mat (mat, strip)` Definition at line 466 of file molecule.py.

`def forcebalance.molecule.AlignToDensity (elem, xyz1, xyz2, binary = False)` Computes a "overlap density" from two frames.

This function can be called by AlignToMoments to get rid of inversion problems

Definition at line 572 of file molecule.py.

Here is the call graph for this function:



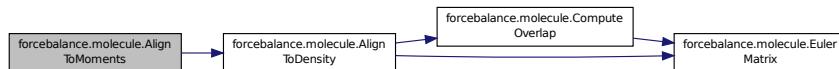
```
def forcebalance.molecule.AlignToMoments( elem, xyz1, xyz2 = None )
```

Pre-aligns molecules to 'moment of inertia'.

If xyz2 is passed in, it will assume that xyz1 is already aligned to the moment of inertia, and it simply does 180-degree rotations to make sure nothing is inverted.

Definition at line 584 of file molecule.py.

Here is the call graph for this function:



```
def forcebalance.molecule.both( A, B, key )
```

Definition at line 504 of file molecule.py.

```
def forcebalance.molecule.BuildLatticeFromLengthsAngles( a, b, c, alpha, beta, gamma )
```

This function takes in three lattice lengths and three lattice angles, and tries to return a complete box specification.

Definition at line 282 of file molecule.py.

```
def forcebalance.molecule.BuildLatticeFromVectors( v1, v2, v3 )
```

This function takes in three lattice vectors and tries to return a complete box specification.

Definition at line 297 of file molecule.py.

```
def forcebalance.molecule.cartesian_product2( arrays )
```

Form a Cartesian product of two NumPy arrays.

Definition at line 645 of file molecule.py.

```
def forcebalance.molecule.ComputeOverlap( theta, elem, xyz1, xyz2 )
```

Computes an 'overlap' between two molecules based on some fictitious density.

Good for fine-tuning alignment but gets stuck in local minima.

Definition at line 555 of file molecule.py.

Here is the call graph for this function:



```
def forcebalance.molecule.CubicLattice( a )
```

This function takes in three lattice lengths and three lattice angles, and tries to return a complete box specification.

Definition at line 262 of file molecule.py.

```
def forcebalance.molecule.diff( A, B, key )
```

Definition at line 507 of file molecule.py.

```
def forcebalance.molecule.either( A, B, key )
```

Definition at line 518 of file molecule.py.

def forcebalance.molecule.elem_from_atomname (*atomname*) Given an atom name, attempt to get the element in most cases.

Definition at line 194 of file molecule.py.

def forcebalance.molecule.EulerMatrix (*T1*, *T2*, *T3*) Constructs an Euler matrix from three Euler angles.

Definition at line 527 of file molecule.py.

def forcebalance.molecule.even_list (*totlen*, *splitsize*) Creates a list of number sequences divided as evenly as possible.

Definition at line 486 of file molecule.py.

def forcebalance.molecule.format_gro_box (*box*) Print a line corresponding to the box vector in accordance with .gro file format.

Parameters

in	<i>box</i>	Box NamedTuple
----	------------	----------------

Definition at line 417 of file molecule.py.

def forcebalance.molecule.format_gro_coord (*resid*, *resname*, *aname*, *seqno*, *xyz*) Print a line in accordance with .gro file format, with six decimal points of precision.

Nine decimal points of precision are necessary to get forces below 1e-3 kJ/mol/nm.

Parameters

in	<i>resid</i>	The number of the residue that the atom belongs to
in	<i>resname</i>	The name of the residue that the atom belongs to
in	<i>aname</i>	The name of the atom
in	<i>seqno</i>	The sequential number of the atom
in	<i>xyz</i>	A 3-element array containing x, y, z coordinates of that atom

Definition at line 396 of file molecule.py.

def forcebalance.molecule.format_xyz_coord (*element*, *xyz*, *tinker = False*) Print a line consisting of (element, x, y, z) in accordance with .xyz file format.

Parameters

in	<i>element</i>	A chemical element of a single atom
in	<i>xyz</i>	A 3-element array containing x, y, z coordinates of that atom

Definition at line 378 of file molecule.py.

def forcebalance.molecule.format_xyzgen_coord (*element*, *xyzgen*) Print a line consisting of (element, p, q, r, s, t, ...) where (p, q, r) are arbitrary atom-wise data (this might happen, for instance, with atomic charges)

Parameters

in	<i>element</i>	A chemical element of a single atom
in	<i>xyzgen</i>	A N-element array containing data for that atom

Definition at line 408 of file molecule.py.

def forcebalance.molecule.get_rotate_translate (*matrix1*, *matrix2*) Definition at line 607 of file molecule.py.

def forcebalance.molecule.getElement (*mass*) Definition at line 189 of file molecule.py.

def forcebalance.molecule.grouper (*n*, *iterable*) Groups a big long iterable into groups of ten or what have you.

Definition at line 480 of file molecule.py.

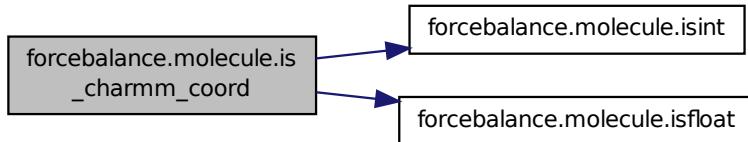
def forcebalance.molecule.is_charmm_coord (*line*) Determines whether a line contains CHARMM data or not.

Parameters

in	<i>line</i>	The line to be tested
----	-------------	-----------------------

Definition at line 444 of file molecule.py.

Here is the call graph for this function:



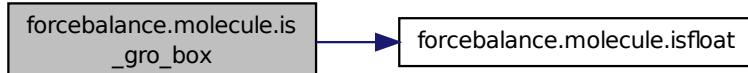
def forcebalance.molecule.is_gro_box (*line*) Determines whether a line contains a GROMACS box vector or not.

Parameters

in	<i>line</i>	The line to be tested
----	-------------	-----------------------

Definition at line 457 of file molecule.py.

Here is the call graph for this function:



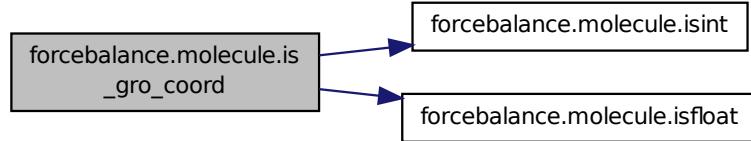
def forcebalance.molecule.is_gro_coord (*line*) Determines whether a line contains GROMACS data or not.

Parameters

in	<i>line</i>	The line to be tested
----	-------------	-----------------------

Definition at line 429 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.isfloat (word) Matches ANY number; it can be a decimal, scientific notation, integer, or what have you.

Definition at line 251 of file molecule.py.

def forcebalance.molecule.isint (word) ONLY matches integers! If you have a decimal point? None shall pass!

Definition at line 246 of file molecule.py.

def forcebalance.molecule.main () Definition at line 3009 of file molecule.py.

def forcebalance.molecule.nodematch (node1, node2) Definition at line 240 of file molecule.py.

def forcebalance.molecule.pvec (vec) Definition at line 475 of file molecule.py.

7.20.2 Variable Documentation

forcebalance.molecule.AllVariableNames = QuantumVariableNames|AtomVariableNames|MetaVariableNames|FrameVariableNames Definition at line 137 of file molecule.py.

tuple forcebalance.molecule.AtomVariableNames = set(['elem', 'partial_charge', 'atomname', 'atomtype', 'tinkersuf', 'resid', 'resname', 'qcsuf', 'qm_ghost', 'chain', 'altloc', 'icode']) Definition at line 120 of file molecule.py.

float forcebalance.molecule.bohrang = 0.529177249 One bohr equals this many angstroms.

Definition at line 238 of file molecule.py.

tuple forcebalance.molecule.Box = namedtuple('Box',[‘a’,‘b’,‘c’,‘alpha’,‘beta’,‘gamma’,‘A’,‘B’,‘C’,‘V’]) Definition at line 258 of file molecule.py.

list forcebalance.molecule.Elements Initial value:

```
1 = ["None",'H','He',
2   'Li','Be','B','C','N','O','F','Ne',
3   'Na','Mg','Al','Si','P','S','Cl','Ar',
4   'K','Ca','Sc','Ti','V','Cr','Mn','Fe','Co','Ni','Cu','Zn','Ga','Ge','As','Se','Br','Kr',
5   'Rb','Sr','Y','Zr','Nb','Mo','Tc','Ru','Rh','Pd','Ag','Cd','In','Sn','Sb','Te','I','Xe',
6   'Cs','Ba','La','Ce','Pr','Nd','Pm','Sm','Eu','Gd','Tb','Dy','Ho','Er','Tm','Yb',
7   'Lu','Hf','Ta','W','Re','Os','Ir','Pt','Au','Hg','Tl','Pb','Bi','Po','At','Rn',
8   'Fr','Ra','Ac','Th','Pa','U','Np','Pu','Am','Cm','Bk','Cf','Es','Fm','Md','No','Lr','Rf','Db',
  Sg,'Bh','Hs','Mt']
```

Definition at line 164 of file molecule.py.

tuple forcebalance.molecule.FrameVariableNames Initial value:

```
1 = set(['xyzs', 'comms', 'boxes', 'qm_hessians', 'qm_forces', 'qm_energies', 'qm_interaction',
2       'qm_espxyzs', 'qm_espvals', 'qm_extchgs', 'qm_mulliken_charges', '
     qm_mulliken_spins'])
```

Definition at line 106 of file molecule.py.

int forcebalance.molecule.have_contact = 0 Definition at line 321 of file molecule.py.

tuple forcebalance.molecule.MetaVariableNames = set(['fnm', 'ftype', 'qcrems', 'qctemplate', 'qcerr', 'charge', 'mult', 'bonds']) Definition at line 133 of file molecule.py.

tuple forcebalance.molecule.PeriodicTable Initial value:

```
1 = OrderedDict([(('H', 1.0079), ('He', 4.0026),
2                 ('Li', 6.941), ('Be', 9.0122), ('B', 10.811), ('C', 12.0107), ('N', 14.00
3                 67), ('O', 15.9994), ('F', 18.9984), ('Ne', 20.1797),
4                 ('Na', 22.9897), ('Mg', 24.305), ('Al', 26.9815), ('Si', 28.0855), ('P',
5                 30.9738), ('S', 32.065), ('Cl', 35.453), ('Ar', 39.948),
6                 ('K', 39.0983), ('Ca', 40.078), ('Sc', 44.9559), ('Ti', 47.867), ('V',
7                 50.9415), ('Cr', 51.9961), ('Mn', 54.938), ('Fe', 55.845), ('Co', 58.9332),
8                 ('Ni', 58.6934), ('Cu', 63.546), ('Zn', 65.39), ('Ga', 69.723), ('Ge',
9                 72.64), ('As', 74.9216), ('Se', 78.96), ('Br', 79.904), ('Kr', 83.8),
10                ('Rb', 85.4678), ('Sr', 87.62), ('Y', 88.9059), ('Zr', 91.224), ('Nb',
11                92.9064), ('Mo', 95.94), ('Tc', 98), ('Ru', 101.07), ('Rh', 102.9055),
12                ('Pd', 106.42), ('Ag', 107.8682), ('Cd', 112.411), ('In', 114.818), ('Sn',
13                118.71), ('Sb', 121.76), ('Te', 127.6), ('I', 126.9045), ('Xe', 131.293),
14                ('Cs', 132.9055), ('Ba', 137.327), ('La', 138.9055), ('Ce', 140.116), ('Pr',
15                140.9077), ('Nd', 144.24), ('Pm', 145), ('Sm', 150.36),
16                ('Eu', 151.964), ('Gd', 157.25), ('Tb', 158.9253), ('Dy', 162.5), ('Ho',
17                164.9303), ('Er', 167.259), ('Tm', 168.9342), ('Yb', 173.04),
18                ('Lu', 174.967), ('Hf', 178.49), ('Ta', 180.9479), ('W', 183.84), ('Re',
19                186.207), ('Os', 190.23), ('Ir', 192.217), ('Pt', 195.078),
20                ('Au', 196.9665), ('Hg', 200.59), ('Tl', 204.3833), ('Pb', 207.2), ('Bi',
21                208.9804), ('Po', 209), ('At', 210), ('Rn', 222),
22                ('Fr', 223), ('Ra', 226), ('Ac', 227), ('Th', 232.0381), ('Pa', 231.0359),
23                ('U', 238.0289), ('Np', 237), ('Pu', 244),
24                ('Am', 243), ('Cm', 247), ('Bk', 247), ('Cf', 251), ('Es', 252), ('Fm',
25                257), ('Md', 258), ('No', 259),
26                ('Lr', 262), ('Rf', 261), ('Db', 262), ('Sg', 266), ('Bh', 264), ('Hs',
27                277), ('Mt', 268)])
```

Definition at line 174 of file molecule.py.

tuple forcebalance.molecule.QuantumVariableNames = set(['qcrems', 'qctemplate', 'charge', 'mult', 'qcsuf', 'qm_ghost']) Definition at line 135 of file molecule.py.

int forcebalance.molecule.radian = 180 Definition at line 259 of file molecule.py.

list forcebalance.molecule.Radii Initial value:

```
1 = [0.31, 0.28, # H and He
2     1.28, 0.96, 0.84, 0.76, 0.71, 0.66, 0.57, 0.58, # First row elements
3     1.66, 1.41, 1.21, 1.11, 1.07, 1.05, 1.02, 1.06, # Second row elements
4     2.03, 1.76, 1.70, 1.60, 1.53, 1.39, 1.61, 1.52, 1.50,
5     1.24, 1.32, 1.22, 1.20, 1.19, 1.20, 1.20, 1.16, # Third row elements, K through Kr
6     2.20, 1.95, 1.90, 1.75, 1.64, 1.54, 1.47, 1.46, 1.42,
7     1.39, 1.45, 1.44, 1.42, 1.39, 1.39, 1.38, 1.39, 1.40, # Fourth row elements, Rb through Xe
8     2.44, 2.15, 2.07, 2.04, 2.03, 2.01, 1.99, 1.98,
9     1.98, 1.96, 1.94, 1.92, 1.92, 1.89, 1.90, 1.87, # Fifth row elements, s and f blocks
10    1.87, 1.75, 1.70, 1.62, 1.51, 1.44, 1.41, 1.36,
11    1.36, 1.32, 1.45, 1.46, 1.48, 1.40, 1.50, 1.50, # Fifth row elements, d and p blocks
12    2.60, 2.21, 2.15, 2.06, 2.00, 1.96, 1.90, 1.87, 1.80, 1.69]
```

Definition at line 150 of file molecule.py.

tuple forcebalance.molecule.splitter = re.compile(r'(\s+|\S+)') Definition at line 255 of file molecule.py.

7.21 forcebalance.moments Namespace Reference

Multipole moment fitting module.

Classes

- class [Moments](#)

Subclass of Target for fitting force fields to multipole moments (from experiment or theory).

Variables

- tuple [logger](#) = getLogger(__name__)

7.21.1 Detailed Description

Multipole moment fitting module.

Author

Lee-Ping Wang

Date

09/2012

7.21.2 Variable Documentation

[tuple forcebalance.moments.logger = getLogger\(__name__\)](#) Definition at line 22 of file moments.py.

7.22 forcebalance.nifty Namespace Reference

Nifty functions, intended to be imported by any module within ForceBalance.

Classes

- class [Pickler_LP](#)
A subclass of the python Pickler that implements pickling of _ElementTree types.
- class [Unpickler_LP](#)
A subclass of the python Unpickler that implements unpickling of _ElementTree types.
- class [LineChunker](#)

Functions

- def [pvec1d](#)
Printout of a 1-D vector.
- def [astr](#)
Write an array to a string so we can use it to key a dictionary.
- def [pmat2d](#)
Printout of a 2-D matrix.
- def [grouper](#)
- def [encode](#)
- def [segments](#)
- def [commadash](#)
- def [uncommadash](#)

- def `extract_int`
Get the representative integer value from an array.
- def `printcool`
Cool-looking printout for slick formatting of output.
- def `printcool_dictionary`
See documentation for printcool; this is a nice way to print out keys/values in a dictionary.
- def `isint`
ONLY matches integers! If you have a decimal point? None shall pass!
- def `isfloat`
Matches ANY number; it can be a decimal, scientific notation, what have you CAUTION - this will also match an integer.
- def `isdecimal`
Matches things with a decimal only; see isint and isfloat.
- def `floatornan`
Returns a big number if we encounter NaN.
- def `col`
Given any list, array, or matrix, return a 1-column matrix.
- def `row`
Given any list, array, or matrix, return a 1-row matrix.
- def `flat`
Given any list, array, or matrix, return a single-index array.
- def `monotonic`
- def `orthogonalize`
Given two vectors vec1 and vec2, project out the component of vec1 that is along the vec2-direction.
- def `invert_svd`
Invert a matrix using singular value decomposition.
- def `get_least_squares`
- def `statisticalinefficiency`
Compute the (cross) statistical inefficiency of (two) timeseries.
- def `multiD_statisticalinefficiency`
- def `lp_dump`
Use this instead of pickle.dump for pickling anything that contains _ElementTree types.
- def `lp_load`
Use this instead of pickle.load for unpickling anything that contains _ElementTree types.
- def `getWorkQueue`
- def `getWQIds`
- def `createWorkQueue`
- def `destroyWorkQueue`
- def `queue_up`
Submit a job to the Work Queue.
- def `queue_up_src_dest`
Submit a job to the Work Queue.
- def `wq_wait1`
This function waits ten seconds to see if a task in the Work Queue has finished.
- def `wq_wait`
This function waits until the work queue is completely empty.
- def `click`
Stopwatch function for timing.

- def `bak`
- def `onefile`
- def `Golnto`
- def `allsplit`
- def `Leave`
- def `MissingFileInspection`
- def `wopen`

If trying to write to a symbolic link, remove it first.
- def `LinkFile`
- def `CopyFile`
- def `link_dir_contents`
- def `remove_if_exists`

Remove the file if it exists (doesn't return an error).
- def `which`
- def `warn_press_key`
- def `warn_once`

Prints a warning but will only do so once in a given run.
- def `concurrent_map`

Similar to the builtin function map().

Variables

- tuple `logger` = getLogger(__name__)
- float `kb` = 0.0083144100163

Boltzmann constant.
- float `eqcgmx` = 2625.5002

Q-Chem to GMX unit conversion for energy.
- float `fqcgmx` = -49621.9

Q-Chem to GMX unit conversion for force.
- float `bohrang` = 0.529177249

One bohr equals this many angstroms.
- string `XMLFILE` = 'x'

Pickle uses 'flags' to pickle and unpickle different variable types.
- `WORK_QUEUE` = None
- tuple `WQIDS` = defaultdict(list)
- list `specific_lst`
- tuple `specific_dct` = dict(list(itertools.chain(*[[j,i[1]] for j in i[0]] for i in `specific_lst`))))

7.22.1 Detailed Description

Nifty functions, intended to be imported by any module within ForceBalance. Table of Contents:

- I/O formatting
- Math: Variable manipulation, linear algebra, least squares polynomial fitting
- Pickle: Expand Python's own pickle to accommodate writing XML etree objects
- Commands for submitting things to the Work Queue
- Various file and process management functions
- Development stuff (not commonly used)

Named after the mighty Sniffy Handy Nifty (King Sniffy)

Author

Lee-Ping Wang

Date

12/2011

7.22.2 Function Documentation

def forcebalance.nifty.allsplit (Dir) Definition at line 852 of file nifty.py.

def forcebalance.nifty.astr (vec1d, precision = 4) Write an array to a string so we can use it to key a dictionary.
Definition at line 60 of file nifty.py.

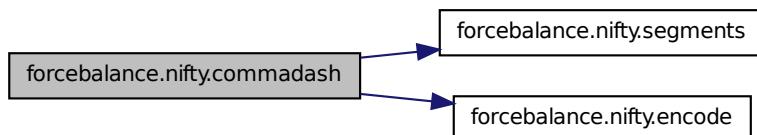
def forcebalance.nifty.bak (path, dest = None) Definition at line 803 of file nifty.py.

def forcebalance.nifty.click () Stopwatch function for timing.
Definition at line 796 of file nifty.py.

def forcebalance.nifty.col (vec) Given any list, array, or matrix, return a 1-column matrix.
Input: vec = The input vector that is to be made into a column
Output: A column matrix
Definition at line 302 of file nifty.py.

def forcebalance.nifty.commadash (I) Definition at line 91 of file nifty.py.

Here is the call graph for this function:



def forcebalance.nifty.concurrent_map (func, data) Similar to the builtin function map().

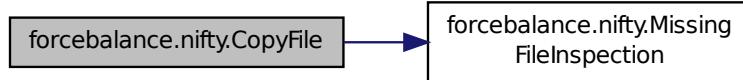
But spawn a thread for each argument and apply `func` concurrently.

Note: unlike `map()`, we cannot take an iterable argument. `data` should be an indexable sequence.

Definition at line 1127 of file nifty.py.

def forcebalance.nifty.CopyFile (src, dest) Definition at line 910 of file nifty.py.

Here is the call graph for this function:



def forcebalance.nifty.createWorkQueue (wq_port, debug = True) Definition at line 643 of file nifty.py.

def forcebalance.nifty.destroyWorkQueue () Definition at line 652 of file nifty.py.

def forcebalance.nifty.encode (I) Definition at line 82 of file nifty.py.

def forcebalance.nifty.extract_int (arr, avgthre, limthre, label = "value", verbose = True) Get the representative integer value from an array.

Sanity check: Make sure the value does not go through big excursions. The integer value is the rounded value of the average. thresh = A threshold to make sure we're not dealing with fluctuations that are too large.

Definition at line 140 of file nifty.py.

def forcebalance.nifty.flat (vec) Given any list, array, or matrix, return a single-index array.

Parameters

in	vec	The data to be flattened
----	-----	--------------------------

Returns

answer The flattened data

Definition at line 321 of file nifty.py.

def forcebalance.nifty.floatornan (word) Returns a big number if we encounter NaN.

Parameters

in	word	The string to be converted
----	------	----------------------------

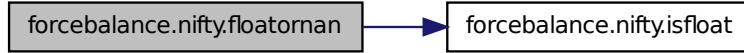
Returns

answer The string converted to a float; if not a float, return 1e10

Todo I could use suggestions for making this better.

Definition at line 284 of file nifty.py.

Here is the call graph for this function:



```
def forcebalance.nifty.get_least_squares( x, y, w=None, thresh=1e-12 )
```

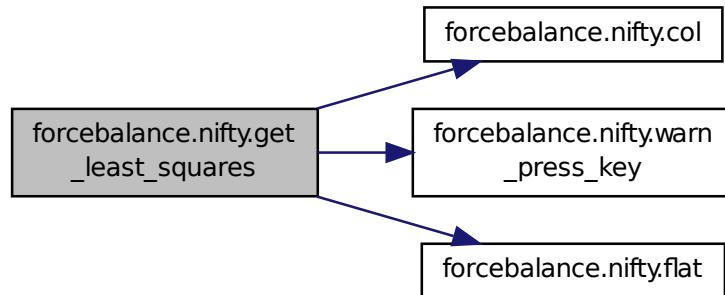
```
1 -- -- |  
2 | 1 (x0) (x0)^2 (x0)^3 |  
3 | 1 (x1) (x1)^2 (x1)^3 |  
4 | 1 (x2) (x2)^2 (x2)^3 |  
5 | 1 (x3) (x3)^2 (x3)^3 |  
6 | 1 (x4) (x4)^2 (x4)^3 |  
7 | -- |  
8 | -- |
```

Parameters

in	X	(2-D array) An array of X-values (see above)
in	Y	(array) An array of Y-values (only used in getting the least squares coefficients)
in	w	(array) An array of weights, hopefully normalized to one.
out	Beta	The least-squares coefficients
out	Hat	The hat matrix that takes linear combinations of data y-values to give fitted y-values (weights)
out	yfit	The fitted y-values
out	MPPI	The Moore-Penrose pseudoinverse (multiply by Y to get least-squares coefficients, multiply by dY/dk to get derivatives of least-squares coefficients)

Definition at line 410 of file nifty.py.

Here is the call graph for this function:



```
def forcebalance.nifty.getWorkQueue( ) Definition at line 635 of file nifty.py.
```

```

def forcebalance.nifty.getWQIds ( ) Definition at line 639 of file nifty.py.

def forcebalance.nifty.GoInto ( Dir ) Definition at line 844 of file nifty.py.

def forcebalance.nifty.grouper ( iterable, n ) Definition at line 75 of file nifty.py.

def forcebalance.nifty.invert_svd ( X, thresh = 1e-12 ) Invert a matrix using singular value decomposition.
Parameters

```

in	<i>X</i>	The matrix to be inverted
in	<i>thresh</i>	The SVD threshold; eigenvalues below this are not inverted but set to zero

Returns

Xt The inverted matrix

Definition at line 369 of file nifty.py.

```

def forcebalance.nifty.isdecimal ( word ) Matches things with a decimal only; see isint and isfloat.
Parameters

```

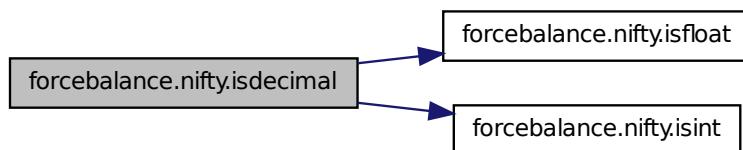
in	<i>word</i>	String (for instance, '123', '153.0', '2.', '-354')
----	-------------	---

Returns

answer Boolean which specifies whether the string is a number with a decimal point

Definition at line 274 of file nifty.py.

Here is the call graph for this function:



```

def forcebalance.nifty.isfloat ( word ) Matches ANY number; it can be a decimal, scientific notation, what have you
CAUTION - this will also match an integer.
Parameters

```

in	<i>word</i>	String (for instance, '123', '153.0', '2.', '-354')
----	-------------	---

Returns

answer Boolean which specifies whether the string is any number

Definition at line 264 of file nifty.py.

```

def forcebalance.nifty.isint ( word ) ONLY matches integers! If you have a decimal point? None shall pass!

```

Parameters

in	word	String (for instance, '123', '153.0', '2.', '-354')
----	------	---

Returns

answer Boolean which specifies whether the string is an integer (only +/- sign followed by digits)

Definition at line 253 of file nifty.py.

def forcebalance.nifty.Leave (Dir) Definition at line 858 of file nifty.py.

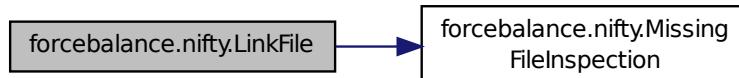
Here is the call graph for this function:



def forcebalance.nifty.link_dir_contents (abssrcdir, absdestdir) Definition at line 920 of file nifty.py.

def forcebalance.nifty.LinkFile (src, dest, nosrcok = False) Definition at line 897 of file nifty.py.

Here is the call graph for this function:



def forcebalance.nifty.lp_dump (obj, file, protocol = None) Use this instead of pickle.dump for pickling anything that contains _ElementTree types.

Definition at line 613 of file nifty.py.

def forcebalance.nifty.lp_load (file) Use this instead of pickle.load for unpickling anything that contains _ElementTree types.

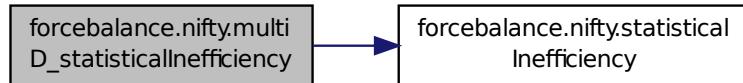
Definition at line 618 of file nifty.py.

def forcebalance.nifty.MissingFileInspection (fnm) Definition at line 879 of file nifty.py.

def forcebalance.nifty.monotonic (arr, start, end) Definition at line 324 of file nifty.py.

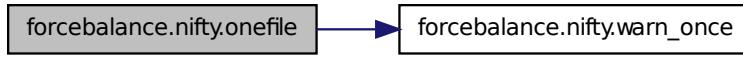
```
def forcebalance.nifty.multiD_statisticalInefficiency ( A_n, B_n = None, fast = False, mintime = 3, warn = True ) Definition at line 539 of file nifty.py.
```

Here is the call graph for this function:



```
def forcebalance.nifty.onefile ( ext, arg = None ) Definition at line 826 of file nifty.py.
```

Here is the call graph for this function:



```
def forcebalance.nifty.orthogonalize ( vec1, vec2 ) Given two vectors vec1 and vec2, project out the component of vec1 that is along the vec2-direction.
```

Parameters

in	vec1	The projectee (i.e. output is some modified version of vec1)
in	vec2	The projector (component subtracted out from vec1 is parallel to this)

Returns

answer A copy of vec1 but with the vec2-component projected out.

Definition at line 356 of file nifty.py.

```
def forcebalance.nifty.pmat2d ( mat2d, precision = 1, format = "e", loglevel = INFO ) Printout of a 2-D matrix.
```

Parameters

in	mat2d	a 2-D matrix
----	-------	--------------

Definition at line 68 of file nifty.py.

```
def forcebalance.nifty.printcool ( text, sym = "#", bold = False, color = 2, ansi = None, bottom = ' - ', minwidth = 50, center = True, sym2 = "=" ) Cool-looking printout for slick formatting of output.
```

Parameters

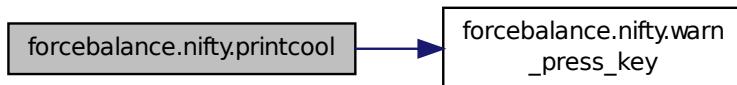
in	<i>text</i>	The string that the printout is based upon. This function will print out the string, ANSI-colored and enclosed in the symbol for example: ##### I am cool #####
in	<i>sym</i>	The surrounding symbol
in	<i>bold</i>	Whether to use bold print
in	<i>color</i>	The ANSI color: 1 red 2 green 3 yellow 4 blue 5 magenta 6 cyan 7 white
in	<i>bottom</i>	The symbol for the bottom bar
in	<i>minwidth</i>	The minimum width for the box, if the text is very short then we insert the appropriate number of padding spaces

Returns

bar The bottom bar is returned for the user to print later, e.g. to mark off a 'section'

Definition at line 184 of file nifty.py.

Here is the call graph for this function:



def forcebalance.nifty.printcool_dictionary(*Dict*, *title* = "General options", *bold* = False, *color* = 2, *keywidth* = 25, *topwidth* = 50, *center* = True, *leftpad* = 0) See documentation for printcool; this is a nice way to print out keys/values in a dictionary.

The keys in the dictionary are sorted before printing out.

Parameters

in	<i>dict</i>	The dictionary to be printed
in	<i>title</i>	The title of the printout

Definition at line 229 of file nifty.py.

Here is the call graph for this function:



def forcebalance.nifty.pvec1d (*vec1d*, *precision* = 1, *format* = "e", *loglevel* = INFO) Printout of a 1-D vector.

Parameters

in	<i>vec1d</i>	a 1-D vector
----	--------------	--------------

Definition at line 52 of file nifty.py.

def forcebalance.nifty.queue.up (*wq*, *command*, *input_files*, *output_files*, *tag* = None, *tgt* = None, *verbose* = True) Submit a job to the Work Queue.

Parameters

in	<i>wq</i>	(Work Queue Object)
in	<i>command</i>	(string) The command to run on the remote worker.
in	<i>input_files</i>	(list of files) A list of locations of the input files.
in	<i>output_files</i>	(list of files) A list of locations of the output files.

Definition at line 667 of file nifty.py.

def forcebalance.nifty.queue.up_src_dest (*wq*, *command*, *input_files*, *output_files*, *tag* = None, *tgt* = None, *verbose* = True) Submit a job to the Work Queue.

This function is a bit fancier in that we can explicitly specify where the input files come from, and where the output files go to.

Parameters

in	<i>wq</i>	(Work Queue Object)
in	<i>command</i>	(string) The command to run on the remote worker.
in	<i>input_files</i>	(list of 2-tuples) A list of local and remote locations of the input files.
in	<i>output_files</i>	(list of 2-tuples) A list of local and remote locations of the output files.

Definition at line 700 of file nifty.py.

def forcebalance.nifty.remove_if_exists (*fnm*) Remove the file if it exists (doesn't return an error).

Definition at line 931 of file nifty.py.

def forcebalance.nifty.row (*vec*) Given any list, array, or matrix, return a 1-row matrix.

Parameters

in	<i>vec</i>	The input vector that is to be made into a row
----	------------	--

Returns

answer A row matrix

Definition at line 312 of file nifty.py.

def forcebalance.nifty.segments (e) Definition at line 85 of file nifty.py.

def forcebalance.nifty.statisticalinefficiency (A_n, B_n = None, fast = False, mintime = 3, warn = True) Compute the (cross) statistical inefficiency of (two) timeseries.

Notes The same timeseries can be used for both A_n and B_n to get the autocorrelation statistical inefficiency. The fast method described in Ref [1] is used to compute g.

References [1] J. D. Chodera, W. C. Swope, J. W. Pitera, C. Seok, and K. A. Dill. Use of the weighted histogram analysis method for the analysis of simulated and parallel tempering simulations. JCTC 3(1):26-41, 2007.

Examples

Compute statistical inefficiency of timeseries data with known correlation time.

```
import timeseries A_n = timeseries.generateCorrelatedTimeseries(N=100000,
tau=5.0) g = statisticalInefficiency(A_n, fast=True)
```

@param[in] A_n (required, numpy array) - A_n[n] is nth value of timeseries A. Length is deduced from vector.

@param[in] B_n (optional, numpy array) - B_n[n] is nth value of timeseries B. Length is deduced from vector. If supplied, the cross-correlation of timeseries A and B will be estimated instead of the autocorrelation of timeseries A.

@param[in] fast (optional, boolean) - if True, will use faster (but less accurate) method to estimate correlation time, described in Ref. [1] (default: False)

@param[in] mintime (optional, int) - minimum amount of correlation function to compute (default: 3) The algorithm terminates after computing the correlation time out to mintime when the correlation function first goes negative. Note that this time may need to be increased if there is a strong initial negative peak in the correlation function.

@return g The estimated statistical inefficiency (equal to 1 + 2 tau, where tau is the correlation time). We enforce g >= 1.0.

Definition at line 486 of file nifty.py.

def forcebalance.nifty.uncommadash (s) Definition at line 101 of file nifty.py.

def forcebalance.nifty.warn_once (warning, warnhash = None) Prints a warning but will only do so once in a given run.

Definition at line 1103 of file nifty.py.

def forcebalance.nifty.warn_press_key (warning, timeout = 10) Definition at line 1091 of file nifty.py.

def forcebalance.nifty.which (fnm) Definition at line 935 of file nifty.py.

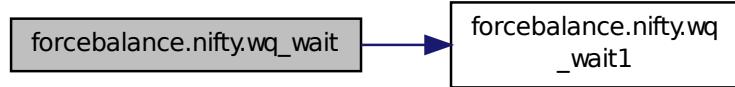
def forcebalance.nifty.wopen (dest) If trying to write to a symbolic link, remove it first.

Definition at line 891 of file nifty.py.

def forcebalance.nifty.wq_wait (wq, wait_time = 10, wait_intvl = 10, print_time = 60, verbose = False) This function waits until the work queue is completely empty.

Definition at line 787 of file nifty.py.

Here is the call graph for this function:



```
def forcebalance.nifty.wq_wait1 ( wq, wait_time = 10, wait_intvl = 1, print_time = 60, verbose = False )
```

This function waits ten seconds to see if a task in the Work Queue has finished.

Definition at line 722 of file nifty.py.

7.22.3 Variable Documentation

float forcebalance.nifty.bohrang = 0.529177249 One bohr equals this many angstroms.

Definition at line 42 of file nifty.py.

float forcebalance.nifty.eqcgmx = 2625.5002 Q-Chem to GMX unit conversion for energy.

Definition at line 38 of file nifty.py.

float forcebalance.nifty.fqcgmx = -49621.9 Q-Chem to GMX unit conversion for force.

Definition at line 40 of file nifty.py.

float forcebalance.nifty.kb = 0.0083144100163 Boltzmann constant.

Definition at line 36 of file nifty.py.

tuple forcebalance.nifty.logger = getLogger(__name__) Definition at line 31 of file nifty.py.

tuple forcebalance.nifty.specific_dct = dict(list(itertools.chain(*[[[j,i[1]] for j in i[0]] for i in specific_lst]))) Definition at line 877 of file nifty.py.

list forcebalance.nifty.specific_lst Initial value:

```
1 = [[(['mdrun','grompp','trjconv','g-energy','g-traj'], "Make sure to install GROMACS and add it to your path  
2     (or set the gmxpath option"),  
3         ['force.mdin', 'stage.leap'], "This file is needed for setting up AMBER force matching  
targets"),  
4             ['conf.pdb', 'mono.pdb'], "This file is needed for setting up OpenMM condensed phase  
property targets"),  
5                 ['liquid.xyz', 'liquid.key', 'mono.xyz', 'mono.key'], "This file is needed for setting up  
OpenMM condensed phase property targets"),  
6                     ['dynamic', 'analyze', 'minimize', 'testgrad', 'vibrate', 'optimize', 'polarize', '  
superpose'], "Make sure to install TINKER and add it to your path (or set the tinkerpath option")],  
7                         ['truncuda.sh', 'npt.py', 'npt.tinker.py'], "This file belongs in the ForceBalance source  
directory, not sure why it is missing"),  
8                             ['input.xyz'], "This file is needed for TINKER molecular property targets"),  
9                               ('.*key$', '.*xyz$'), "I am guessing this file is probably needed by TINKER"),  
10                                 ('.*gro$', '.*top$', '.*itp$', '.*mdp$', '.*ndx$'), "I am guessing this file is probably  
needed by GROMACS")  
10 ]
```

Definition at line 865 of file nifty.py.

forcebalance.nifty.WORK_QUEUE = None Definition at line 630 of file nifty.py.

tuple forcebalance.nifty.WQIDS = defaultdict(list) Definition at line 633 of file nifty.py.

string forcebalance.nifty.XMLFILE = 'x' Pickle uses 'flags' to pickle and unpickle different variable types.

Here we use the letter 'x' to signify that the variable type is an XML file.

Definition at line 559 of file nifty.py.

7.23 forcebalance.objective Namespace Reference

ForceBalance objective function.

Classes

- class **Objective**
Objective function.
- class **Penalty**
Penalty functions for regularizing the force field optimizer.

Variables

- tuple **logger** = getLogger(__name__)
- dictionary **Implemented_Tests**
The table of implemented Targets.
- list **Letters** = ['X','G','H']
This is the canonical lettering that corresponds to : objective function, gradient, Hessian.

7.23.1 Detailed Description

ForceBalance objective function.

7.23.2 Variable Documentation

dictionary forcebalance.objectiveImplemented_Tests Initial value:

```
1 = {
2   'ABINITIO_GMX':AbInitio_GMX,
3   'ABINITIO_TINKER':AbInitio_TINKER,
4   'ABINITIO_OPENMM':AbInitio_OpenMM,
5   'ABINITIO_AMBER':AbInitio_AMBER,
6   'ABINITIO_INTERNAL':AbInitio_Internal,
7   'VIBRATION_TINKER':Vibration_TINKER,
8   'VIBRATION_GMX':Vibration_GMX,
9   'THERMO_GMX':Thermo_GMX,
10  'LIQUID_OPENMM':Liquid_OpenMM,
11  'LIQUID_TINKER':Liquid_TINKER,
12  'LIQUID_GMX':Liquid_GMX,
13  'LIPID_GMX':Lipid_GMX,
14  'COUNTERPOISE':Counterpoise,
15  'THCDF_PSI4':THCDF_Psi4,
16  'RDVR3_PSI4':RDVR3_Psi4,
17  'INTERACTION_GMX':Interaction_GMX,
18  'INTERACTION_TINKER':Interaction_TINKER,
19  'INTERACTION_OPENMM':Interaction_OpenMM,
20  'BINDINGENERGY_TINKER':BindingEnergy_TINKER,
21  'BINDINGENERGY_GMX':BindingEnergy_GMX,
22  'BINDINGENERGY_OPENMM':BindingEnergy_OpenMM,
23  'MOMENTS_TINKER':Moments_TINKER,
24  'MOMENTS_GMX':Moments_GMX,
25  'MOMENTS_OPENMM':Moments_OpenMM,
26  'REMOTE_TARGET':RemoteTarget,
27 }
```

The table of implemented Targets.
Definition at line 68 of file objective.py.

list forcebalance.objective.Letters = ['X','G','H'] This is the canonical lettering that corresponds to : objective function, gradient, Hessian.

Definition at line 97 of file objective.py.

tuple forcebalance.objective.logger = getLogger(__name__) Definition at line 17 of file objective.py.

7.24 forcebalance.openmmio Namespace Reference

[OpenMM](#) input/output.

Classes

- class [OpenMM_Reader](#)
Class for parsing OpenMM force field files.
- class [OpenMM](#)
Derived from Engine object for carrying out general purpose OpenMM calculations.
- class [Liquid_OpenMM](#)
Condensed phase property matching using OpenMM.
- class [AbInitio_OpenMM](#)
Force and energy matching using OpenMM.
- class [BindingEnergy_OpenMM](#)
Binding energy matching using OpenMM.
- class [Interaction_OpenMM](#)
Interaction matching using OpenMM.
- class [Moments_OpenMM](#)
Multipole moment matching using OpenMM.

Functions

- def [energy_components](#)
- def [get_multipoles](#)
Return the current multipole moments in Debye and Buckingham units.
- def [get_dipole](#)
Return the current dipole moment in Debye.
- def [PrepareVirtualSites](#)
Prepare a list of function wrappers and vsite parameters from the system.
- def [ResetVirtualSites_fast](#)
Given a set of OpenMM-compatible positions and a System object, compute the correct virtual site positions according to the System.
- def [ResetVirtualSites](#)
Given a set of OpenMM-compatible positions and a System object, compute the correct virtual site positions according to the System.
- def [GetVirtualSiteParameters](#)
Return an array of all virtual site parameters in the system.
- def [CopyAmoebaBondParameters](#)
- def [CopyAmoebaOutOfPlaneBendParameters](#)
- def [CopyAmoebaAngleParameters](#)

- def `CopyAmoebaInPlaneAngleParameters`
- def `CopyAmoebaVdwParameters`
- def `CopyAmoebaMultipoleParameters`
- def `CopyHarmonicBondParameters`
- def `CopyHarmonicAngleParameters`
- def `CopyPeriodicTorsionParameters`
- def `CopyNonbondedParameters`
- def `do_nothing`
- def `CopySystemParameters`

Copy parameters from one system (i.e.
- def `UpdateSimulationParameters`
- def `SetAmoebaVirtualExclusions`
- def `MTSVVVRIntegrator`

Create a multiple timestep velocity verlet with velocity randomization (VVVR) integrator.

Variables

- tuple `logger` = getLogger(`_name_`)
 - dictionary `suffix_dict`
 - string `pdict` = "XML_Override"
- pdict is a useless variable if the force field is XML.*

7.24.1 Detailed Description

[OpenMM](#) input/output.

Author

Lee-Ping Wang

Date

04/2012

7.24.2 Function Documentation

def forcebalance.openmmio.CopyAmoebaAngleParameters (*src*, *dest*) Definition at line 227 of file openmmio.py.

def forcebalance.openmmio.CopyAmoebaBondParameters (*src*, *dest*) Definition at line 213 of file openmmio.py.

def forcebalance.openmmio.CopyAmoebaInPlaneAngleParameters (*src*, *dest*) Definition at line 236 of file openmmio.py.

def forcebalance.openmmio.CopyAmoebaMultipoleParameters (*src*, *dest*) Definition at line 249 of file openmmio.py.

def forcebalance.openmmio.CopyAmoebaOutOfPlaneBendParameters (*src*, *dest*) Definition at line 219 of file openmmio.py.

def forcebalance.openmmio.CopyAmoebaVdwParameters (*src*, *dest*) Definition at line 245 of file openmmio.py.

```
def forcebalance.openmmio.CopyHarmonicAngleParameters ( src, dest ) Definition at line 257 of file openmmio.py.
```

```
def forcebalance.openmmio.CopyHarmonicBondParameters ( src, dest ) Definition at line 253 of file openmmio.py.
```

```
def forcebalance.openmmio.CopyNonbondedParameters ( src, dest ) Definition at line 265 of file openmmio.py.
```

```
def forcebalance.openmmio.CopyPeriodicTorsionParameters ( src, dest ) Definition at line 261 of file openmmio.py.
```

```
def forcebalance.openmmio.CopySystemParameters ( src, dest ) Copy parameters from one system (i.e. that which is created by a new force field) sto another system (i.e. the one stored inside the Target object). DANGER: These need to be implemented manually!!!
Definition at line 279 of file openmmio.py.
```

```
def forcebalance.openmmio.do_nothing ( src, dest ) Definition at line 272 of file openmmio.py.
```

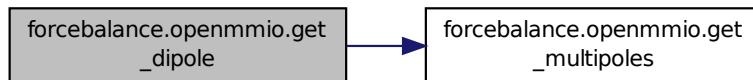
```
def forcebalance.openmmio.energy_components ( Sim, verbose = False ) Definition at line 38 of file openmmio.py.
```

```
def forcebalance.openmmio.get_dipole ( simulation, q = None, mass = None, positions = None ) Return the current dipole moment in Debye.
```

Note that this quantity is meaningless if the system carries a net charge.

Definition at line 107 of file openmmio.py.

Here is the call graph for this function:



```
def forcebalance.openmmio.get_multipoles ( simulation, q = None, mass = None, positions = None, rmcom = True ) Return the current multipole moments in Debye and Buckingham units.
```

Definition at line 48 of file openmmio.py.

```
def forcebalance.openmmio.GetVirtualSiteParameters ( system ) Return an array of all virtual site parameters in the system.
```

Used for comparison purposes.

Definition at line 194 of file openmmio.py.

```
def forcebalance.openmmio.MTSVVVRIntegrator( temperature, collision_rate, timestep, system, ninnersteps = 4 ) Create a multiple timestep velocity verlet with velocity randomization (VVVR) integrator.
```

ARGUMENTS

temperature (Quantity compatible with kelvin) - the temperature
collision_rate (Quantity compatible with 1/picoseconds) - the collision rate
timestep (Quantity compatible with femtoseconds) - the integration timestep
system (simtk.openmm.System) - system whose forces will be partitioned
ninnersteps (int) - number of inner timesteps (default: 4)

RETURNS

integrator (openmm.CustomIntegrator) - a VVVR integrator

NOTES

This integrator is equivalent to a Langevin integrator in the velocity Verlet discretization with a timestep correction to ensure that the field-free diffusion constant is timestep invariant. The inner velocity Verlet discretization is transformed into a multiple timestep algorithm.

REFERENCES

VVVR Langevin integrator:

- <http://arxiv.org/abs/1301.3800>
- <http://arxiv.org/abs/1107.2967> (to appear in PRX 2013)

TODO

Move initialization of 'sigma' to setting the per-particle variables.

Definition at line 357 of file openmmio.py.

```
def forcebalance.openmmio.PrepareVirtualSites( system ) Prepare a list of function wrappers and vsite parameters from the system.
```

Definition at line 112 of file openmmio.py.

```
def forcebalance.openmmio.ResetVirtualSites( positions, system ) Given a set of OpenMM-compatible positions and a System object, compute the correct virtual site positions according to the System.
```

Definition at line 167 of file openmmio.py.

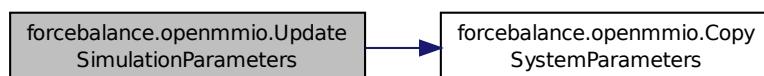
```
def forcebalance.openmmio.ResetVirtualSites.fast( positions, vsinfo ) Given a set of OpenMM-compatible positions and a System object, compute the correct virtual site positions according to the System.
```

Definition at line 152 of file openmmio.py.

```
def forcebalance.openmmio.SetAmoebaVirtualExclusions( system ) Definition at line 304 of file openmmio.py.
```

```
def forcebalance.openmmio.UpdateSimulationParameters( src_system, dest_simulation ) Definition at line 298 of file openmmio.py.
```

Here is the call graph for this function:



7.24.3 Variable Documentation

```
tuple forcebalance.openmmio.logger = getLogger(__name__) Definition at line 29 of file openmmio.py.
```

```
string forcebalance.openmmio.pdict = "XML_Override" pdict is a useless variable if the force field is XML.  
Definition at line 436 of file openmmio.py.
```

dictionary forcebalance.openmmio.suffix_dict Initial value:

```
1 = { "HarmonicBondForce" : {"Bond" : ["class1", "class2"]},  
2     "HarmonicAngleForce" : {"Angle" : ["class1", "class2", "class3"],},  
3     "PeriodicTorsionForce" : {"Proper" : ["class1", "class2", "class3", "class4"],},  
4     "NonbondedForce" : {"Atom" : ["type"]},  
5     "AmoebaBondForce" : {"Bond" : ["class1", "class2"]},  
6     "AmoebaAngleForce" : {"Angle" : ["class1", "class2", "class3"]},  
7     "AmoebaStretchBendForce" : {"StretchBend" : ["class1", "class2", "class3"]},  
8     "AmoebaVdwForce" : {"Vdw" : ["class"]},  
9     "AmoebaMultipoleForce" : {"Multipole" : ["type", "kz", "kx"], "Polarize" : ["type"]},  
10    "AmoebaUreyBradleyForce" : {"UreyBradley" : ["class1", "class2", "class3"]},  
11    "Residues.Residue" : {"VirtualSite" : ["index"]}  
12 }
```

Definition at line 422 of file openmmio.py.

7.25 forcebalance.optimizer Namespace Reference

Optimization algorithms.

Classes

- class [Optimizer](#)
Optimizer class.

Functions

- def [Counter](#)
- def [First](#)
- def [GoodStep](#)

Variables

- tuple [logger](#) = getLogger(__name__)
- int [ITERATION](#) = 0
- int [GOODSTEP](#) = 0
- int [ITERINIT](#) = 0

7.25.1 Detailed Description

Optimization algorithms. My current implementation is to have a single optimizer class with several methods contained inside.

Author

Lee-Ping Wang

Date

12/2011

7.25.2 Function Documentation

def forcebalance.optimizer.Counter() Definition at line 32 of file optimizer.py.

```
def forcebalance.optimizer.First( ) Definition at line 36 of file optimizer.py.  
  
def forcebalance.optimizer.GoodStep( ) Definition at line 40 of file optimizer.py.
```

7.25.3 Variable Documentation

```
int forcebalance.optimizer.GOODSTEP = 0 Definition at line 27 of file optimizer.py.
```

```
int forcebalance.optimizer.ITERATION = 0 Definition at line 25 of file optimizer.py.
```

```
int forcebalance.optimizer.ITERINIT = 0 Definition at line 30 of file optimizer.py.
```

```
tuple forcebalance.optimizer.logger = getLogger(__name__) Definition at line 22 of file optimizer.py.
```

7.26 forcebalance.output Namespace Reference

Classes

- class [ForceBalanceLogger](#)
This logger starts out with a default handler that writes to stdout addHandler removes this default the first time another handler is added.
- class [RawStreamHandler](#)
Exactly like output.StreamHandler except it does no extra formatting before sending logging messages to the stream.
- class [RawFileHandler](#)
Exactly like output.FileHandler except it does no extra formatting before sending logging messages to the file.
- class [CleanStreamHandler](#)
Similar to [RawStreamHandler](#) except it does not write terminal escape codes.
- class [CleanFileHandler](#)
File handler that does not write terminal escape codes and carriage returns to files.
- class [ModLogger](#)

7.27 forcebalance.parser Namespace Reference

Input file parser for ForceBalance jobs.

Functions

- def [read_mvals](#)
- def [read_pvals](#)
- def [read_priors](#)
- def [read_internals](#)
- def [printsection](#)
Print out a section of the input file in a parser-compliant and readable format.
- def [parse_inputs](#)
Parse through the input file and read all user-supplied options.

Variables

- tuple `logger` = getLogger(`_name_`)
- dictionary `gen_opts_types`

Default general options.
- dictionary `tgt_opts_types`

Default fitting target options.
- tuple `all_opts_names` = list(itertools.chain(*[i.keys() for i in gen_opts_types.values()]))
- list `iocc` = []

Check for uniqueness of option names.
- dictionary `gen_opts_defaults` = {}

Default general options - basically a collapsed version of gen_opts_types.
- dictionary `subdict` = {}
- dictionary `tgt_opts_defaults` = {}

Default target options - basically a collapsed version of tgt_opts_types.
- dictionary `bkwd`

Option maps for maintaining backward compatibility.
- list `mainsections` = ["SIMULATION", "TARGET", "OPTIONS", "END", "NONE"]

Listing of sections in the input file.
- dictionary `ParsTab`

ParsTab that refers to subsection parsers.

7.27.1 Detailed Description

Input file parser for ForceBalance jobs. Additionally, the location for all default options.

Although I will do my best to write good documentation, for many programs the input parser becomes the most up-to-date source for documentation. So this is a great place to write lots of comments for those who implement new functionality.

There are two types of sections for options - GENERAL and TARGET. Since there can be many fitting targets within a single job (i.e. we may wish to fit water trimers and hexamers, which constitutes two fitting targets) the input is organized into sections, like so:

```
$options
gen_option_1 Big
gen_option_2 Mao
$target
tgt_option_1 Sniffy
tgt_option_2 Schmao
$target
tgt_option_1 Nifty
tgt_option_2 Jiffy
$end
```

In this case, two sets of target options are generated in addition to the general option.

(Note: "Target" used to be called "Simulation". Backwards compatibility is maintained.)

Each option is meant to be parsed as a certain variable type.

- String option values are read in directly; note that only the first two words in the line are processed
- Some strings are capitalized when they are read in; this is mainly for function tables like OptTab and TgtTab
- List option types will pick up all of the words on the line and use them as values, plus if the option occurs more than once it will aggregate all of the values.
- Integer and float option types are read in a pretty straightforward way

- Boolean option types are always set to true, unless the second word is '0', 'no', or 'false' (not case sensitive)
- Section option types are meant to treat more elaborate inputs, such as the user pasting in output parameters from a previous job as input, or a specification of internal coordinate system. I imagine that for every section type I would have to write my own parser. Maybe a ParsTab of parsing functions would work. :)

To add a new option, simply add it to the dictionaries below and give it a default value if desired. If you add an entirely new type, make sure to implement the interpretation of that type in the parse_inputs function.

Author

Lee-Ping Wang

Date

11/2012

7.27.2 Function Documentation

def forcebalance.parser.parse_inputs (*input_file = None*) Parse through the input file and read all user-supplied options.

This is usually the first thing that happens when an executable script is called. Our parser first loads the default options, and then updates these options as it encounters keywords.

Each keyword corresponds to a variable type; each variable type (e.g. string, integer, float, boolean) is treated differently. For more elaborate inputs, there is a 'section' variable type.

There is only one set of general options, but multiple sets of target options. Each target has its own section delimited by the \$target keyword, and we build a list of target options.

Parameters

in	<i>input_file</i>	The name of the input file.
----	-------------------	-----------------------------

Returns

options General options.

tgt_opts List of fitting target options.

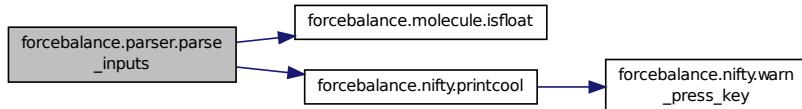
Todo Implement internal coordinates.

Implement sampling correction.

Implement charge groups.

Definition at line 438 of file parser.py.

Here is the call graph for this function:



def forcebalance.parser.printsection (*heading, optdict, typedict*) Print out a section of the input file in a parser-compliant and readable format.

At the time of writing of this function, it's mainly intended to be called by MakeInputFile.py. The heading is printed first (it is something like \$options or \$target). Then it loops through the variable types (strings, allcaps, etc...) and the keys in each variable type. The one-line description of each key is printed out as a comment, and then the key itself is printed out along with the value provided in optdict. If optdict is None, then the default value is printed out instead.

Parameters

in	<i>heading</i>	Heading, either \$options or \$target
in	<i>optdict</i>	Options dictionary or None.
in	<i>typedict</i>	Option type dictionary, either gen_opts_types or tgt_opts_types specified in this file.

Returns

Answer List of strings for the section that we are printing out.

Definition at line 341 of file parser.py.

def forcebalance.parser.read_internals (*fobj*) Definition at line 315 of file parser.py.

def forcebalance.parser.read_mvals (*fobj*) Definition at line 290 of file parser.py.

def forcebalance.parser.read_priors (*fobj*) Definition at line 306 of file parser.py.

def forcebalance.parser.read_pvals (*fobj*) Definition at line 298 of file parser.py.

7.27.3 Variable Documentation

tuple forcebalance.parser.all_opts_names = list(itertools.chain(*[i.keys() for i in gen_opts_types.values()])) Definition at line 243 of file parser.py.

dictionary forcebalance.parser.bkwd Initial value:

```
1 = {"simtype" : "type",
2     "masterfile" : "inter.txt",
3     "openmm.cuda.precision" : "openmm.precision",
4     "mdrun.threads" : "md.threads",
5     "mts.vvvr" : "mts.integrator",
6     "amoeba.polarization" : "amoeba.pol",
7     "liquid.prod.steps" : "liquid_md.steps",
8     "gas.prod.steps" : "gas_md.steps",
9     "liquid.equ.steps" : "liquid_eq.steps",
10    "gas.equ.steps" : "gas_eq.steps",
11    "lipid.prod.steps" : "lipid_md.steps",
12    "lipid.equ.steps" : "lipid_eq.steps",
13 }
```

Option maps for maintaining backward compatibility.

Definition at line 273 of file parser.py.

dictionary forcebalance.parser.gen_opts_defaults = {} Default general options - basically a collapsed veresion of gen_opts_types.

Definition at line 257 of file parser.py.

dictionary forcebalance.parser.gen_opts_types Default general options.

Note that the documentation is included in part of the key; this will aid in automatic doc-extraction. :) In the 5-tuple we have: Default value, priority (larger number means printed first), short docstring, description of scope, list of filter strings for pulling out pertinent targets (MakeInputFile.py)

Definition at line 65 of file parser.py.

list forcebalance.parser.iocc = [] Check for uniqueness of option names.

Definition at line 246 of file parser.py.

tuple forcebalance.parser.logger = getLogger(__name__) Definition at line 60 of file parser.py.

list forcebalance.parser.mainsections = ["SIMULATION","TARGET","OPTIONS","END","NONE"] Listing of sections in the input file.

Definition at line 288 of file parser.py.

dictionary forcebalance.parser.ParsTab Initial value:

```
1 = {"read_mvals" : read_mvals,
2     "read_pvals" : read_pvals,
3     "priors"     : read_priors,
4     "internal"   : read_internals
5 }
```

ParsTab that refers to subsection parsers.

Definition at line 319 of file parser.py.

dictionary forcebalance.parser.subdict = {} Definition at line 259 of file parser.py.

dictionary forcebalance.parser.tgt_opts_defaults = {} Default target options - basically a collapsed version of tgt_opts_types.

Definition at line 265 of file parser.py.

dictionary forcebalance.parser.tgt_opts_types Default fitting target options.

Definition at line 135 of file parser.py.

7.28 forcebalance.psi4io Namespace Reference

PSI4 force field input/output.

Classes

- class [GBS_Reader](#)
Interaction type -> Parameter Dictionary.
- class [THCDF_Psi4](#)
- class [Grid_Reader](#)
Finite state machine for parsing DVR grid files.
- class [RDVR3_Psi4](#)
Subclass of Target for R-DVR3 grid fitting.

Variables

- tuple [logger = getLogger\(__name__\)](#)

7.28.1 Detailed Description

PSI4 force field input/output. This serves as a good template for writing future force matching I/O modules for other programs because it's so simple.

Author

Lee-Ping Wang

Date

01/2012

7.28.2 Variable Documentation

tuple `forcebalance.psi4io.logger = getLogger(__name__)` Definition at line 24 of file `psi4io.py`.

7.29 forcebalance.PT Namespace Reference

Variables

- dictionary `PeriodicTable`
- list `Elements`

7.29.1 Variable Documentation

list `forcebalance.PT.Elements` Initial value:

```
1 = ["None",'H','He',
2      'Li','Be','B','C','N','O','F','Ne',
3      'Na','Mg','Al','Si','P','S','Cl','Ar',
4      'K','Ca','Sc','Ti','V','Cr','Mn','Fe','Co','Ni','Cu','Zn','Ga','Ge','As','Se','Br','Kr',
5      'Rb','Sr','Y','Zr','Nb','Mo','Tc','Ru','Rh','Pd','Ag','Cd','In','Sn','Sb','Te','I','Xe',
6      'Cs','Ba','La','Ce','Pr','Nd','Pm','Sm','Eu','Gd','Tb','Dy','Ho','Er','Tm','Yb',
7      'Lu','Hf','Ta','W','Re','Os','Ir','Pt','Au','Hg','Tl','Pb','Bi','Po','At','Rn',
8      'Fr','Ra','Ac','Th','Pa','U','Np','Pu','Am','Cm','Bk','Cf','Es','Fm','Md','No','Lr','Rf','Db',
     Sg,'Bh','Hs','Mt']
```

Definition at line 18 of file `PT.py`.

dictionary `forcebalance.PT.PeriodicTable` Initial value:

```
1 = {'H' : 1.0079, 'He' : 4.0026,
2      'Li' : 6.941, 'Be' : 9.0122, 'B' : 10.811, 'C' : 12.0107, 'N' : 14.0067, 'O' : 15.9994, 'F'
     : 18.9984, 'Ne' : 20.1797,
3      'Na' : 22.9897, 'Mg' : 24.305, 'Al' : 26.9815, 'Si' : 28.0855, 'P' : 30.9738, 'S' : 32.065
     , 'Cl' : 35.453, 'Ar' : 39.948,
4      'K' : 39.0983, 'Ca' : 40.078, 'Sc' : 44.9559, 'Ti' : 47.867, 'V' : 50.9415, 'Cr' : 51.9961
     , 'Mn' : 54.938, 'Fe' : 55.845, 'Co' : 58.9332,
5      'Ni' : 58.6934, 'Cu' : 63.546, 'Zn' : 65.39, 'Ga' : 69.723, 'Ge' : 72.64, 'As' : 74.9216,
     'Se' : 78.96, 'Br' : 79.904, 'Kr' : 83.8,
6      'Rb' : 85.4678, 'Sr' : 87.62, 'Y' : 88.9059, 'Zr' : 91.224, 'Nb' : 92.9064, 'Mo' : 95.94,
     'Tc' : 98, 'Ru' : 101.07, 'Rh' : 102.9055,
7      'Pd' : 106.42, 'Ag' : 107.8682, 'Cd' : 112.411, 'In' : 114.818, 'Sn' : 118.71, 'Sb' : 121.
    76, 'Te' : 127.6, 'I' : 126.9045, 'Xe' : 131.293,
8      'Cs' : 132.9055, 'Ba' : 137.327, 'La' : 138.9055, 'Ce' : 140.116, 'Pr' : 140.9077, 'Nd' :
    144.24, 'Pm' : 145, 'Sm' : 150.36,
9      'Eu' : 151.964, 'Gd' : 157.25, 'Tb' : 158.9253, 'Dy' : 162.5, 'Ho' : 164.9303, 'Er' : 167.
    259, 'Tm' : 168.9342, 'Yb' : 173.04,
10     'Lu' : 174.967, 'Hf' : 178.49, 'Ta' : 180.9479, 'W' : 183.84, 'Re' : 186.207, 'Os' : 190.2
    3, 'Ir' : 192.217, 'Pt' : 195.078,
11     'Au' : 196.9665, 'Hg' : 200.59, 'Tl' : 204.3833, 'Pb' : 207.2, 'Bi' : 208.9804, 'Po' : 209
     , 'At' : 210, 'Rn' : 222,
12     'Fr' : 223, 'Ra' : 226, 'Ac' : 227, 'Th' : 232.0381, 'Pa' : 231.0359, 'U' : 238.0289, 'Np'
     : 237, 'Pu' : 244,
13     'Am' : 243, 'Cm' : 247, 'Bk' : 247, 'Cf' : 251, 'Es' : 252, 'Fm' : 257, 'Md' : 258, 'No' :
    259,
     'Lr' : 262, 'Rf' : 261, 'Db' : 262, 'Sg' : 266, 'Bh' : 264, 'Hs' : 277, 'Mt' : 268}
```

Definition at line 3 of file `PT.py`.

7.30 forcebalance.qchemio Namespace Reference

Q-Chem input file parser.

Classes

- class `QCIn_Reader`

Finite state machine for parsing Q-Chem input files.

Functions

- def `QChem_Dielectric_Energy`

Variables

- tuple `logger` = getLogger(`__name__`)
- list `ndtypes` = [None]
Types of counterpoise correction cptypes = [None, 'BASS', 'BASSP'] Types of NDDO correction.
- dictionary `pdict`
Section -> Interaction type dictionary.

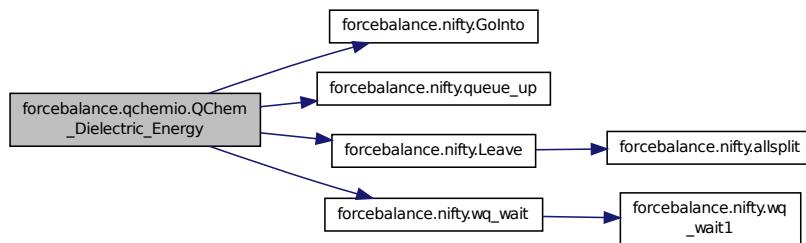
7.30.1 Detailed Description

Q-Chem input file parser.

7.30.2 Function Documentation

def forcebalance.qchemio.QChem_Dielectric_Energy (`fnm`, `wq`) Definition at line 74 of file qchemio.py.

Here is the call graph for this function:



7.30.3 Variable Documentation

tuple forcebalance.qchemio.logger = getLogger(`__name__`) Definition at line 11 of file qchemio.py.

list forcebalance.qchemio.ndtypes = [None] Types of counterpoise correction cptypes = [None, 'BASS', 'BASSP']
Types of NDDO correction.

Definition at line 16 of file qchemio.py.

dictionary forcebalance.qchemio.pdict Initial value:

```
1 = {'BASS': {0:'A', 1:'C'},  
2      'BASSP' :{0:'A', 1:'B', 2:'C'}  
3      }
```

Section -> Interaction type dictionary.

`fdict = { 'basis' : bastypes }` Interaction type -> Parameter Dictionary.

Definition at line 23 of file qchemio.py.

7.31 forcebalance.quantity Namespace Reference

Classes

- class [Quantity](#)
Base class for thermodynamical quantity used for fitting.
- class [Quantity_Density](#)
- class [Quantity_H_vap](#)

Functions

- def [mean_stderr](#)
Return mean and standard deviation of a time series ts.
- def [energy_derivatives](#)
Compute the first derivatives of a set of snapshot energies with respect to the force field parameters.

Variables

- tuple [logger](#) = getLogger(__name__)

7.31.1 Function Documentation

def forcebalance.quantity.energy_derivatives (engine, FF, mvals, h, pgrad, length, AGrad = True)

Compute the first derivatives of a set of snapshot energies with respect to the force field parameters.

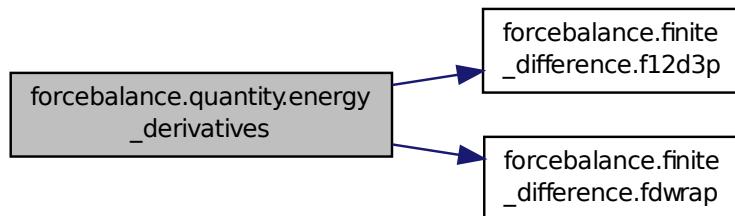
The function calls the finite difference subroutine on the energy_driver subroutine also in this script.

Parameters engine : Engine Use this Engine (GMX,TINKER,OPENMM etc.) object to get the energy snapshots. FF : FF Force field object. mvals : list Mathematical parameter values. h : float Finite difference step size. length : int Number of snapshots (length of energy trajectory). AGrad : Boolean Switch that turns derivatives on or off; if off, return all zeros.

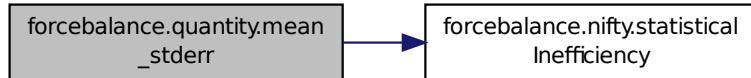
Returns G : np.array Derivative of the energy in a FF.np x length array.

Definition at line 50 of file quantity.py.

Here is the call graph for this function:



```
def forcebalance.quantity.mean_stderr( ts )  Return mean and standard deviation of a time series ts.  
Definition at line 17 of file quantity.py.  
Here is the call graph for this function:
```



7.31.2 Variable Documentation

tuple `forcebalance.quantity.logger = getLogger(__name__)` Definition at line 12 of file quantity.py.

7.32 forcebalance.target Namespace Reference

Classes

- class [Target](#)
Base class for all fitting targets.
- class [RemoteTarget](#)

Variables

- tuple `logger = getLogger(__name__)`

7.32.1 Variable Documentation

tuple `forcebalance.target.logger = getLogger(__name__)` Definition at line 17 of file target.py.

7.33 forcebalance.thermo Namespace Reference

Classes

- class [Thermo](#)
A target for fitting general experimental data sets.
- class [Point](#)

Variables

- tuple `logger = getLogger(__name__)`

7.33.1 Variable Documentation

tuple `forcebalance.thermo.logger = getLogger(__name__)` Definition at line 15 of file thermo.py.

7.34 forcebalance.tinkerio Namespace Reference

[TINKER](#) input/output.

Classes

- class [Tinker_Reader](#)
Finite state machine for parsing [TINKER](#) force field files.
- class [TINKER](#)
Engine for carrying out general purpose [TINKER](#) calculations.
- class [Liquid_TINKER](#)
Condensed phase property matching using [TINKER](#).
- class [AbInitio_TINKER](#)
Subclass of Target for force and energy matching using [TINKER](#).
- class [BindingEnergy_TINKER](#)
Binding energy matching using [TINKER](#).
- class [Interaction_TINKER](#)
Subclass of Target for interaction matching using [TINKER](#).
- class [Moments_TINKER](#)
Subclass of Target for multipole moment matching using [TINKER](#).
- class [Vibration_TINKER](#)
Vibrational frequency matching using [TINKER](#).

Functions

- def [write_key](#)
Create or edit a [TINKER](#) .key file.

Variables

- list [allp](#)
- list [eckeys](#)
- tuple [logger](#) = getLogger(__name__)
- dictionary [pdct](#)

7.34.1 Detailed Description

[TINKER](#) input/output. This serves as a good template for writing future force matching I/O modules for other programs because it's so simple.

Author

Lee-Ping Wang

Date

01/2012

7.34.2 Function Documentation

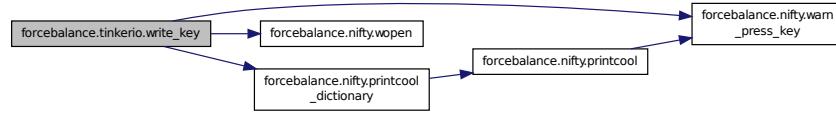
```
def forcebalance.tinkerio.write_key( fout, options, fin = None, defaults = {}, verbose = False, prmfnm = None, chk = [] ) Create or edit a TINKER .key file.
```

Parameters

in	<i>fout</i>	Output file name, can be the same as input file name.
in	<i>options</i>	Dictionary containing .key options. Existing options are replaced, new options are added at the end. Passing None causes options to be deleted. To pass an option without an argument, use ".
in	<i>fin</i>	Input file name.
in	<i>defaults</i>	Default options to add to the mdp only if they don't already exist.
in	<i>verbose</i>	Print out all modifications to the file.
in	<i>prmfnm</i>	TINKER parameter file name.
in	<i>chk</i>	Crash if the key file does NOT have these options by the end.

Definition at line 179 of file tinkerio.py.

Here is the call graph for this function:



7.34.3 Variable Documentation

list forcebalance.tinkerio.allp Initial value:

```

1 = ['atom', 'vdw', 'vdw14', 'vdwpr', 'hbond', 'bond', 'bond5', 'bond4',
2      'bond3', 'electneg', 'angle', 'angle5', 'angle4', 'angle3', 'anglef',
3      'strbnd', 'ureybrad', 'angang', 'opbend', 'opdist', 'improper', 'imptors',
4      'torsion', 'torsion5', 'torsion4', 'pitors', 'strtors', 'tortors', 'charge',
5      'dipole', 'dipole5', 'dipole4', 'dipole3', 'multipole', 'polarize', 'piatom',
6      'pibond', 'pibond5', 'pibond4', 'metal', 'biotype', 'mmffvdw', 'mmffbond',
7      'mmffbonder', 'mmffangle', 'mmffstrbnd', 'mmffopbend', 'mmfftorsion', 'mmffbci',
8      'mmffpbc1', 'mmffequiv', 'mmffdefstbn', 'mmffcovrad', 'mmffprop', 'mmffarom']
  
```

Definition at line 35 of file tinkerio.py.

list forcebalance.tinkerio.eckey Initial value:

```

1 = ['Angle-Angle', 'Angle Bending', 'Atomic Multipoles', 'Bond Stretching', 'Charge-Charge',
2      'Charge-Dipole', 'Dipole-Dipole', 'Extra Energy Terms', 'Geometric Restraints', 'Implicit
     Solvation',
3      'Improper Dihedral', 'Improper Torsion', 'Metal Ligand Field', 'Out-of-Plane Bend', 'Out-of-Plane
     Distance',
4      'Pi-Orbital Torsion', 'Polarization', 'Reaction Field', 'Stretch-Bend', 'Stretch-Torsion',
5      'Torsional Angle', 'Torsion-Torsion', 'Urey-Bradley', 'Van der Waals']
  
```

Definition at line 45 of file tinkerio.py.

tuple forcebalance.tinkerio.logger = getLogger(__name__) Definition at line 52 of file tinkerio.py.

dictionary forcebalance.tinkerio.pdict Initial value:

```

1 = {'VDW' : {'Atom':[1], 2:'S',3:'T',4:'D'}, # Van der Waals distance, well depth, distance from
     bonded neighbor?
2     'BOND' : {'Atom':[1,2], 3:'K',4:'B'}, # Bond force constant and equilibrium distance
     (Angstrom)
3     'ANGLE' : {'Atom':[1,2,3], 4:'K',5:'B'}, # Angle force constant and equilibrium angle
4     'STRBND' : {'Atom':[1,2,3], 4:'K1',5:'K2'}, # Two stretch-bend force constants (usually
     same)
5     'OPBEND' : {'Atom':[1,2,3,4], 5:'K'}, # Out-of-plane bending force constant
     'UREYBRAD' : {'Atom':[1,2,3], 4:'K',5:'B'}, # Urey-Bradley force constant and equilibrium
  
```

```

7      distance (Angstrom)
8          'TORSION'    : ({'Atom':[1,2,3,4], 5:'1K', 6:'1B',
9                           8:'2K', 9:'2B', 11:'3K', 12:'3B'}), # Torsional force constants and equilibrium
10         phi-angles
11         'PITORS'     : {'Atom':[1,2], 3:'K'},           # Pi-torsion force constants (usually 6.85 ..)
12             # Note torsion-torsion (CMAP) not implemented at this time.
13         'MCHARGE'    : {'Atom':[1,2,3], 4:''},           # Atomic charge
14         'DIPOLE'     : {0:'X',1:'Y',2:'Z'},            # Dipole moment in local frame
15         'QUADX'      : {0:'X'},                         # Quadrupole moment, X component
16         'QUADY'      : {0:'X',1:'Y'},                  # Quadrupole moment, Y component
17         'QUADZ'      : {0:'X',1:'Y',2:'Z'},            # Quadrupole moment, Z component
18         'POLARIZE'   : {'Atom':[1], 2:'A',3:'T'},        # Atomic dipole polarizability
19         'BOND-CUBIC' : {'Atom':[], 0:''},              # Below are global parameters.
20             # Ignored for now: stretch/bend coupling, out-of-plane
21             # torsional parameters, pi-torsion, torsion-torsion
22         bending,
23     }

```

Definition at line 54 of file tinkerio.py.

7.35 forcebalance.vibration Namespace Reference

Vibrational mode fitting module.

Classes

- class [Vibration](#)

Subclass of Target for fitting force fields to vibrational spectra (from experiment or theory).

Functions

- def [count_assignment](#)

Variables

- tuple [logger](#) = getLogger(__name__)

7.35.1 Detailed Description

Vibrational mode fitting module.

Author

Lee-Ping Wang

Date

08/2012

7.35.2 Function Documentation

def forcebalance.vibration.count_assignment (*assignment*, *verbose* = *True*) Definition at line 25 of file vibration.py.

7.35.3 Variable Documentation

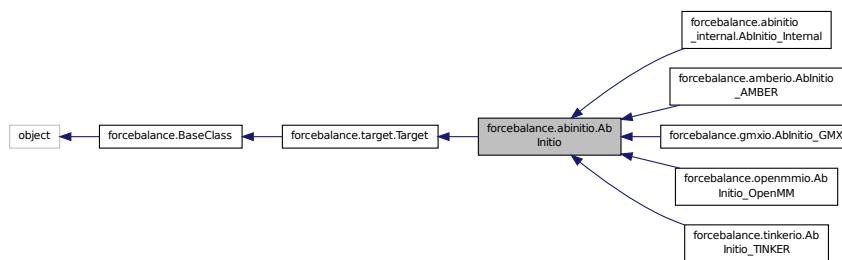
tuple forcebalance.vibration.logger = getLogger(__name__) Definition at line 23 of file vibration.py.

8 Class Documentation

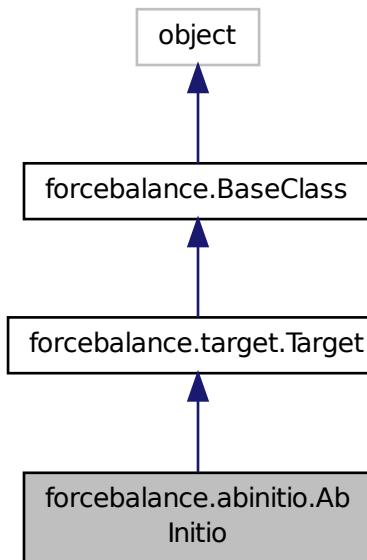
8.1 forcebalance.abinitio.AbInitio Class Reference

Subclass of Target for fitting force fields to ab initio data.

Inheritance diagram for forcebalance.abinitio.AbInitio:



Collaboration diagram for forcebalance.abinitio.AbInitio:



Public Member Functions

- def `_init_`
Initialization; define a few core concepts.
- def `build_invdist`
- def `compute_netforce_torque`

- def `read_reference_data`
Read the reference ab initio data from a file such as qdata.txt.
- def `indicate`
- def `energy_all`
- def `energy_force_all`
- def `energy_force_transform`
- def `energy_one`
- def `energy_force_one`
- def `energy_force_transform_one`
- def `get_energy_force`
LPW 06-30-2013.
- def `get_resp`
Electrostatic potential fitting.
- def `get`
- def `get_X`
Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
Computes the objective function contribution and its gradient.
- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- **boltz_wts**
Initialize the base class.
- **qmboltz_wts**
QM Boltzmann weights.
- **eqm**
Reference (QM) energies.
- **emd0**
Energies of the sampling simulation.
- **fqm**
Reference (QM) forces.
- **espxyz**
ESP grid points.
- **espval**
ESP values.
- **qfnm**
The qdata.txt file that contains the QM energies and forces.
- **qmatoms**
The number of atoms in the QM calculation (Irrelevant if not fitting forces)
- **e_err**
Qualitative Indicator: average energy error (in kJ/mol)
- **e_err_pct**
- **f_err**
Qualitative Indicator: average force error (fractional)
- **f_err_pct**
- **esp_err**
Qualitative Indicator: "relative RMS" for electrostatic potential.
- **nf_err**
- **nf_err_pct**
- **tq_err_pct**
- **use_nft**
Whether to compute net forces and torques, or not.
- **ns**
Read in the trajectory file.
- **mol**
- **nparticles**
The number of (atoms + drude particles + virtual sites)
- **engine**
Build keyword dictionaries to pass to engine.
- **AtomLists**
Lists of atoms to do net force/torque fitting and excluding virtual sites.
- **AtomMask**
- **new_vsites**
Read in the reference data.
- **save_vmvalls**
Save the mvalls from the last time we updated the vsites.
- **force_map**

- `nnf`
- `ntq`
- `force`
- `w_force`
- `nesp`
- `fitatoms`
- `whamboltz`
- `nftqm`
- `fref`
- `w_energy`
- `w_netforce`
- `w_torque`
- `e_ref`
- `f_ref`
- `nf_ref`
- `tq_ref`
- `tq_err`
- `w_resp`
- `invdists`
- `respterm`
- `objective`
- `rd`

Root directory of the whole project.
- `pgrad`

Iteration where we turn on zero-gradient skipping.
- `tempbase`

Relative directory of target.
- `tempdir`
- `rundir`

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- `FF`

Need the forcefield (here for now)
- `xct`

Counts how often the objective function was computed.
- `gct`

Counts how often the gradient was computed.
- `hct`

Counts how often the Hessian was computed.
- `read_indicate`

Whether to read indicate.log from file when restarting an aborted run.
- `write_indicate`

Whether to write indicate.log at every iteration (true for all but remote.)
- `read_objective`

Whether to read objective.p from file when restarting an aborted run.
- `write_objective`

Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.1.1 Detailed Description

Subclass of Target for fitting force fields to ab initio data.

Currently Gromacs-X2, Gromacs, Tinker, OpenMM and AMBER are supported.

We introduce the following concepts:

- The number of snapshots
- The reference energies and forces (eqm, fqm) and the file they belong in (qdata.txt)
- The sampling simulation energies (emd0)
- The WHAM Boltzmann weights (these are computed externally and passed in)
- The QM Boltzmann weights (computed internally using the difference between eqm and emd0)

There are also these little details:

- Switches for whether to turn on certain Boltzmann weights (they stack)
- Temperature for the QM Boltzmann weights
- Whether to fit a subset of atoms

This subclass contains the 'get' method for building the objective function from any simulation software (a driver to run the program and read output is still required). The 'get' method can be overridden by subclasses like AbInitio_GMX. Definition at line 47 of file abinitio.py.

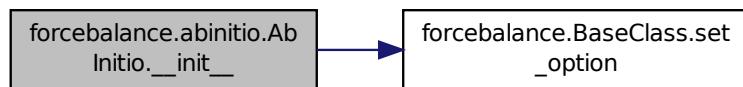
8.1.2 Constructor & Destructor Documentation

```
def forcebalance.abinitio.AbInitio.__init__( self, options, tgt_opts, forcefield ) Initialization; define a few core concepts.
```

Todo Obtain the number of true atoms (or the particle -> atom mapping) from the force field.

Definition at line 57 of file abinitio.py.

Here is the call graph for this function:



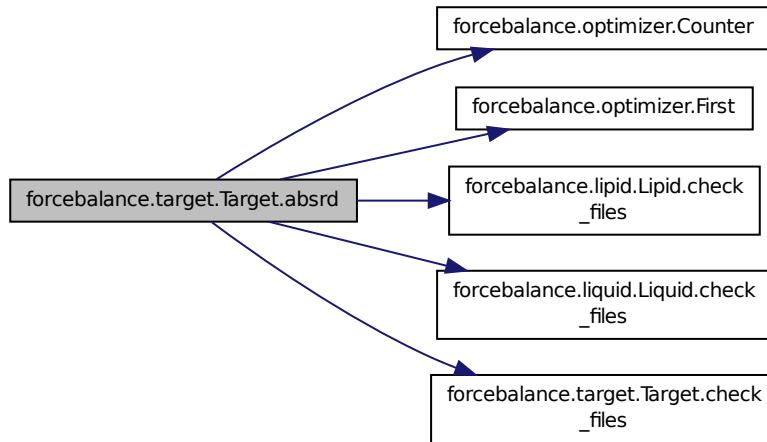
8.1.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory  
specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.AblInitio.build_invdist ( self, mvals ) Definition at line 171 of file abinitio.py.
```

```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence  
of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.abinitio.AblInitio.compute_netforce_torque ( self, xyz, force, QM = False ) Definition at  
line 200 of file abinitio.py.
```

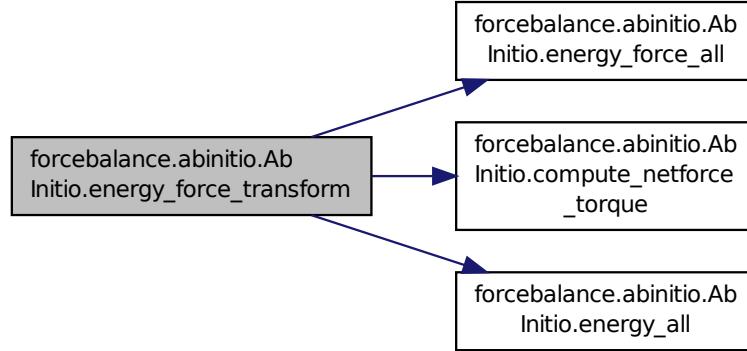
```
def forcebalance.abinitio.AblInitio.energy_all ( self ) Definition at line 472 of file abinitio.py.
```

```
def forcebalance.abinitio.AblInitio.energy_force_all ( self ) Definition at line 478 of file abinitio.py.
```

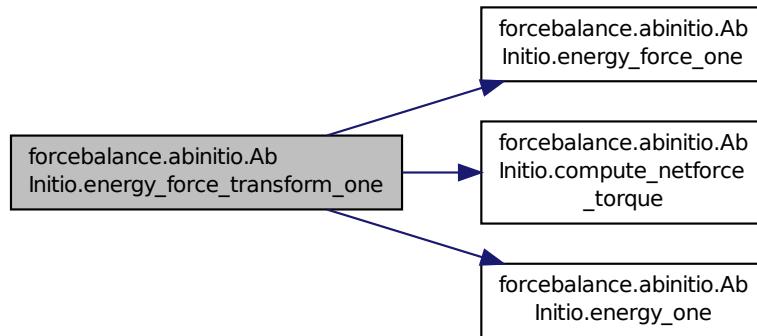
```
def forcebalance.abinitio.AblInitio.energy_force_one ( self, i ) Definition at line 507 of file abinitio.py.
```

```
def forcebalance.abinitio.AblInitio.energy_force_transform ( self ) Definition at line 484 of file abinitio.py.
```

Here is the call graph for this function:



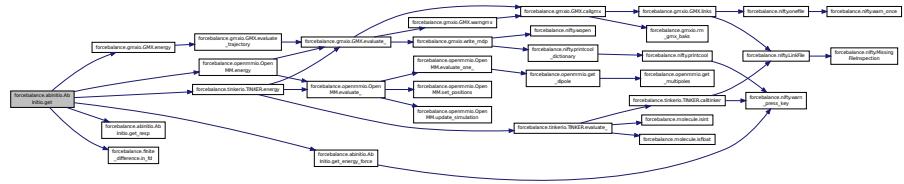
def forcebalance.abinitio.AbInitio.energy_force_transform_one (self, i) Definition at line 513 of file abinitio.py.
Here is the call graph for this function:



def forcebalance.abinitio.AbInitio.energy_one (self, i) Definition at line 501 of file abinitio.py.

def forcebalance.abinitio.AbInitio.get (self, mvals, AGrad = False, AHess = False) Definition at line 1152 of file abinitio.py.

Here is the call graph for this function:



def forcebalance.abinitio.ABInitio.get_energy_force (self, mvals, AGrad = False, AHess = False) LPW
06-30-2013.

This subroutine builds the objective function (and optionally its derivatives) from a general simulation software. This is in contrast to using GROMACS-X2, which computes the objective function and prints it out; then 'get' only needs to call GROMACS and read it in.

This subroutine interfaces with simulation software 'drivers'. The driver is only expected to give the energy and forces.

Now this subroutine may sound trivial since the objective function is simply a least-squares quantity $(M-Q)^2$ - but there are a number of nontrivial considerations. I will list them here.

0) Polytensor formulation: Because there may exist covariance between different components of the force (or covariance between the energy and the force), we build the objective function by taking outer products of vectors that have the form [E F_1x F_1y F_1z F_2x F_2y ...], and then we trace it with the inverse of the covariance matrix to get the objective function.

This version implements both the polytensor formulation and the standard formulation.

1) Boltzmann weights and normalization: Each snapshot has its own Boltzmann weight, which may or may not be normalized. This subroutine does the normalization automatically.

2) Subtracting out the mean energy gap: The zero-point energy difference between reference data and simulation is meaningless. This subroutine subtracts it out.

3) Hybrid ensembles: This program builds a combined objective function from both MM and QM ensembles, which is rigorously better than using a single ensemble

Note that this subroutine does not do **EVERYTHING** that GROMACS-X2 can do, which includes:

Note that this subroutine does not do EVERYTHING that CHIMESSE XL can do, which includes:
 1) Internal coordinate systems 2) 'Sampling correction' (deprecated, since it doesn't seem to work) 3) Analytic derivatives

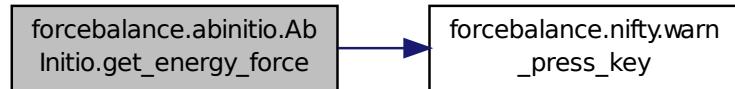
In the previous code (ForTune) this subroutine used analytic first derivatives of the energy and force to build the derivatives of the objective function. Here I will take a simplified approach, because building the derivatives are cumbersome. For now we will return the objective function ONLY. A two-point central difference should give us the first and diagonal second derivative anyhow.

Todo Parallelization over snapshots is not implemented yet.

```
@param[in] mvals Mathematical parameter values  
@param[in] AGrad Switch to turn on analytic gradient  
@param[in] AHess Switch to turn on analytic Hessian  
@return Answer Contribution to the objective function
```

Definition at line 588 of file abinitio.py.

Here is the call graph for this function:



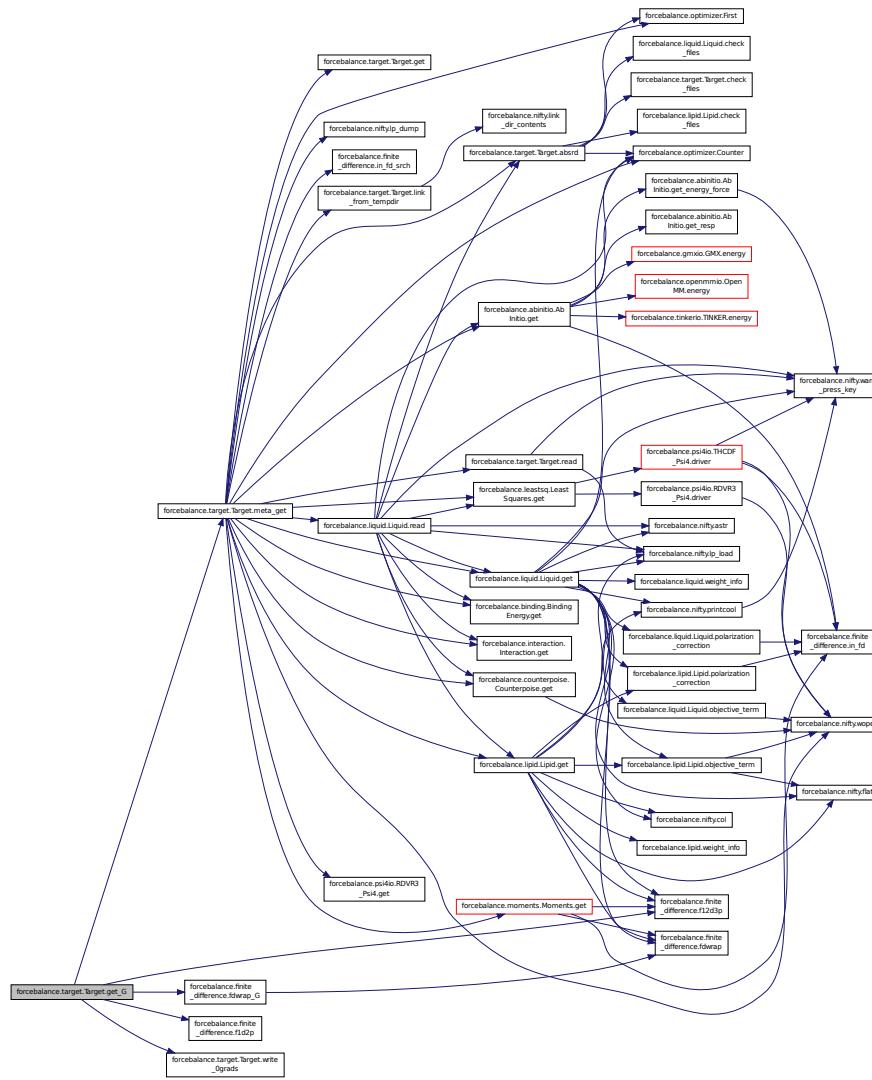
```
def forcebalance.target.Target.get_G( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



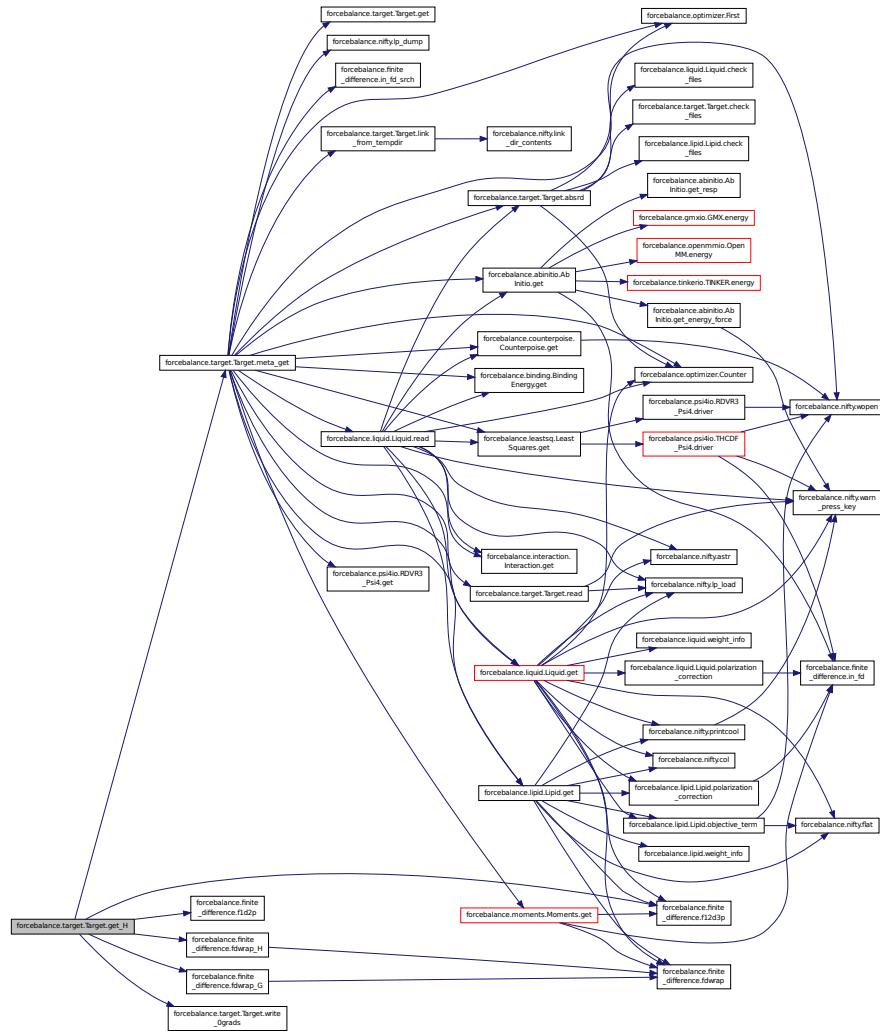
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.ABInitio.get_resp ( self, mvals, AGrad = False, AHess = False ) Electrostatic potential fitting.
```

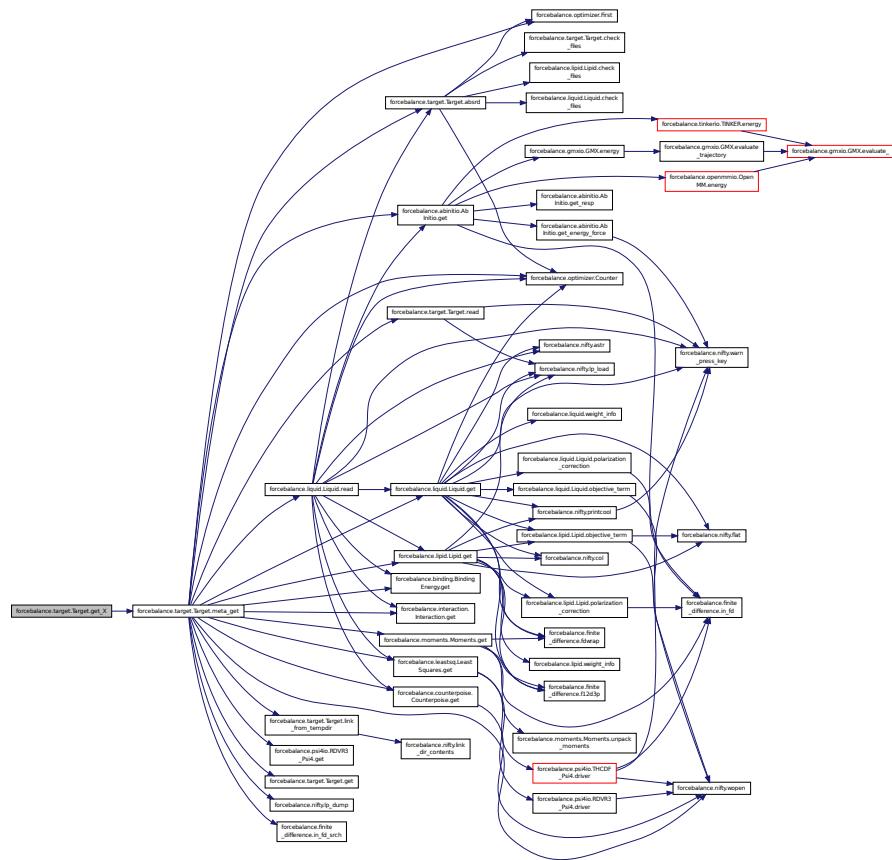
Implements the RESP objective function. (In Python so obviously not optimized.) This function takes the mathematical parameter values and returns the charges on the ATOMS (fancy mapping going on)

Definition at line 1053 of file abinitio.py.

def forcebalance.target.Target.get_X(self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

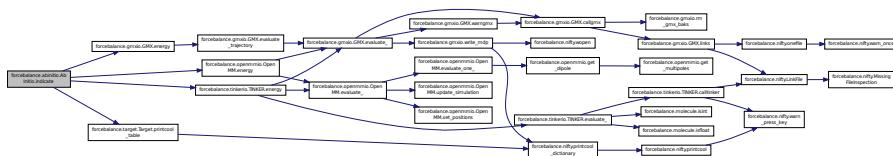
Definition at line 184 of file target.py.

Here is the call graph for this function:



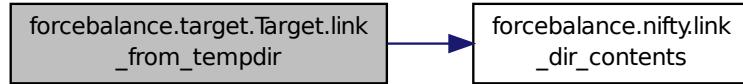
def forcebalance.abinitio.AblInitio.optimize (self) Definition at line 448 of file abinitio.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

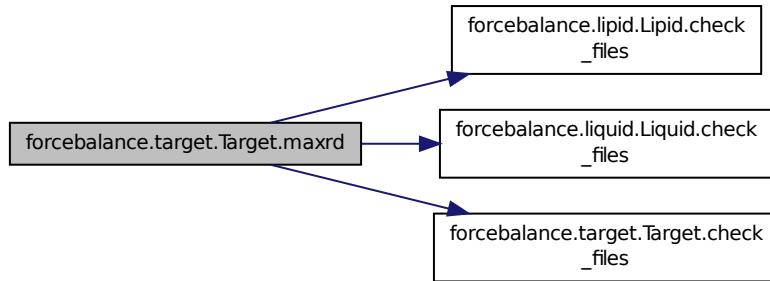
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

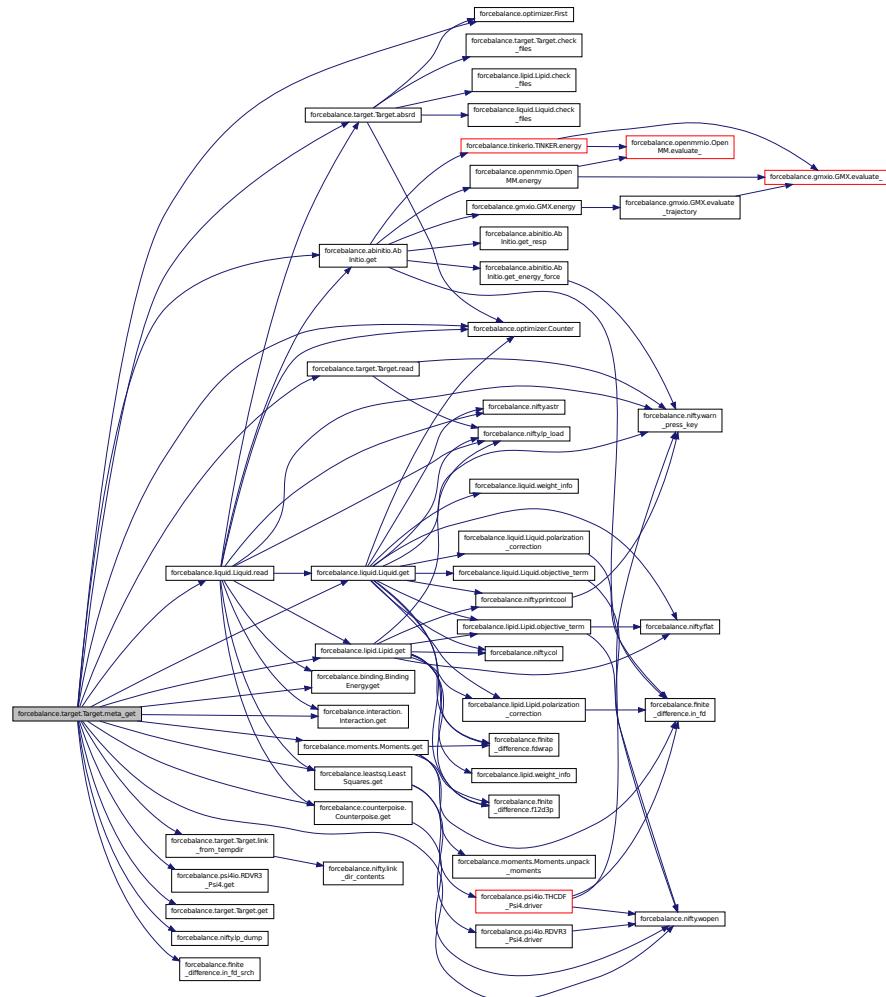


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

Here is the call graph for this function:

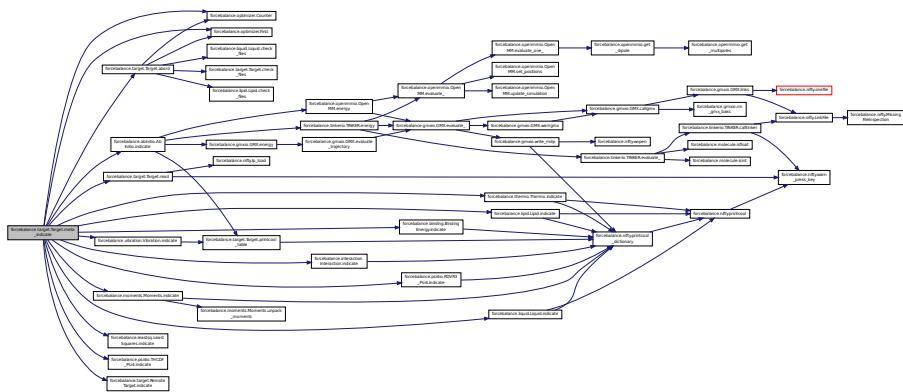


def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.

Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

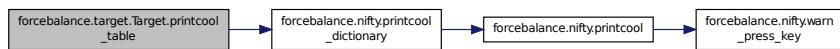
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

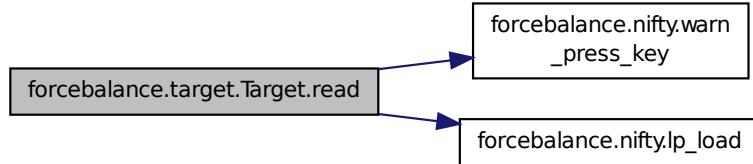
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.read_0grads ( self ) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.
```

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

```
def forcebalance.abinitio.AblInitio.read_reference_data ( self ) Read the reference ab initio data from a file such as qdata.txt.
```

Todo Add an option for picking any slice out of qdata.txt, helpful for cross-validation

Todo Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

After reading in the information from qdata.txt, it is converted into the GROMACS energy units (kind of an arbitrary choice); forces (kind of a misnomer in qdata.txt) are multiplied by -1 to convert gradients to forces.

We also subtract out the mean energies of all energy arrays because energy/force matching does not account for zero-point energy differences between MM and QM (i.e. energy of electrons in core orbitals).

The configurations in force/energy matching typically come from a the thermodynamic ensemble of the MM force field at some temperature (by running MD, for example), and for many reasons it is helpful to introduce non-Boltzmann weights in front of these configurations. There are two options: WHAM Boltzmann weights (for combining the weights of several simulations together) and QM Boltzmann weights (for converting MM weights into QM weights). Note that the two sets of weights 'stack'; i.e. they can be used at the same time.

A 'hybrid' ensemble is possible where we use 50% MM and 50% QM weights. Please read more in LPW and Troy Van Voorhis, JCP Vol. 133, Pg. 231101 (2010), doi:10.1063/1.3519043.

Todo The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Finally, note that using non-Boltzmann weights degrades the statistical information content of the snapshots. This problem will generally become worse if the ensemble to which we're reweighting is dramatically different from the one we're sampling from. We end up with a set of Boltzmann weights like [1e-9, 1e-9, 1.0, 1e-9, 1e-9 ...] and this is essentially just one snapshot. I believe Troy is working on something to cure this problem.

Here, we have a measure for the information content of our snapshots, which comes easily from the definition of information entropy:

```
S = -1*Sum_i(P_i*log(P_i))
InfoContent = exp(-S)
```

With uniform weights, InfoContent is equal to the number of snapshots; with horrible weights, InfoContent is closer to one.

Definition at line 329 of file abinitio.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

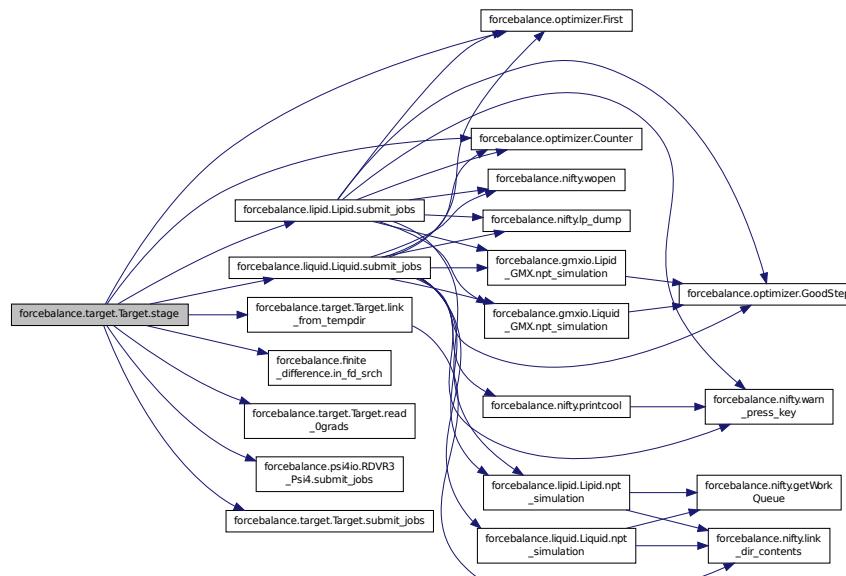
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

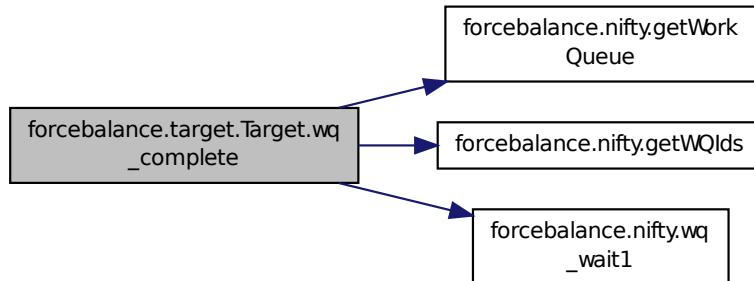


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_Ograds ( self, Ans ) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.1.4 Member Data Documentation

forcebalance.abinitio.ABInitio.AtomLists Lists of atoms to do net force/torque fitting and excluding virtual sites.

Definition at line 160 of file abinitio.py.

forcebalance.abinitio.ABInitio.AtomMask Definition at line 161 of file abinitio.py.

forcebalance.abinitio.ABInitio.boltz_wts Initialize the base class.

Number of snapshots Whether to use WHAM Boltzmann weights Whether to use the Sampling Correction Whether to match Absolute Energies (make sure you know what you're doing) Whether to use the Covariance Matrix Whether to use QM Boltzmann weights The temperature for QM Boltzmann weights Number of atoms that we are fitting Whether to fit Energies. Whether to fit Forces. Whether to fit Electrostatic Potential. Weights for the three components. Option for how much data to write to disk. Whether to do energy and force calculations for the whole trajectory, or to do one calculation per snapshot. OpenMM-only option - whether to run the energies and forces internally. Whether we have virtual sites (set at the global option level) Attenuate the weights as a function of energy What is the energy denominator? (Valid for 'attenuate') Set upper cutoff energy WHAM Boltzmann weights

Definition at line 116 of file abinitio.py.

forcebalance.abinitio.ABInitio.e_err Qualitative Indicator: average energy error (in kJ/mol)

Definition at line 134 of file abinitio.py.

forcebalance.abinitio.ABInitio.e_err_pct Definition at line 135 of file abinitio.py.

forcebalance.abinitio.AbInitio.e.ref Definition at line 1030 of file abinitio.py.

forcebalance.abinitio.AbInitio.emd0 Energies of the sampling simulation.
Definition at line 122 of file abinitio.py.

forcebalance.abinitio.AbInitio.engine Build keyword dictionaries to pass to engine.
Create engine object.
Definition at line 158 of file abinitio.py.

forcebalance.abinitio.AbInitio.eqm Reference (QM) energies.
Definition at line 120 of file abinitio.py.

forcebalance.abinitio.AbInitio.esp_err Qualitative Indicator: "relative RMS" for electrostatic potential.
Definition at line 140 of file abinitio.py.

forcebalance.abinitio.AbInitio.espval ESP values.
Definition at line 128 of file abinitio.py.

forcebalance.abinitio.AbInitio.espxyz ESP grid points.
Definition at line 126 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err Qualitative Indicator: average force error (fractional)
Definition at line 137 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err_pct Definition at line 138 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_ref Definition at line 1034 of file abinitio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.abinitio.AbInitio.fitatoms Definition at line 366 of file abinitio.py.

forcebalance.abinitio.AbInitio.force Definition at line 361 of file abinitio.py.

forcebalance.abinitio.AbInitio.force_map Definition at line 209 of file abinitio.py.

forcebalance.abinitio.AbInitio.fqm Reference (QM) forces.
Definition at line 124 of file abinitio.py.

forcebalance.abinitio.AbInitio.fref Definition at line 442 of file abinitio.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.abinitio.AbInitio.invdists Definition at line 1061 of file abinitio.py.

forcebalance.abinitio.ABInitio.mol Definition at line 148 of file abinitio.py.

forcebalance.abinitio.ABInitio.nesp Definition at line 363 of file abinitio.py.

forcebalance.abinitio.ABInitio.new_vsites Read in the reference data.

The below two options are related to whether we want to rebuild virtual site positions. Rebuild the distance matrix if virtual site positions have changed

Definition at line 166 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err Definition at line 141 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err_pct Definition at line 142 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_ref Definition at line 1038 of file abinitio.py.

forcebalance.abinitio.ABInitio.nftqm Definition at line 438 of file abinitio.py.

forcebalance.abinitio.ABInitio.nnf Definition at line 267 of file abinitio.py.

forcebalance.abinitio.ABInitio.nparticles The number of (atoms + drude particles + virtual sites)

Definition at line 153 of file abinitio.py.

forcebalance.abinitio.ABInitio.ns Read in the trajectory file.

Definition at line 147 of file abinitio.py.

forcebalance.abinitio.ABInitio.ntq Definition at line 268 of file abinitio.py.

forcebalance.abinitio.ABInitio.objective Definition at line 1172 of file abinitio.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.abinitio.ABInitio.qfnm The qdata.txt file that contains the QM energies and forces.

Definition at line 130 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmatoms The number of atoms in the QM calculation (Irrelevant if not fitting forces)

Definition at line 132 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmboltz_wts QM Boltzmann weights.

Definition at line 118 of file abinitio.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.abinitio.ABInitio.respterm Definition at line 1140 of file abinitio.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.abinitio.ABInitio.save_vmvales Save the mvales from the last time we updated the vsites.

Definition at line 168 of file abinitio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.abinitio.ABInitio.tq_err Definition at line 1042 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_err_pct Definition at line 143 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_ref Definition at line 1041 of file abinitio.py.

forcebalance.abinitio.ABInitio.use_nft Whether to compute net forces and torques, or not.

Definition at line 145 of file abinitio.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.abinitio.ABInitio.w_energy Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_force Definition at line 362 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_netforce Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_resp Definition at line 1054 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_torque Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.whamboltz Definition at line 382 of file abinitio.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

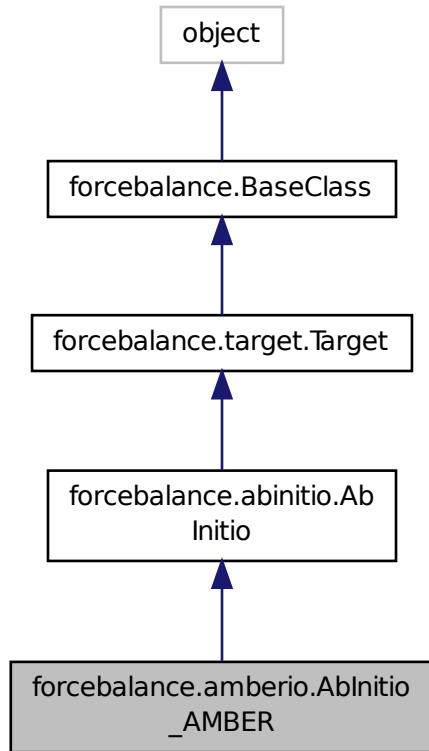
The documentation for this class was generated from the following file:

- [abinitio.py](#)

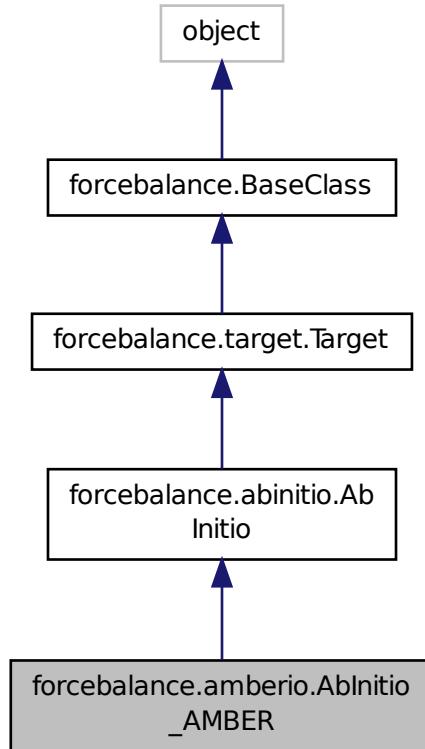
8.2 forcebalance.amberio.ABInitio_AMBER Class Reference

Subclass of Target for force and energy matching using AMBER.

Inheritance diagram for forcebalance.amberio.AbInitio_AMBER:



Collaboration diagram for forcebalance.amberio.AbInitio_AMBER:



Public Member Functions

- def `_init_`
- def `prepare_temp_directory`
- def `energy_force_driver_all_external_`
- def `energy_force_driver_all`
- def `build_invdist`
- def `compute_netforce_torque`
- def `read_reference_data`

Read the reference ab initio data from a file such as qdata.txt.

- def `indicate`
- def `energy_all`
- def `energy_force_all`
- def `energy_force_transform`
- def `energy_one`
- def `energy_force_one`
- def `energy_force_transform_one`
- def `get_energy_force`

LPW 06-30-2013.

- def `get_resp`
Electrostatic potential fitting.
- def `get`
- def `get_X`
Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
Computes the objective function contribution and its gradient.
- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `coords`
Name of the trajectory, we need this BEFORE initializing the SuperClass.
- `all_at_once`
all_at_once is not implemented.
- `boltz_wts`
Initialize the base class.
- `qmboltz_wts`
QM Boltzmann weights.

- **eqm**
Reference (QM) energies.
- **emd0**
Energies of the sampling simulation.
- **fqm**
Reference (QM) forces.
- **espxyz**
ESP grid points.
- **espval**
ESP values.
- **qfnm**
The qdata.txt file that contains the QM energies and forces.
- **qatoms**
The number of atoms in the QM calculation (Irrelevant if not fitting forces)
- **e_err**
Qualitative Indicator: average energy error (in kJ/mol)
- **e_err_pct**
- **f_err**
Qualitative Indicator: average force error (fractional)
- **f_err_pct**
- **esp_err**
Qualitative Indicator: "relative RMS" for electrostatic potential.
- **nf_err**
- **nf_err_pct**
- **tq_err_pct**
- **use_nft**
Whether to compute net forces and torques, or not.
- **ns**
Read in the trajectory file.
- **mol**
- **nparticles**
The number of (atoms + drude particles + virtual sites)
- **engine**
Build keyword dictionaries to pass to engine.
- **AtomLists**
Lists of atoms to do net force/torque fitting and excluding virtual sites.
- **AtomMask**
- **new_vsites**
Read in the reference data.
- **save_vmvalls**
Save the mvalls from the last time we updated the vsites.
- **force_map**
- **nnf**
- **ntq**
- **force**
- **w_force**
- **nesp**
- **fitatoms**

- `whamboltz`
- `nftqm`
- `fref`
- `w_energy`
- `w_netforce`
- `w_torque`
- `e_ref`
- `f_ref`
- `nf_ref`
- `tq_ref`
- `tq_err`
- `w_resp`
- `invdists`
- `respterm`
- `objective`
- `rd`

Root directory of the whole project.
- `pgrad`

Iteration where we turn on zero-gradient skipping.
- `tempbase`

Relative directory of target.
- `tempdir`
- `rundir`

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- `FF`

Need the forcefield (here for now)
- `xct`

Counts how often the objective function was computed.
- `gct`

Counts how often the gradient was computed.
- `hct`

Counts how often the Hessian was computed.
- `read_indicate`

Whether to read indicate.log from file when restarting an aborted run.
- `write_indicate`

Whether to write indicate.log at every iteration (true for all but remote.)
- `read_objective`

Whether to read objective.p from file when restarting an aborted run.
- `write_objective`

Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.2.1 Detailed Description

Subclass of Target for force and energy matching using AMBER.

Implements the prepare and energy_force_driver methods. The get method is in the base class.

Definition at line 171 of file amberio.py.

8.2.2 Constructor & Destructor Documentation

```
def forcebalance.amberio.AbInitio_AMBER.__init__( self, options, tgt_opts, forcefield ) Definition at line 174  
of file amberio.py.
```

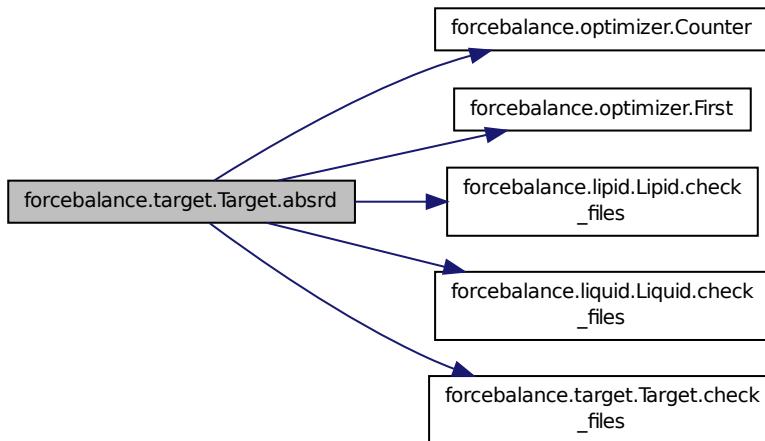
8.2.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd( self, inum = None ) [inherited] Supply the correct directory  
specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.build_invdist( self, mvals ) [inherited] Definition at line 171 of file  
abinitio.py.
```

```
def forcebalance.target.Target.check_files( self, there ) [inherited] Check this directory for the presence  
of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

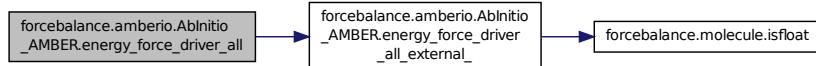
```
def forcebalance.abinitio.AbInitio.compute_netforce_torque( self, xyz, force, QM = False )  
[inherited] Definition at line 200 of file abinitio.py.
```

```
def forcebalance.abinitio.AbInitio.energy_all( self ) [inherited] Definition at line 472 of file abinitio.py.
```

```
def forcebalance.abinitio.AbInitio.energy_force_all( self ) [inherited] Definition at line 478 of file abinitio.py.
```

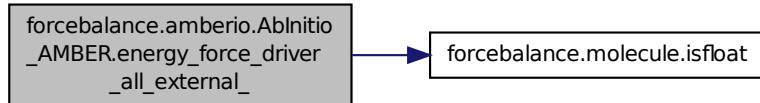
```
def forcebalance.amberio.ABInitio_AMBER.energy_force_driver_all ( self ) Definition at line 228 of file amberio.py.
```

Here is the call graph for this function:



```
def forcebalance.amberio.ABInitio_AMBER.energy_force_driver_all_external ( self ) Definition at line 190 of file amberio.py.
```

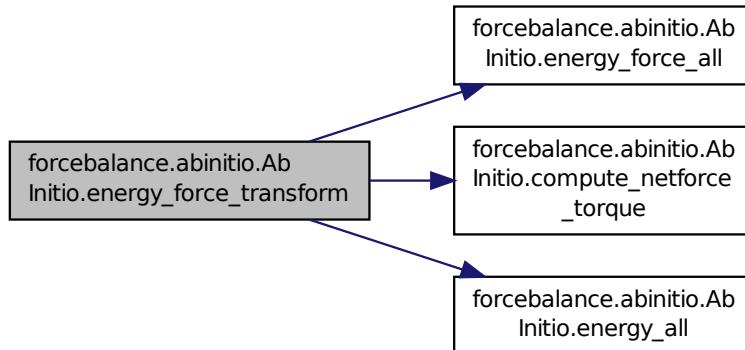
Here is the call graph for this function:



```
def forcebalance.abinitio.ABInitio.energy_force_one ( self, i ) [inherited] Definition at line 507 of file abinitio.py.
```

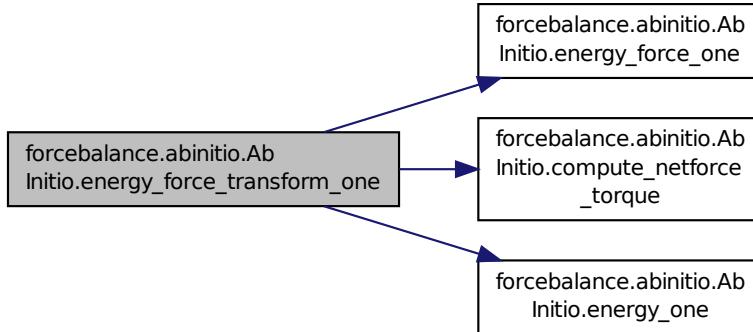
```
def forcebalance.abinitio.ABInitio.energy_force_transform ( self ) [inherited] Definition at line 484 of file abinitio.py.
```

Here is the call graph for this function:



def forcebalance.abinitio.ABInitio.energy_force.transform.one (self, i) [inherited] Definition at line 513 of file abinitio.py.

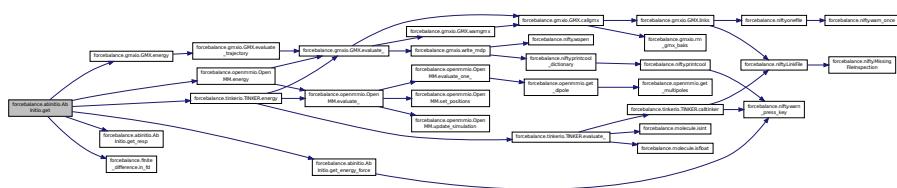
Here is the call graph for this function:



def forcebalance.abinitio.ABInitio.energy_one(self, i) [inherited] Definition at line 501 of file abinitio.py.

def forcebalance.abinitio.ABInitio.get(self, mvals, AGrad = False, AHess = False) [inherited]
Definition at line 1152 of file abinitio.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.ABInitio.get_energy_force ( self, mvals, AGrad = False, AHess = False )  
[inherited] LPW 06-30-2013.
```

This subroutine builds the objective function (and optionally its derivatives) from a general simulation software. This is in contrast to using GROMACS-X2, which computes the objective function and prints it out; then 'get' only needs to call GROMACS and read it in.

This subroutine interfaces with simulation software 'drivers'. The driver is only expected to give the energy and forces.

Now this subroutine may sound trivial since the objective function is simply a least-squares quantity $(M-Q)^2$ - but there are a number of nontrivial considerations. I will list them here.

0) Polytensor formulation: Because there may exist covariance between different components of the force (or covariance between the energy and the force), we build the objective function by taking outer products of vectors that have the form [E F_1x F_1y F_1z F_2x F_2y ...], and then we trace it with the inverse of the covariance matrix to get the objective function.

This version implements both the polytensor formulation and the standard formulation.

1) Boltzmann weights and normalization: Each snapshot has its own Boltzmann weight, which may or may not be normalized. This subroutine does the normalization automatically.

2) Subtracting out the mean energy gap: The zero-point energy difference between reference data and simulation is meaningless. This subroutine subtracts it out.

3) Hybrid ensembles: This program builds a combined objective function from both MM and QM ensembles, which is rigorously better than using a single ensemble.

Note that this subroutine does not do EVERYTHING that GROMACS-X2 can do, which includes:

1) Internal coordinate systems 2) 'Sampling correction' (deprecated, since it doesn't seem to work) 3) Analytic derivatives

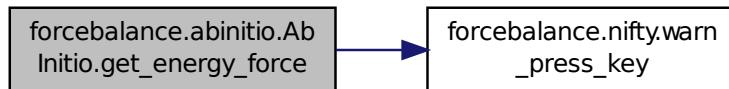
In the previous code (ForTune) this subroutine used analytic first derivatives of the energy and force to build the derivatives of the objective function. Here I will take a simplified approach, because building the derivatives are cumbersome. For now we will return the objective function ONLY. A two-point central difference should give us the first and diagonal second derivative anyhow.

Todo Parallelization over snapshots is not implemented yet

```
@param[in] mvals Mathematical parameter values
@param[in] AGrad Switch to turn on analytic gradient
@param[in] AHess Switch to turn on analytic Hessian
@return Answer Contribution to the objective function
```

Definition at line 588 of file abinitio.py.

Here is the call graph for this function:



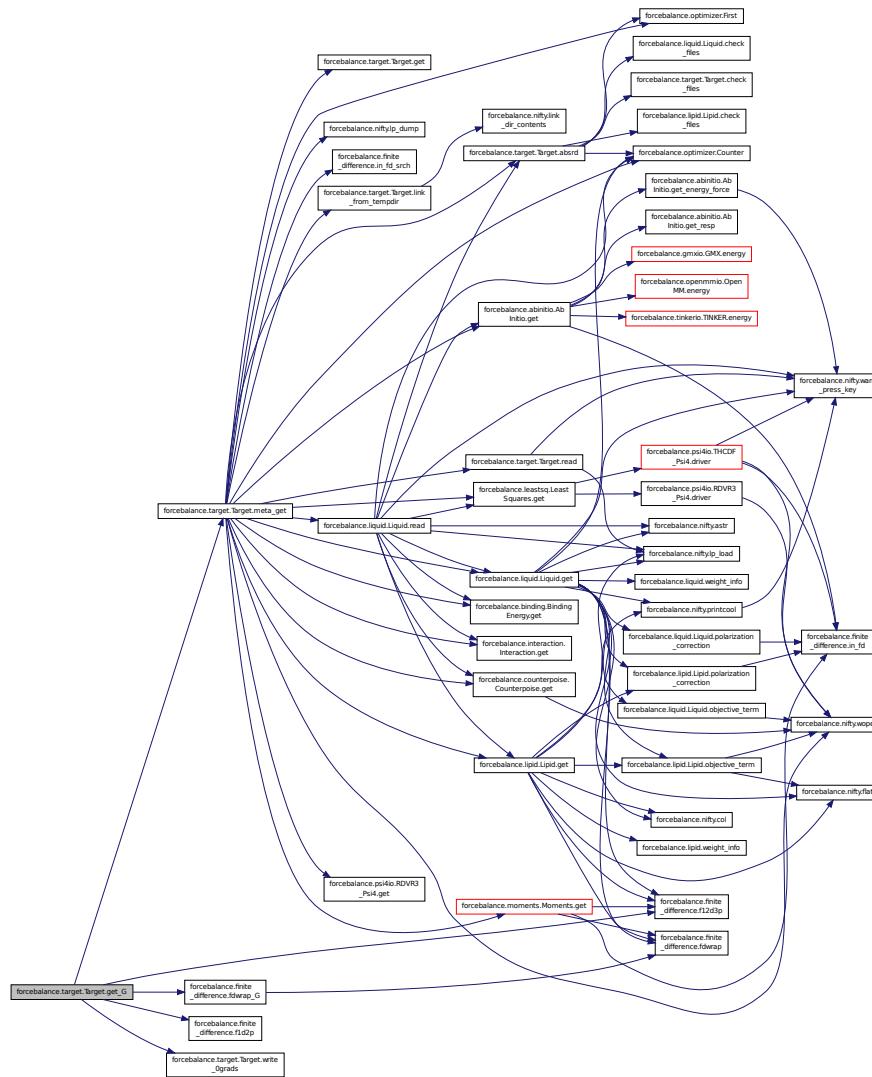
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



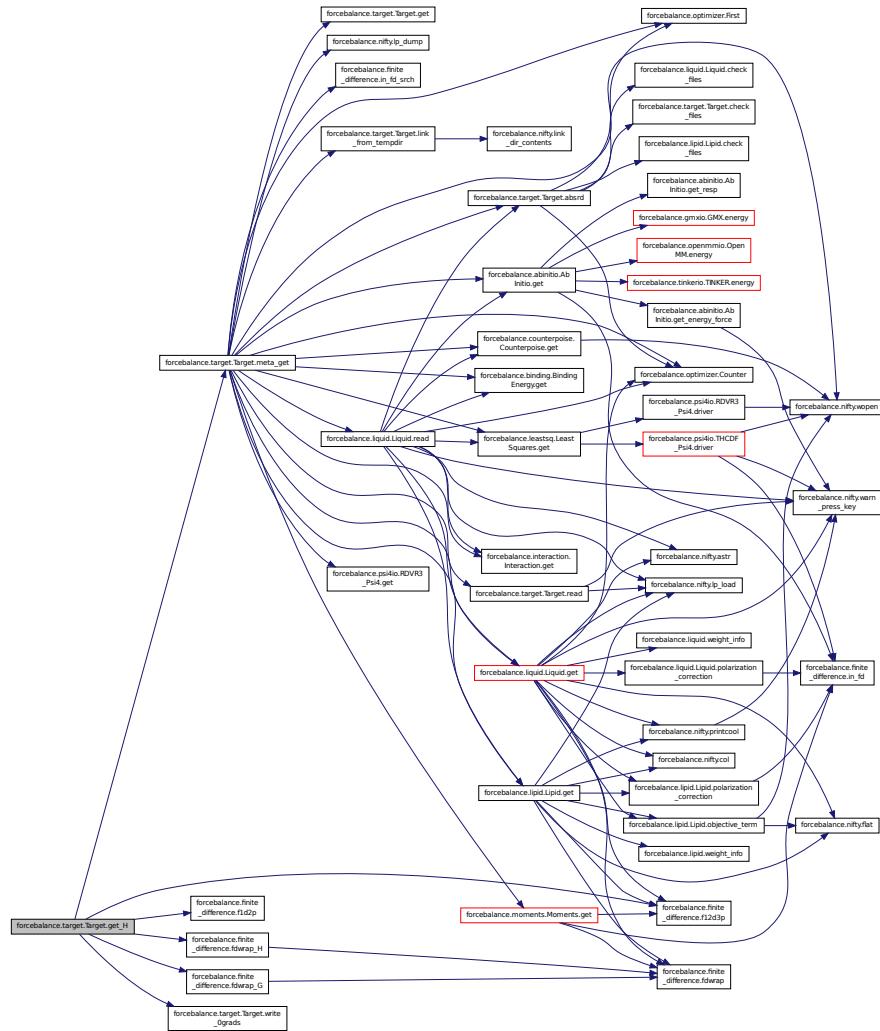
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.get_resp ( self, mvals, AGrad = False, AHess = False )  
[inherited] Electrostatic potential fitting.
```

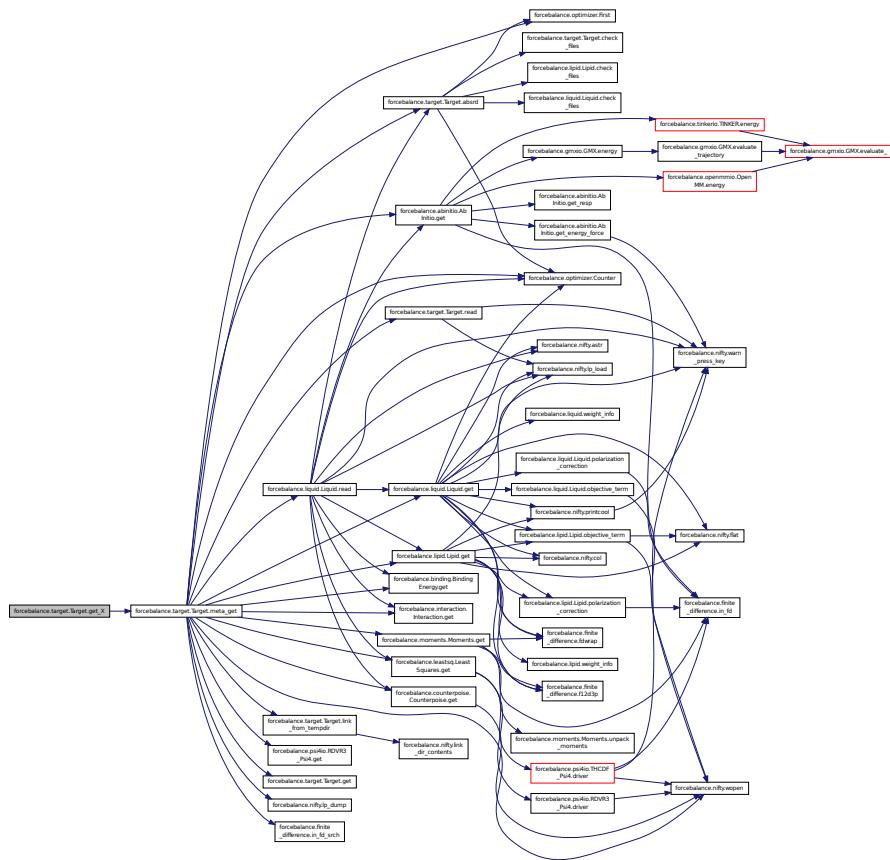
Implements the RESP objective function. (In Python so obviously not optimized.) This function takes the mathematical parameter values and returns the charges on the ATOMS (fancy mapping going on)

Definition at line 1053 of file abinitio.py.

def forcebalance.target.Target.get_X(self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

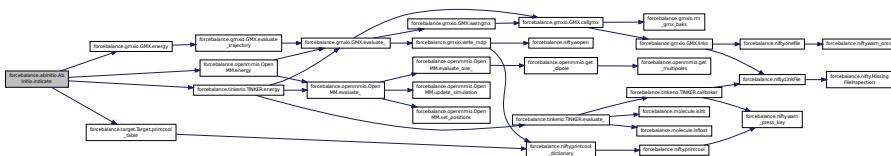
Definition at line 184 of file target.py.

Here is the call graph for this function:



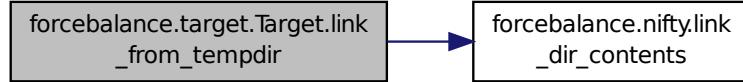
def forcebalance.abinitio.ABInitio.indicate (self) [inherited] Definition at line 448 of file abinitio.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

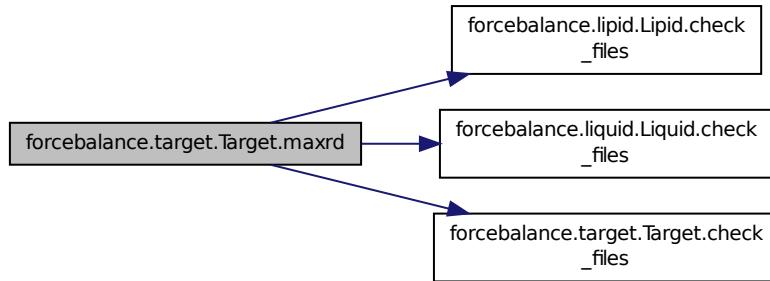
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

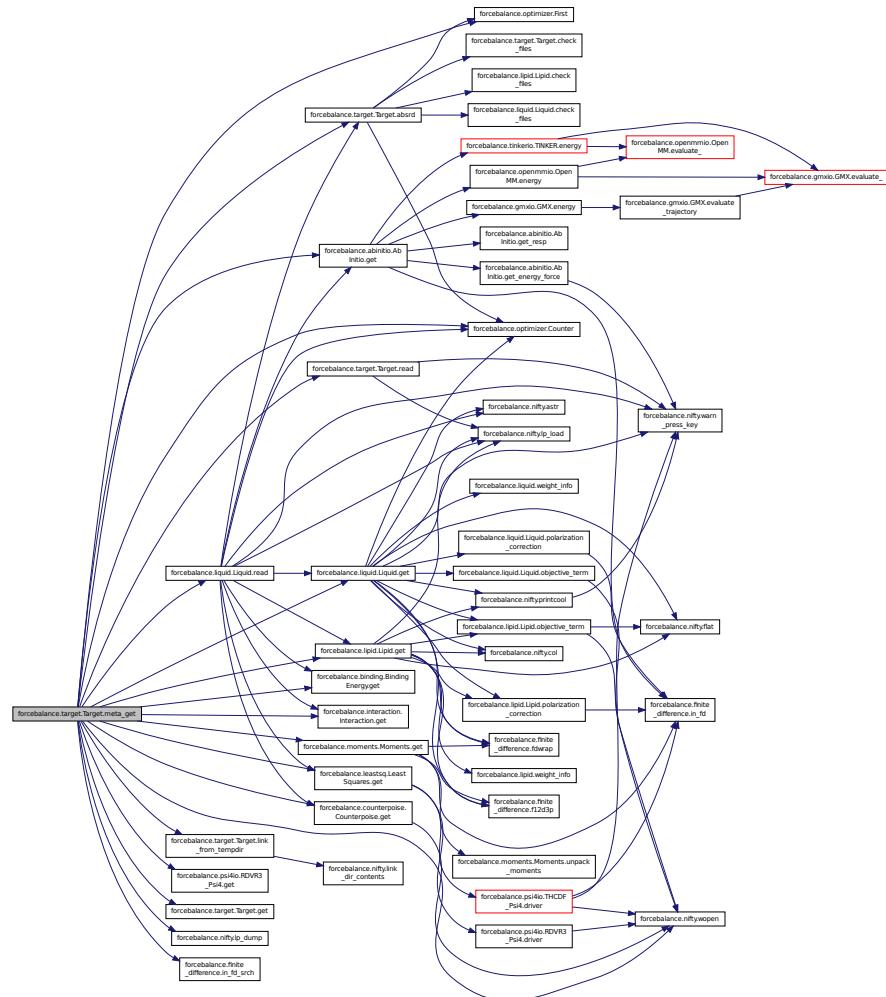


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

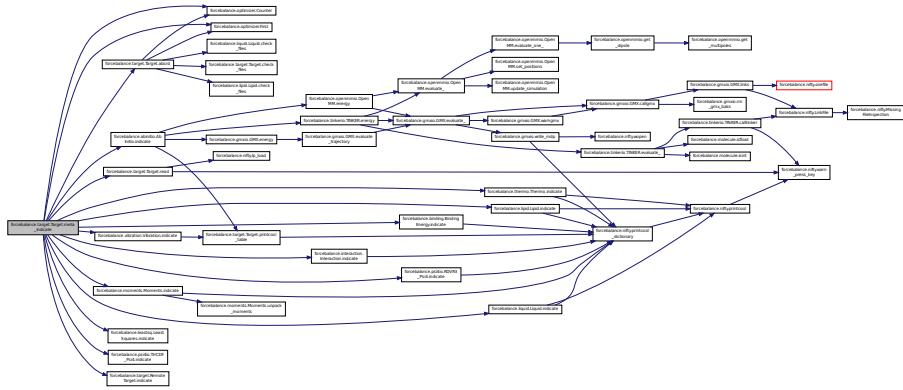
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



def forcebalance.amberio.ABInitio_AMBER.prepare_temp_directory (self, options, tgt_opts) Definition at line 181 of file amberio.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

Here is the call graph for this function:

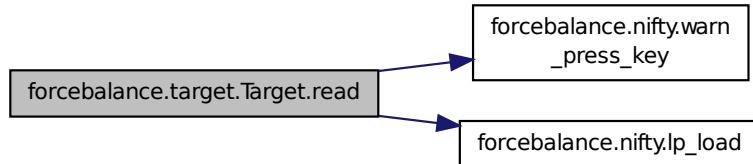


```
def forcebalance.target.Target.read ( self, mvals, AGrad = False, AHess = False ) [inherited]
```

Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.read_0grads ( self ) [inherited]
```

Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

```
def forcebalance.abinitio.AbInitio.read_reference_data ( self ) [inherited]
```

Read the reference ab initio data from a file such as qdata.txt.

Todo Add an option for picking any slice out of qdata.txt, helpful for cross-validation

Todo Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

After reading in the information from qdata.txt, it is converted into the GROMACS energy units (kind of an arbitrary choice); forces (kind of a misnomer in qdata.txt) are multiplied by -1 to convert gradients to forces.

We also subtract out the mean energies of all energy arrays because energy/force matching does not account for zero-point energy differences between MM and QM (i.e. energy of electrons in core orbitals).

The configurations in force/energy matching typically come from a the thermodynamic ensemble of the MM force field at some temperature (by running MD, for example), and for many reasons it is helpful to introduce non-Boltzmann weights in front of these configurations. There are two options: WHAM Boltzmann weights (for combining the weights of several simulations together) and QM Boltzmann weights (for converting MM weights into QM weights). Note that the two sets of weights 'stack'; i.e. they can be used at the same time.

A 'hybrid' ensemble is possible where we use 50% MM and 50% QM weights. Please read more in LPW and Troy Van Voorhis, JCP Vol. 133, Pg. 231101 (2010), doi:10.1063/1.3519043.

Todo The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Finally, note that using non-Boltzmann weights degrades the statistical information content of the snapshots. This problem will generally become worse if the ensemble to which we're reweighting is dramatically different from the one we're sampling from. We end up with a set of Boltzmann weights like [1e-9, 1e-9, 1.0, 1e-9, 1e-9 ...] and this is essentially just one snapshot. I believe Troy is working on something to cure this problem.

Here, we have a measure for the information content of our snapshots, which comes easily from the definition of information entropy:

```
S = -1*Sum_i(P_i*log(P_i))
InfoContent = exp(-S)
```

With uniform weights, InfoContent is equal to the number of snapshots; with horrible weights, InfoContent is closer to one.

Definition at line 329 of file abinitio.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

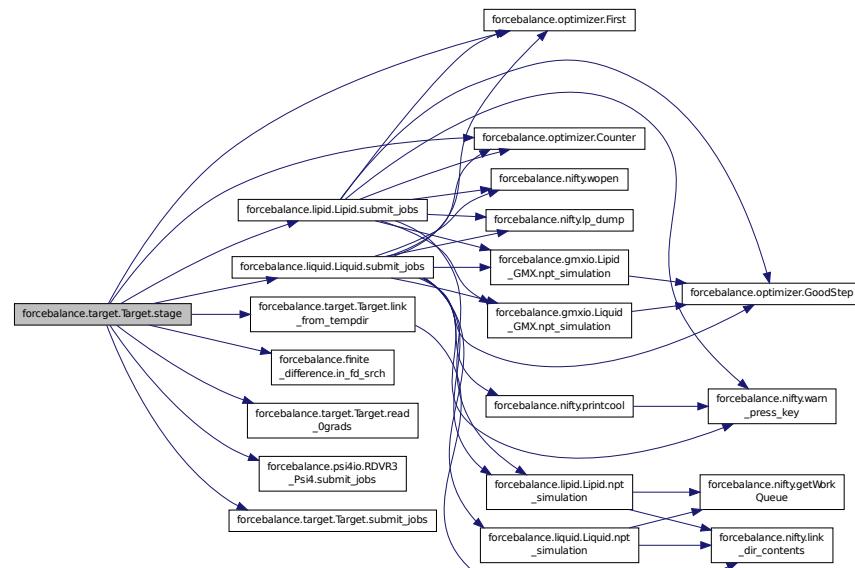
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

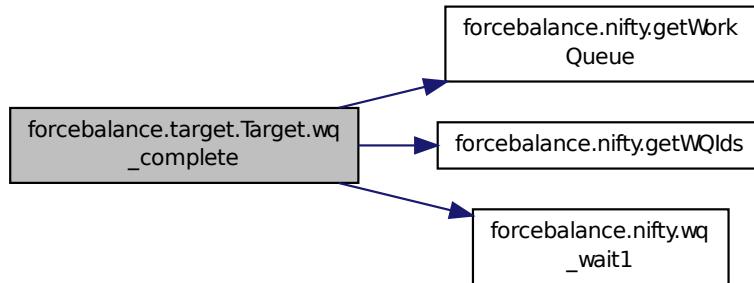


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work  
Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_0grads ( self, Ans ) [inherited] Write a file to the target directory  
containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.2.4 Member Data Documentation

```
forcebalance.amberio.AbInitio_AMBER.all_at_once all_at_once is not implemented.
```

Definition at line 179 of file amberio.py.

```
forcebalance.abinitio.AbInitio.AtomLists [inherited] Lists of atoms to do net force/torque fitting and excluding virtual sites.
```

Definition at line 160 of file abinitio.py.

```
forcebalance.abinitio.AbInitio.AtomMask [inherited] Definition at line 161 of file abinitio.py.
```

```
forcebalance.abinitio.AbInitio.boltz_wts [inherited] Initialize the base class.
```

Number of snapshots Whether to use WHAM Boltzmann weights Whether to use the Sampling Correction Whether to match Absolute Energies (make sure you know what you're doing) Whether to use the Covariance Matrix Whether to use QM Boltzmann weights The temperature for QM Boltzmann weights Number of atoms that we are fitting Whether to fit Energies. Whether to fit Forces. Whether to fit Electrostatic Potential. Weights for the three components. Option for how much data to write to disk. Whether to do energy and force calculations for the whole trajectory, or to do one calculation per snapshot. OpenMM-only option - whether to run the energies and forces internally. Whether we have virtual sites (set at the global option level) Attenuate the weights as a function of energy What is the energy denominator? (Valid for 'attenuate') Set upper cutoff energy WHAM Boltzmann weights

Definition at line 116 of file abinitio.py.

forcebalance.amberio.ABInitio_AMBER.coords Name of the trajectory, we need this BEFORE initializing the Super-Class.

Definition at line 176 of file amberio.py.

forcebalance.abinitio.ABInitio.e_err [inherited] Qualitative Indicator: average energy error (in kJ/mol)
Definition at line 134 of file abinitio.py.

forcebalance.abinitio.ABInitio.e_err_pct [inherited] Definition at line 135 of file abinitio.py.

forcebalance.abinitio.ABInitio.e_ref [inherited] Definition at line 1030 of file abinitio.py.

forcebalance.abinitio.ABInitio.emd0 [inherited] Energies of the sampling simulation.
Definition at line 122 of file abinitio.py.

forcebalance.abinitio.ABInitio.engine [inherited] Build keyword dictionaries to pass to engine.
Create engine object.
Definition at line 158 of file abinitio.py.

forcebalance.abinitio.ABInitio.eqm [inherited] Reference (QM) energies.
Definition at line 120 of file abinitio.py.

forcebalance.abinitio.ABInitio.esp_err [inherited] Qualitative Indicator: "relative RMS" for electrostatic potential.
Definition at line 140 of file abinitio.py.

forcebalance.abinitio.ABInitio.espval [inherited] ESP values.
Definition at line 128 of file abinitio.py.

forcebalance.abinitio.ABInitio.espxyz [inherited] ESP grid points.
Definition at line 126 of file abinitio.py.

forcebalance.abinitio.ABInitio.f_err [inherited] Qualitative Indicator: average force error (fractional)
Definition at line 137 of file abinitio.py.

forcebalance.abinitio.ABInitio.f_err_pct [inherited] Definition at line 138 of file abinitio.py.

forcebalance.abinitio.ABInitio.f_ref [inherited] Definition at line 1034 of file abinitio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.abinitio.ABInitio.fitatoms [inherited] Definition at line 366 of file abinitio.py.

forcebalance.abinitio.ABInitio.force [inherited] Definition at line 361 of file abinitio.py.

forcebalance.abinitio.ABInitio.force_map [inherited] Definition at line 209 of file abinitio.py.

forcebalance.abinitio.ABInitio.fqm [inherited] Reference (QM) forces.
Definition at line 124 of file abinitio.py.

forcebalance.abinitio.AbInitio.fref [inherited] Definition at line 442 of file abinitio.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.abinitio.AbInitio.invdists [inherited] Definition at line 1061 of file abinitio.py.

forcebalance.abinitio.AbInitio.mol [inherited] Definition at line 148 of file abinitio.py.

forcebalance.abinitio.AbInitio.nesp [inherited] Definition at line 363 of file abinitio.py.

forcebalance.abinitio.AbInitio.new_vsites [inherited] Read in the reference data.

The below two options are related to whether we want to rebuild virtual site positions. Rebuild the distance matrix if virtual site positions have changed
Definition at line 166 of file abinitio.py.

forcebalance.abinitio.AbInitio.nf_err [inherited] Definition at line 141 of file abinitio.py.

forcebalance.abinitio.AbInitio.nf_err_pct [inherited] Definition at line 142 of file abinitio.py.

forcebalance.abinitio.AbInitio.nf_ref [inherited] Definition at line 1038 of file abinitio.py.

forcebalance.abinitio.AbInitio.nftqm [inherited] Definition at line 438 of file abinitio.py.

forcebalance.abinitio.AbInitio.nnf [inherited] Definition at line 267 of file abinitio.py.

forcebalance.abinitio.AbInitio.nparticles [inherited] The number of (atoms + drude particles + virtual sites)
Definition at line 153 of file abinitio.py.

forcebalance.abinitio.AbInitio.ns [inherited] Read in the trajectory file.

Definition at line 147 of file abinitio.py.

forcebalance.abinitio.AbInitio.ntq [inherited] Definition at line 268 of file abinitio.py.

forcebalance.abinitio.AbInitio.objective [inherited] Definition at line 1172 of file abinitio.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.
Dictionary of whether to call the derivatives.
Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.abinitio.AbInitio.qfnm [inherited] The qdata.txt file that contains the QM energies and forces.
Definition at line 130 of file abinitio.py.

forcebalance.abinitio.AblInitio.qmatoms [inherited] The number of atoms in the QM calculation (Irrelevant if not fitting forces)

Definition at line 132 of file abinitio.py.

forcebalance.abinitio.AblInitio.qmboltz_wts [inherited] QM Boltzmann weights.

Definition at line 118 of file abinitio.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.abinitio.AblInitio.respterm [inherited] Definition at line 1140 of file abinitio.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number. The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.abinitio.AblInitio.save_vmvabs [inherited] Save the mvabs from the last time we updated the vsites.

Definition at line 168 of file abinitio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.abinitio.AblInitio.tq_err [inherited] Definition at line 1042 of file abinitio.py.

forcebalance.abinitio.AblInitio.tq_err_pct [inherited] Definition at line 143 of file abinitio.py.

forcebalance.abinitio.AblInitio.tq_ref [inherited] Definition at line 1041 of file abinitio.py.

forcebalance.abinitio.ABInitio.use_nft [inherited] Whether to compute net forces and torques, or not.
Definition at line 145 of file abinitio.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.abinitio.ABInitio.w_energy [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_force [inherited] Definition at line 362 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_netforce [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_resp [inherited] Definition at line 1054 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_torque [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.whamboltz [inherited] Definition at line 382 of file abinitio.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

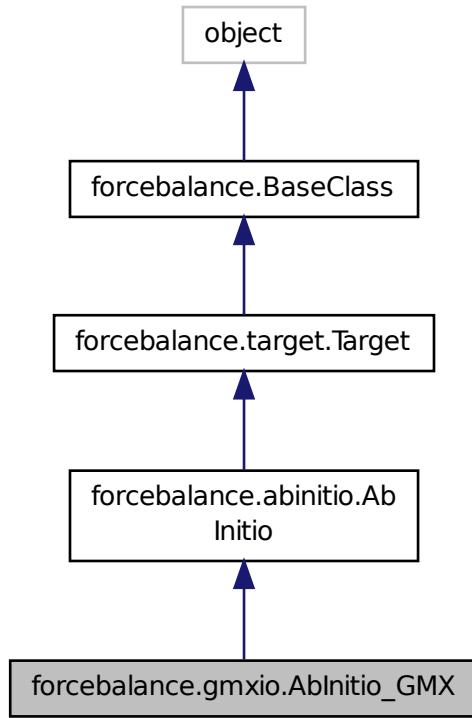
The documentation for this class was generated from the following file:

- [amberio.py](#)

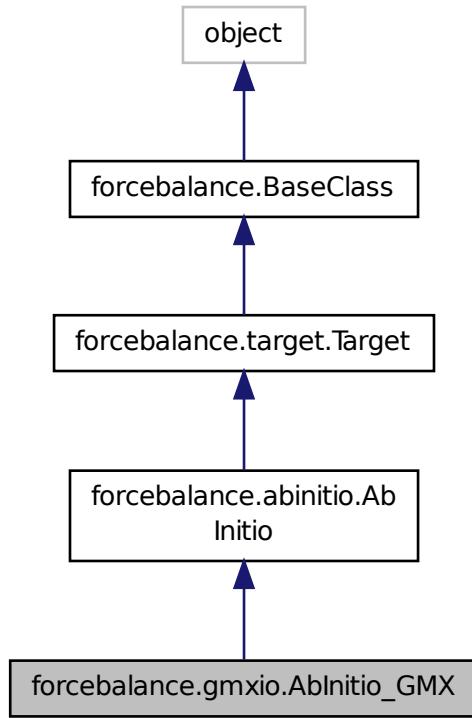
8.3 forcebalance.gmxio.ABInitio_GMX Class Reference

Subclass of ABInitio for force and energy matching using GROMACS.

Inheritance diagram for forcebalance.gmxio.AbInitio_GMX:



Collaboration diagram for forcebalance.gmxio.AbInitio_GMX:



Public Member Functions

- def `_init_`
- def `build_invdist`
- def `compute_netforce_torque`
- def `read_reference_data`

Read the reference ab initio data from a file such as qdata.txt.

- def `indicate`
- def `energy_all`
- def `energy_force_all`
- def `energy_force_transform`
- def `energy_one`
- def `energy_force_one`
- def `energy_force_transform_one`
- def `get_energy_force`

LPW 06-30-2013.

- def `get_resp`

Electrostatic potential fitting.

- def `get`

- def `get_X`
Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
Computes the objective function contribution and its gradient.
- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
Default file names for coordinates, top and mdp files.
- `boltz_wts`
Initialize the base class.
- `qmboltz_wts`
QM Boltzmann weights.
- `eqm`
Reference (QM) energies.
- `emd0`
Energies of the sampling simulation.
- `fqm`

Reference (QM) forces.

- [espxyz](#)
ESP grid points.
- [espval](#)
ESP values.
- [qfnm](#)
The qdata.txt file that contains the QM energies and forces.
- [qatoms](#)
The number of atoms in the QM calculation (Irrelevant if not fitting forces)
- [e_err](#)
Qualitative Indicator: average energy error (in kJ/mol)
- [e_err_pct](#)
- [f_err](#)
Qualitative Indicator: average force error (fractional)
- [f_err_pct](#)
- [esp_err](#)
Qualitative Indicator: "relative RMS" for electrostatic potential.
- [nf_err](#)
- [nf_err_pct](#)
- [tq_err_pct](#)
- [use_nft](#)
Whether to compute net forces and torques, or not.
- [ns](#)
Read in the trajectory file.
- [mol](#)
- [nparticles](#)
The number of (atoms + drude particles + virtual sites)
- [engine](#)
Build keyword dictionaries to pass to engine.
- [AtomLists](#)
Lists of atoms to do net force/torque fitting and excluding virtual sites.
- [AtomMask](#)
- [new_vsites](#)
Read in the reference data.
- [save_vmvalls](#)
Save the mvalls from the last time we updated the vsites.
- [force_map](#)
- [nnf](#)
- [ntq](#)
- [force](#)
- [w_force](#)
- [nesp](#)
- [fitatoms](#)
- [whamboltz](#)
- [nftqm](#)
- [fref](#)
- [w_energy](#)
- [w_netforce](#)

- `w_torque`
- `e_ref`
- `f_ref`
- `nf_ref`
- `tq_ref`
- `tq_err`
- `w_resp`
- `invdists`
- `respterm`
- `objective`
- `rd`

Root directory of the whole project.
- `pgrad`

Iteration where we turn on zero-gradient skipping.
- `tempbase`

Relative directory of target.
- `tempdir`
- `rundir`

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- `FF`

Need the forcefield (here for now)
- `xct`

Counts how often the objective function was computed.
- `gct`

Counts how often the gradient was computed.
- `hct`

Counts how often the Hessian was computed.
- `read_indicate`

Whether to read indicate.log from file when restarting an aborted run.
- `write_indicate`

Whether to write indicate.log at every iteration (true for all but remote.)
- `read_objective`

Whether to read objective.p from file when restarting an aborted run.
- `write_objective`

Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.3.1 Detailed Description

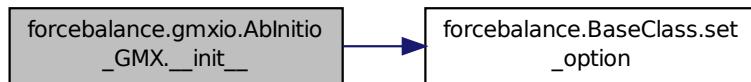
Subclass of AbInitio for force and energy matching using GROMACS.

Definition at line 1449 of file gmxio.py.

8.3.2 Constructor & Destructor Documentation

```
def forcebalance.gmxio.AbInitio_GMX.__init__ ( self, options, tgt_opts, forcefield ) Definition at line 1450 of file gmxio.py.
```

Here is the call graph for this function:



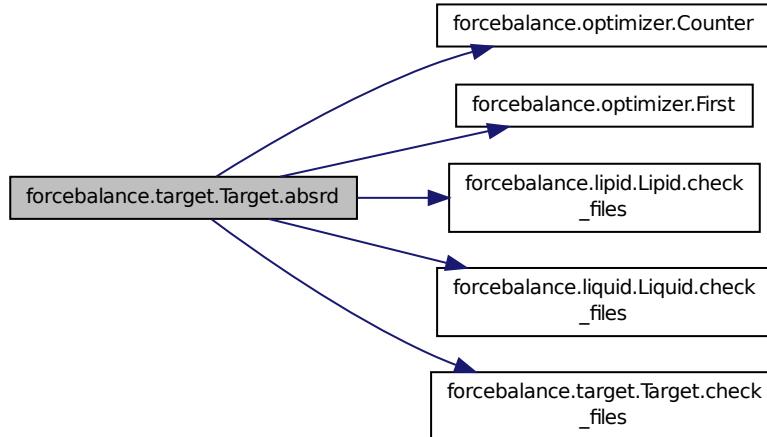
8.3.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.build_invdist ( self, mvals ) [inherited] Definition at line 171 of file abinitio.py.
```

```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.abinitio.AbInitio.compute_netforce_torque ( self, xyz, force, QM = False )  
[inherited] Definition at line 200 of file abinitio.py.
```

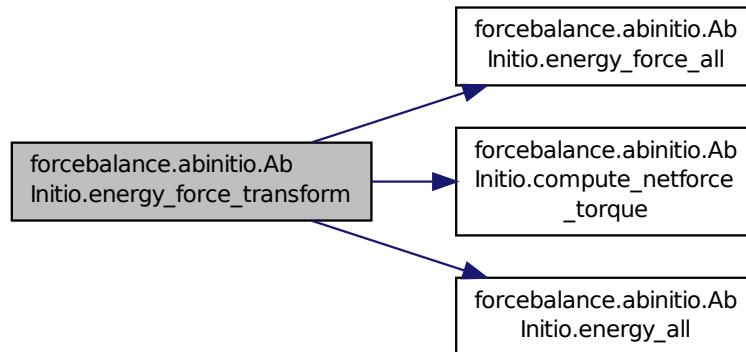
```
def forcebalance.abinitio.AbInitio.energy_all ( self ) [inherited] Definition at line 472 of file abinitio.py.
```

```
def forcebalance.abinitio.AbInitio.energy_force_all ( self ) [inherited] Definition at line 478 of file abinitio.py.
```

```
def forcebalance.abinitio.AbInitio.energy_force_one ( self, i ) [inherited] Definition at line 507 of file abinitio.py.
```

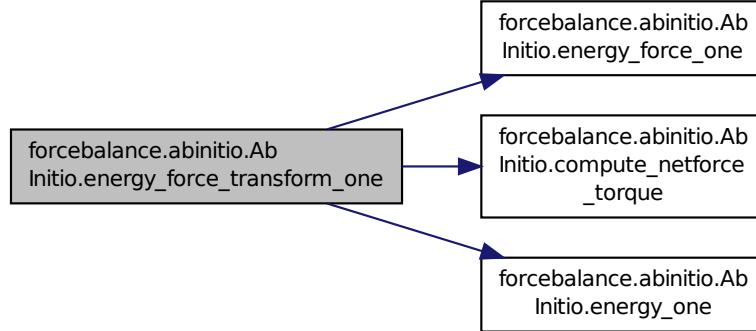
```
def forcebalance.abinitio.AbInitio.energy_force_transform ( self ) [inherited] Definition at line 484 of file abinitio.py.
```

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.energy_force_transform_one ( self, i ) [inherited] Definition at line 513 of file abinitio.py.
```

Here is the call graph for this function:

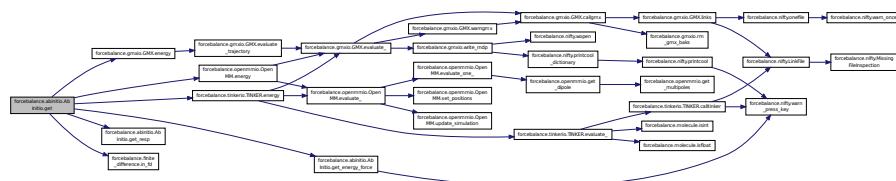


def forcebalance.abinitio.AbInitio.energy_one (self, i) [inherited] Definition at line 501 of file abinitio.py.

def forcebalance.abinitio.AbInitio.get (self, mvals, AGrad = False, AHess = False) [inherited]

Definition at line 1152 of file abinitio.py.

Here is the call graph for this function:



def forcebalance.abinitio.AbInitio.get_energy_force (self, mvals, AGrad = False, AHess = False) [inherited] LPW 06-30-2013.

This subroutine builds the objective function (and optionally its derivatives) from a general simulation software. This is in contrast to using GROMACS-X2, which computes the objective function and prints it out; then 'get' only needs to call GROMACS and read it in.

This subroutine interfaces with simulation software 'drivers'. The driver is only expected to give the energy and forces.

Now this subroutine may sound trivial since the objective function is simply a least-squares quantity $(M-Q)^2$ - but there are a number of nontrivial considerations. I will list them here.

0) Polytensor formulation: Because there may exist covariance between different components of the force (or covariance between the energy and the force), we build the objective function by taking outer products of vectors that have the form $[E F_{1x} F_{1y} F_{1z} F_{2x} F_{2y} \dots]$, and then we trace it with the inverse of the covariance matrix to get the objective function.

This version implements both the polytensor formulation and the standard formulation.

1) Boltzmann weights and normalization: Each snapshot has its own Boltzmann weight, which may or may not be normalized. This subroutine does the normalization automatically.

2) Subtracting out the mean energy gap: The zero-point energy difference between reference data and simulation is meaningless. This subroutine subtracts it out.

3) Hybrid ensembles: This program builds a combined objective function from both MM and QM ensembles, which is rigorously better than using a single ensemble.

Note that this subroutine does not do EVERYTHING that GROMACS-X2 can do, which includes:

1) Internal coordinate systems 2) 'Sampling correction' (deprecated, since it doesn't seem to work) 3) Analytic derivatives

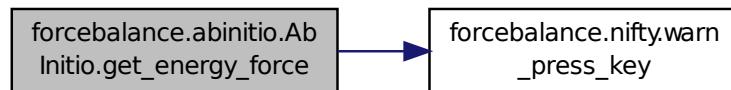
In the previous code (ForTune) this subroutine used analytic first derivatives of the energy and force to build the derivatives of the objective function. Here I will take a simplified approach, because building the derivatives are cumbersome. For now we will return the objective function ONLY. A two-point central difference should give us the first and diagonal second derivative anyhow.

Todo Parallelization over snapshots is not implemented yet

```
@param[in] mvals Mathematical parameter values
@param[in] AGrad Switch to turn on analytic gradient
@param[in] AHess Switch to turn on analytic Hessian
@return Answer Contribution to the objective function
```

Definition at line 588 of file abinitio.py.

Here is the call graph for this function:



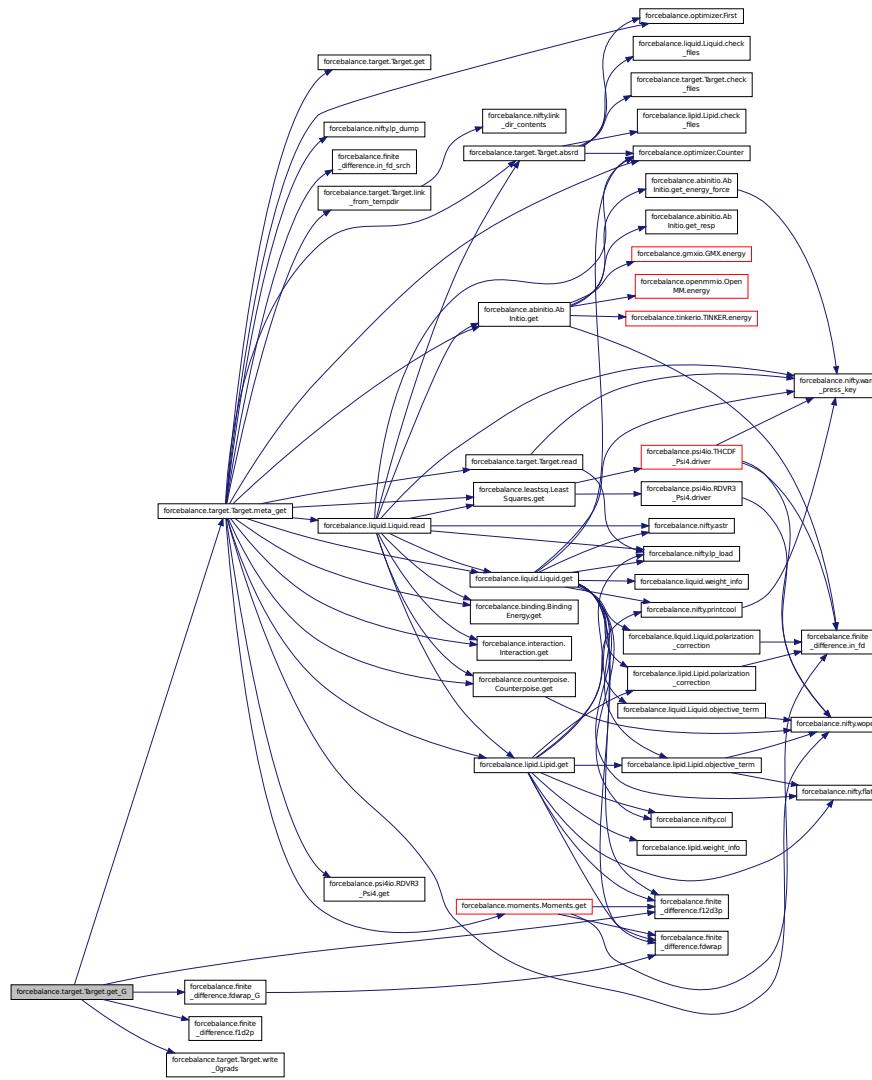
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



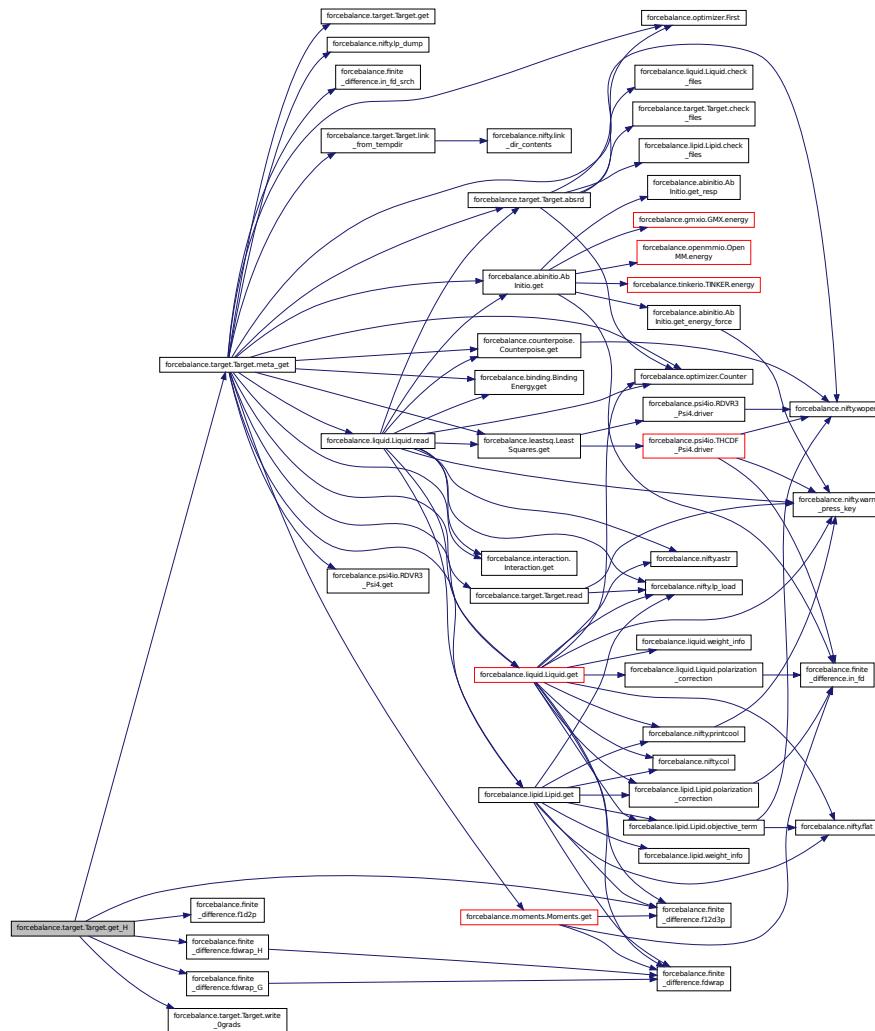
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.get_resp ( self, mvals, AGrad = False, AHess = False )
[inherited] Electrostatic potential fitting.
```

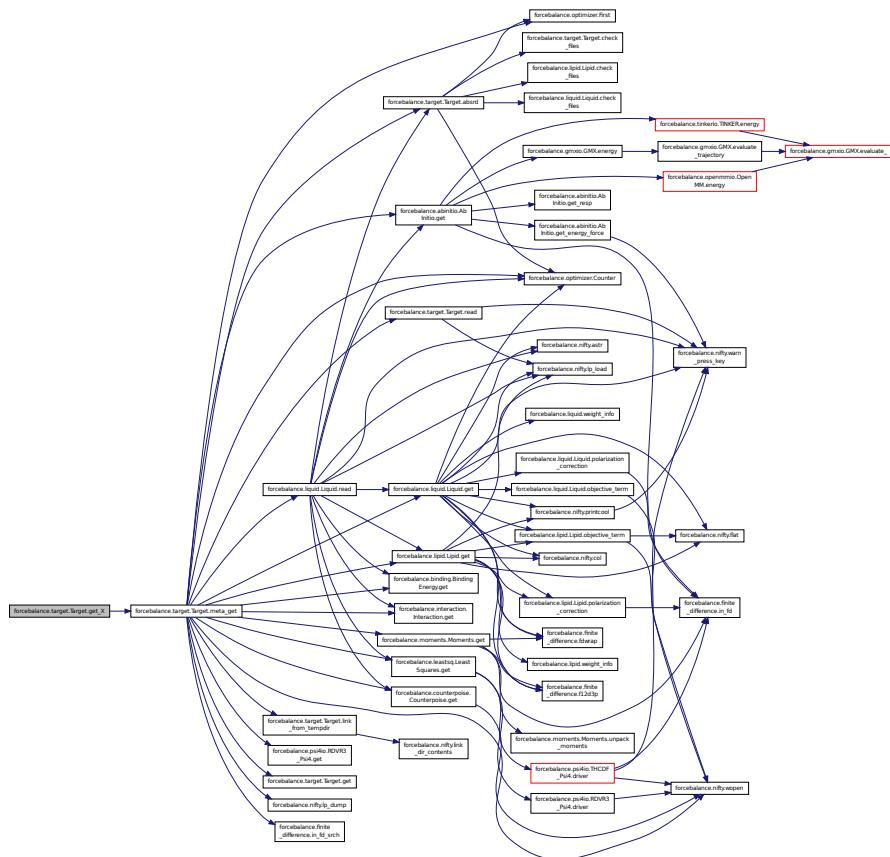
Implements the RESP objective function. (In Python so obviously not optimized.) This function takes the mathematical parameter values and returns the charges on the ATOMS (fancy mapping going on)

Definition at line 1053 of file abinitio.py.

```
def forcebalance.target.Target.get_X ( self, mvals = None ) [inherited] Computes the objective function contribution without any parametric derivatives.
```

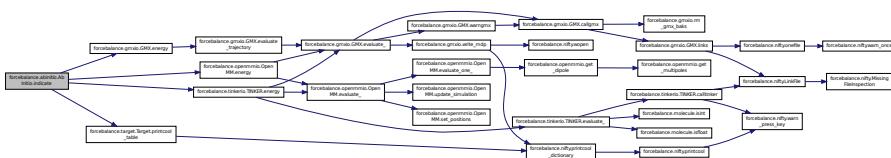
Definition at line 184 of file target.py.

Here is the call graph for this function:



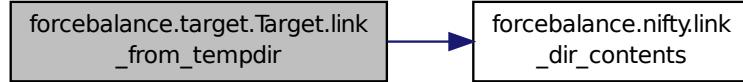
def forcebalance.abinitio.ABInitio.indicate (self) [inherited] Definition at line 448 of file abinitio.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.link_from_tempdir( self, absdestdir ) [inherited] Definition at line 315 of file target.py.
```

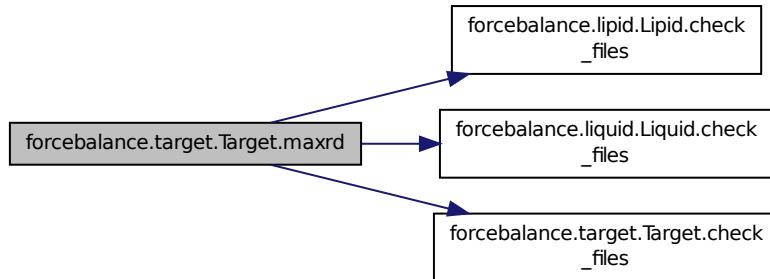
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

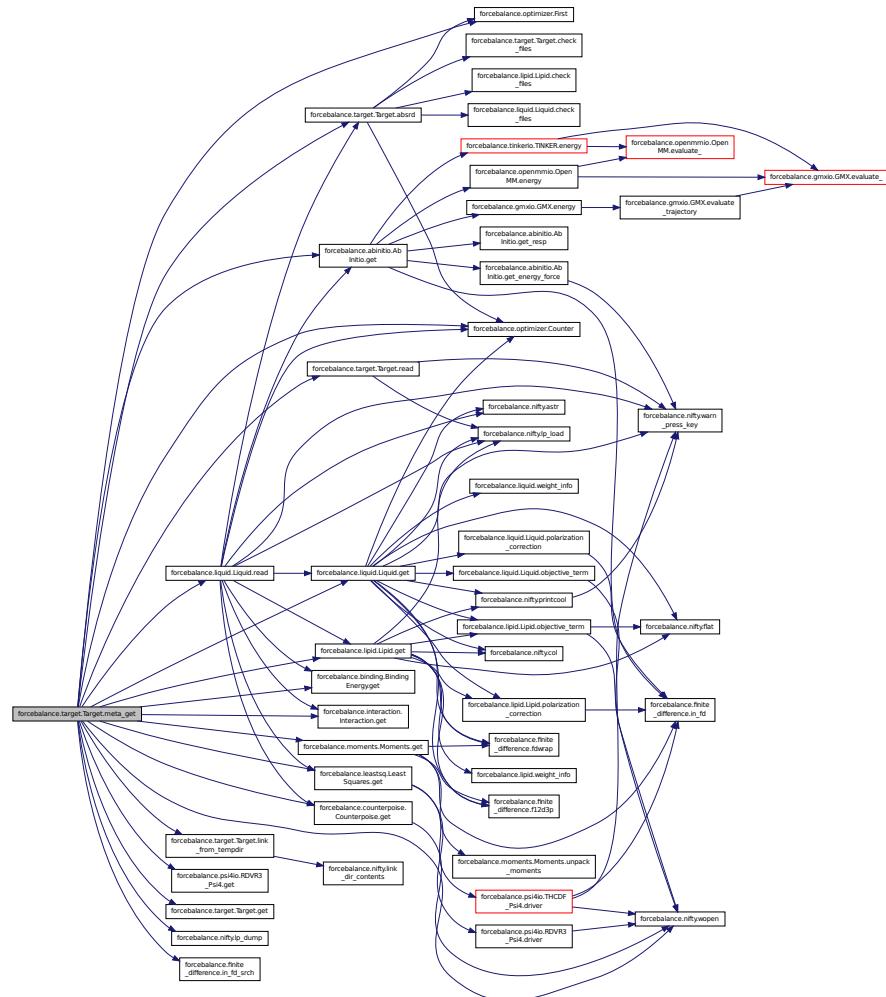


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

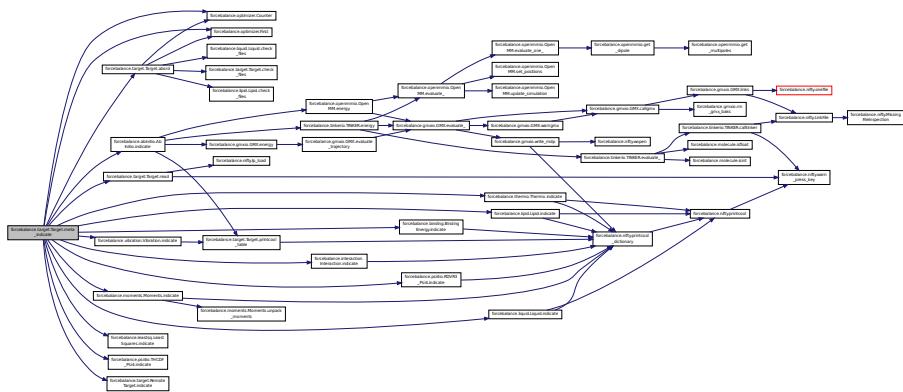
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

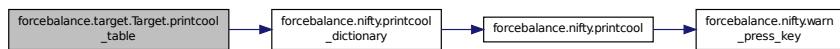
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

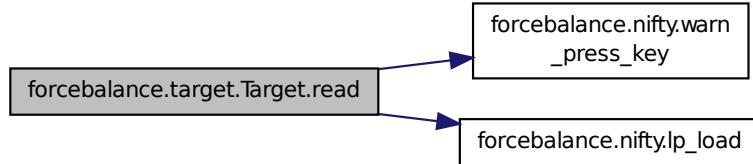
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.abinitio.AbInitio.read_reference_data (self) [inherited] Read the reference ab initio data from a file such as qdata.txt.

Todo Add an option for picking any slice out of qdata.txt, helpful for cross-validation

Todo Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

After reading in the information from qdata.txt, it is converted into the GROMACS energy units (kind of an arbitrary choice); forces (kind of a misnomer in qdata.txt) are multiplied by -1 to convert gradients to forces.

We also subtract out the mean energies of all energy arrays because energy/force matching does not account for zero-point energy differences between MM and QM (i.e. energy of electrons in core orbitals).

The configurations in force/energy matching typically come from a the thermodynamic ensemble of the MM force field at some temperature (by running MD, for example), and for many reasons it is helpful to introduce non-Boltzmann weights in front of these configurations. There are two options: WHAM Boltzmann weights (for combining the weights of several simulations together) and QM Boltzmann weights (for converting MM weights into QM weights). Note that the two sets of weights 'stack'; i.e. they can be used at the same time.

A 'hybrid' ensemble is possible where we use 50% MM and 50% QM weights. Please read more in LPW and Troy Van Voorhis, JCP Vol. 133, Pg. 231101 (2010), doi:10.1063/1.3519043.

Todo The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Finally, note that using non-Boltzmann weights degrades the statistical information content of the snapshots. This problem will generally become worse if the ensemble to which we're reweighting is dramatically different from the one we're sampling from. We end up with a set of Boltzmann weights like [1e-9, 1e-9, 1.0, 1e-9, 1e-9 ...] and this is essentially just one snapshot. I believe Troy is working on something to cure this problem.

Here, we have a measure for the information content of our snapshots, which comes easily from the definition of information entropy:

```
S = -1*Sum_i(P_i*log(P_i))
InfoContent = exp(-S)
```

With uniform weights, InfoContent is equal to the number of snapshots; with horrible weights, InfoContent is closer to one.

Definition at line 329 of file abinitio.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

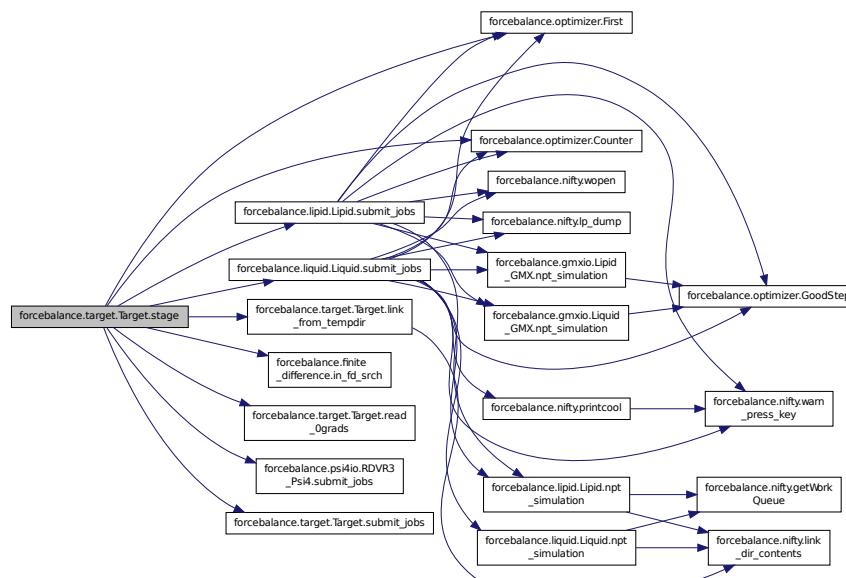
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

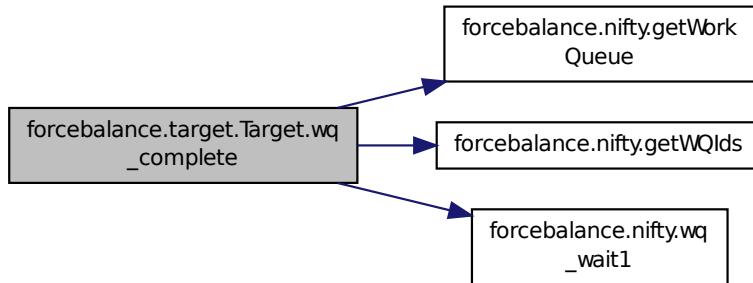


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work  
Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_Ograds ( self, Ans ) [inherited] Write a file to the target directory  
containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.3.4 Member Data Documentation

```
forcebalance.abinitio.ABInitio.AtomLists [inherited] Lists of atoms to do net force/torque fitting and excluding virtual sites.
```

Definition at line 160 of file abinitio.py.

```
forcebalance.abinitio.ABInitio.AtomMask [inherited] Definition at line 161 of file abinitio.py.
```

```
forcebalance.abinitio.ABInitio.boltz_wts [inherited] Initialize the base class.
```

Number of snapshots Whether to use WHAM Boltzmann weights Whether to use the Sampling Correction Whether to match Absolute Energies (make sure you know what you're doing) Whether to use the Covariance Matrix Whether to use QM Boltzmann weights The temperature for QM Boltzmann weights Number of atoms that we are fitting Whether to fit Energies. Whether to fit Forces. Whether to fit Electrostatic Potential. Weights for the three components. Option for how much data to write to disk. Whether to do energy and force calculations for the whole trajectory, or to do one calculation per snapshot. OpenMM-only option - whether to run the energies and forces internally. Whether we have virtual sites (set at the global option level) Attenuate the weights as a function of energy What is the energy denominator? (Valid for 'attenuate') Set upper cutoff energy WHAM Boltzmann weights

Definition at line 116 of file abinitio.py.

```
forcebalance.abinitio.ABInitio.e_err [inherited] Qualitative Indicator: average energy error (in kJ/mol)
```

Definition at line 134 of file abinitio.py.

```
forcebalance.abinitio.ABInitio.e_err_pct [inherited] Definition at line 135 of file abinitio.py.
```

forcebalance.abinitio.AbInitio.e.ref [inherited] Definition at line 1030 of file abinitio.py.

forcebalance.abinitio.AbInitio.emd0 [inherited] Energies of the sampling simulation.
Definition at line 122 of file abinitio.py.

forcebalance.abinitio.AbInitio.engine [inherited] Build keyword dictionaries to pass to engine.
Create engine object.
Definition at line 158 of file abinitio.py.

forcebalance.gmxio.AbInitio_GMX.engine Default file names for coordinates, top and mdp files.
Definition at line 1455 of file gmxio.py.

forcebalance.abinitio.AbInitio.eqm [inherited] Reference (QM) energies.
Definition at line 120 of file abinitio.py.

forcebalance.abinitio.AbInitio.esp_err [inherited] Qualitative Indicator: "relative RMS" for electrostatic potential.
Definition at line 140 of file abinitio.py.

forcebalance.abinitio.AbInitio.espval [inherited] ESP values.
Definition at line 128 of file abinitio.py.

forcebalance.abinitio.AbInitio.espxyz [inherited] ESP grid points.
Definition at line 126 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err [inherited] Qualitative Indicator: average force error (fractional)
Definition at line 137 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err_pct [inherited] Definition at line 138 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_ref [inherited] Definition at line 1034 of file abinitio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.abinitio.AbInitio.fitatoms [inherited] Definition at line 366 of file abinitio.py.

forcebalance.abinitio.AbInitio.force [inherited] Definition at line 361 of file abinitio.py.

forcebalance.abinitio.AbInitio.force_map [inherited] Definition at line 209 of file abinitio.py.

forcebalance.abinitio.AbInitio.fqm [inherited] Reference (QM) forces.
Definition at line 124 of file abinitio.py.

forcebalance.abinitio.AbInitio.fref [inherited] Definition at line 442 of file abinitio.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.abinitio.ABInitio.invdist [inherited] Definition at line 1061 of file abinitio.py.

forcebalance.abinitio.ABInitio.mol [inherited] Definition at line 148 of file abinitio.py.

forcebalance.abinitio.ABInitio.nesp [inherited] Definition at line 363 of file abinitio.py.

forcebalance.abinitio.ABInitio.new_vsites [inherited] Read in the reference data.

The below two options are related to whether we want to rebuild virtual site positions. Rebuild the distance matrix if virtual site positions have changed

Definition at line 166 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err [inherited] Definition at line 141 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err_pct [inherited] Definition at line 142 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_ref [inherited] Definition at line 1038 of file abinitio.py.

forcebalance.abinitio.ABInitio.nftqm [inherited] Definition at line 438 of file abinitio.py.

forcebalance.abinitio.ABInitio.nnf [inherited] Definition at line 267 of file abinitio.py.

forcebalance.abinitio.ABInitio.nparticles [inherited] The number of (atoms + drude particles + virtual sites)
Definition at line 153 of file abinitio.py.

forcebalance.abinitio.ABInitio.ns [inherited] Read in the trajectory file.

Definition at line 147 of file abinitio.py.

forcebalance.abinitio.ABInitio.ntq [inherited] Definition at line 268 of file abinitio.py.

forcebalance.abinitio.ABInitio.objective [inherited] Definition at line 1172 of file abinitio.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.abinitio.ABInitio.qfnm [inherited] The qdata.txt file that contains the QM energies and forces.
Definition at line 130 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmatoms [inherited] The number of atoms in the QM calculation (Irrelevant if not fitting forces)

Definition at line 132 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmboltz_wts [inherited] QM Boltzmann weights.

Definition at line 118 of file abinitio.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.abinitio.ABInitio.respterm [inherited] Definition at line 1140 of file abinitio.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.abinitio.ABInitio.save_vmvales [inherited] Save the mvales from the last time we updated the vsites.

Definition at line 168 of file abinitio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.abinitio.ABInitio.tq_err [inherited] Definition at line 1042 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_err_pct [inherited] Definition at line 143 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_ref [inherited] Definition at line 1041 of file abinitio.py.

forcebalance.abinitio.ABInitio.use_nft [inherited] Whether to compute net forces and torques, or not.

Definition at line 145 of file abinitio.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.abinitio.ABInitio.w_energy [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_force [inherited] Definition at line 362 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_netforce [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_resp [inherited] Definition at line 1054 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_torque [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.whamboltz [inherited] Definition at line 382 of file abinitio.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

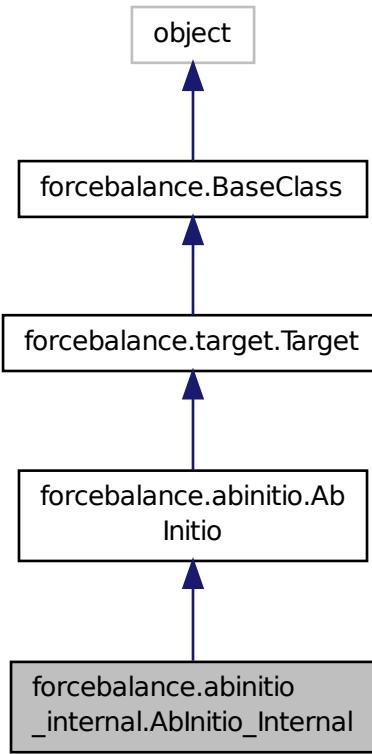
The documentation for this class was generated from the following file:

- [gmxio.py](#)

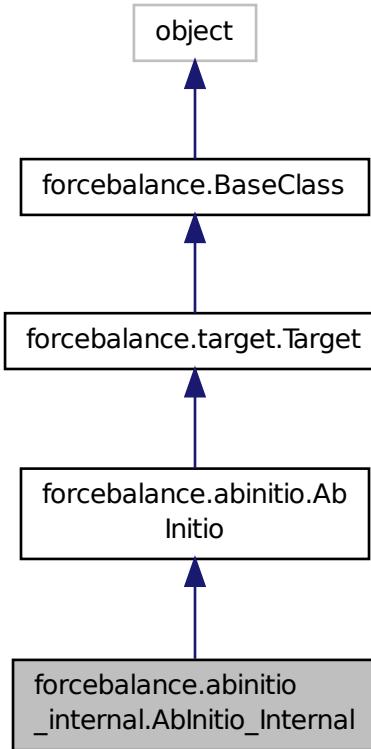
8.4 forcebalance.abinitio_internal.ABInitio_Internal Class Reference

Subclass of Target for force and energy matching using an internal implementation.

Inheritance diagram for forcebalance.abinitio_internal.AbInitio_Internal:



Collaboration diagram for forcebalance.abinitio_internal.AbInitio_Internal:



Public Member Functions

- def `_init_`
- def `energy_force_driver_all`

Here we actually compute the interactions and return the energies and forces.

- def `build_invdist`
- def `compute_netforce_torque`
- def `read_reference_data`

Read the reference ab initio data from a file such as qdata.txt.

- def `indicate`
- def `energy_all`
- def `energy_force_all`
- def `energy_force_transform`
- def `energy_one`
- def `energy_force_one`
- def `energy_force_transform_one`
- def `get_energy_force`

LPW 06-30-2013.

- def `get_resp`
Electrostatic potential fitting.
- def `get`
- def `get_X`
Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
Computes the objective function contribution and its gradient.
- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `coords`
Name of the trajectory, we need this BEFORE initializing the SuperClass.
- `boltz_wts`
Initialize the base class.
- `qm_boltz_wts`
QM Boltzmann weights.
- `eqm`
Reference (QM) energies.

- **emd0**
Energies of the sampling simulation.
- **fqm**
Reference (QM) forces.
- **espxyz**
ESP grid points.
- **espval**
ESP values.
- **qfnm**
The qdata.txt file that contains the QM energies and forces.
- **qatoms**
The number of atoms in the QM calculation (Irrelevant if not fitting forces)
- **e_err**
Qualitative Indicator: average energy error (in kJ/mol)
- **e_err_pct**
- **f_err**
Qualitative Indicator: average force error (fractional)
- **f_err_pct**
- **esp_err**
Qualitative Indicator: "relative RMS" for electrostatic potential.
- **nf_err**
- **nf_err_pct**
- **tq_err_pct**
- **use_nft**
Whether to compute net forces and torques, or not.
- **ns**
Read in the trajectory file.
- **mol**
- **nparticles**
The number of (atoms + drude particles + virtual sites)
- **engine**
Build keyword dictionaries to pass to engine.
- **AtomLists**
Lists of atoms to do net force/torque fitting and excluding virtual sites.
- **AtomMask**
- **new_vsites**
Read in the reference data.
- **save_vmvalls**
Save the mvalls from the last time we updated the vsites.
- **force_map**
- **nnf**
- **ntq**
- **force**
- **w_force**
- **nesp**
- **fitatoms**
- **whamboltz**
- **nftqm**

- `fref`
- `w_energy`
- `w_netforce`
- `w_torque`
- `e_ref`
- `f_ref`
- `nf_ref`
- `tq_ref`
- `tq_err`
- `w_resp`
- `invdists`
- `respterm`
- `objective`
- `rd`
`Root directory of the whole project.`
- `pgrad`
`Iteration where we turn on zero-gradient skipping.`
- `tempbase`
`Relative directory of target.`
- `tempdir`
- `rundir`
`self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.`
- `FF`
`Need the forcefield (here for now)`
- `xct`
`Counts how often the objective function was computed.`
- `gct`
`Counts how often the gradient was computed.`
- `hct`
`Counts how often the Hessian was computed.`
- `read_indicate`
`Whether to read indicate.log from file when restarting an aborted run.`
- `write_indicate`
`Whether to write indicate.log at every iteration (true for all but remote.)`
- `read_objective`
`Whether to read objective.p from file when restarting an aborted run.`
- `write_objective`
`Whether to write objective.p at every iteration (true for all but remote.)`
- `verbose_options`
- `PrintOptionDict`

8.4.1 Detailed Description

Subclass of Target for force and energy matching using an internal implementation.

Implements the `prepare` and `energy_force_driver` methods. The `get` method is in the superclass.

The purpose of this class is to provide an extremely simple test case that does not require the user to install any external software. It only runs with one of the included sample test calculations (`internal_tip3p`), and the objective function is energy matching.

Warning

This class is only intended to work with a very specific test case (internal.tip3p). This is because the topology and ordering of the atoms is hard-coded (12 water molecules with 3 atoms each).

This class does energy matching only (no forces)

Definition at line 37 of file abinitio_internal.py.

8.4.2 Constructor & Destructor Documentation

def forcebalance.abinitio_internal.AbInitio_Internal.__init__ (self, options, tgt_opts, forcefield) Definition at line 40 of file abinitio_internal.py.

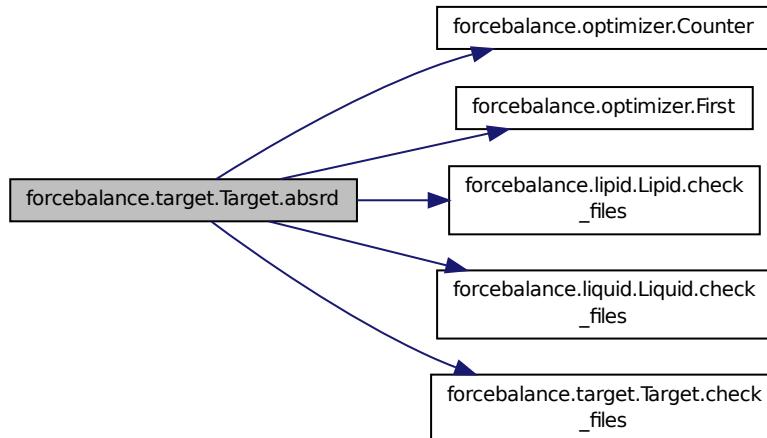
8.4.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited] Definition at line 28 of file __init__.py.

def forcebalance.target.Target.absrd (self, inum = None) [inherited] Supply the correct directory specified by user's "read" option.

Definition at line 393 of file target.py.

Here is the call graph for this function:



def forcebalance.abinitio.AbInitio.build_invdist (self, mvals) [inherited] Definition at line 171 of file abinitio.py.

def forcebalance.target.Target.check_files (self, there) [inherited] Check this directory for the presence of readable files when the 'read' option is set.

Definition at line 364 of file target.py.

def forcebalance.abinitio.AbInitio.compute_netforce_torque (self, xyz, force, QM = False) [inherited] Definition at line 200 of file abinitio.py.

```
def forcebalance.abinitio.AbInitio.energy_all( self ) [inherited] Definition at line 472 of file abinitio.py.
```

```
def forcebalance.abinitio.AbInitio.energy_force_all( self ) [inherited] Definition at line 478 of file abinitio.py.
```

def forcebalance.abinitio_internal.AbInitio_Internal.energy_force_driver_all (self) Here we actually compute the interactions and return the energies and forces.

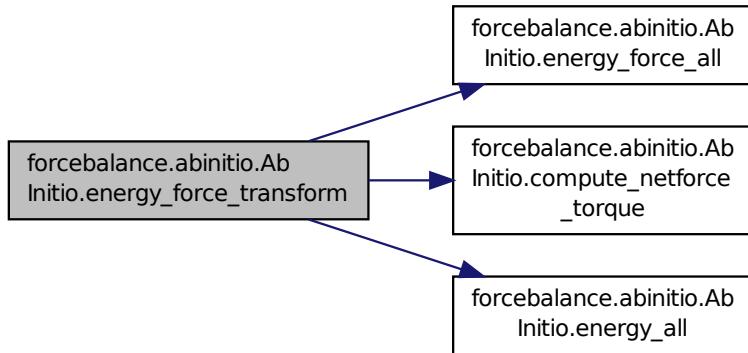
I verified this to give the same answer as GROMACS.

Definition at line 50 of file abinitio_internal.py.

```
def forcebalance.abinitio.AbInitio.energy_force_one ( self, i ) [inherited] Definition at line 507 of file abinitio.py.
```

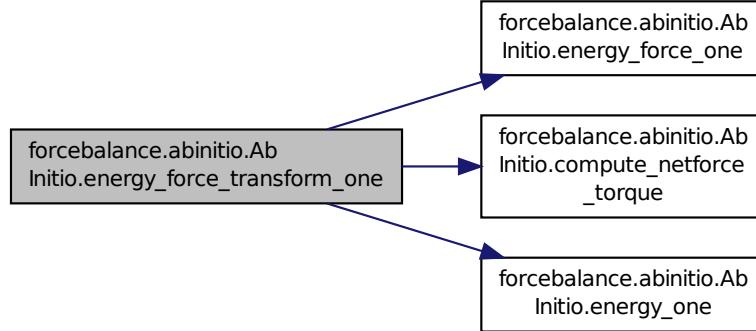
```
def forcebalance.abinitio.AbInitio.energy_force_transform ( self ) [inherited] Definition at line 484 of file abinitio.py.
```

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.energy_force_transform_one ( self, i ) [inherited] Definition at line 513 of file abinitio.py.
```

Here is the call graph for this function:

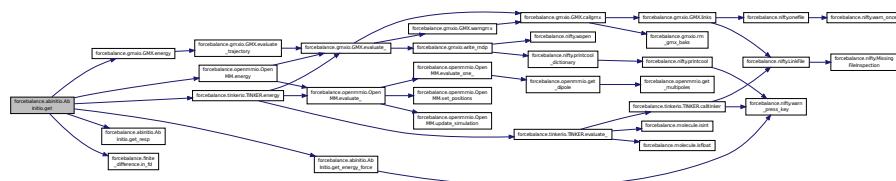


def forcebalance.abinitio.AbInitio.energy_one (self, i) [inherited] Definition at line 501 of file abinitio.py.

def forcebalance.abinitio.AbInitio.get (self, mvals, AGrad = False, AHess = False) [inherited]

Definition at line 1152 of file abinitio.py.

Here is the call graph for this function:



def forcebalance.abinitio.AbInitio.get_energy_force (self, mvals, AGrad = False, AHess = False) [inherited] LPW 06-30-2013.

This subroutine builds the objective function (and optionally its derivatives) from a general simulation software. This is in contrast to using GROMACS-X2, which computes the objective function and prints it out; then 'get' only needs to call GROMACS and read it in.

This subroutine interfaces with simulation software 'drivers'. The driver is only expected to give the energy and forces.

Now this subroutine may sound trivial since the objective function is simply a least-squares quantity $(M-Q)^2$ - but there are a number of nontrivial considerations. I will list them here.

0) Polytensor formulation: Because there may exist covariance between different components of the force (or covariance between the energy and the force), we build the objective function by taking outer products of vectors that have the form $[E \ F_{1x} \ F_{1y} \ F_{1z} \ F_{2x} \ F_{2y} \dots]$, and then we trace it with the inverse of the covariance matrix to get the objective function.

This version implements both the polytensor formulation and the standard formulation.

1) Boltzmann weights and normalization: Each snapshot has its own Boltzmann weight, which may or may not be normalized. This subroutine does the normalization automatically.

2) Subtracting out the mean energy gap: The zero-point energy difference between reference data and simulation is meaningless. This subroutine subtracts it out.

3) Hybrid ensembles: This program builds a combined objective function from both MM and QM ensembles, which is rigorously better than using a single ensemble.

Note that this subroutine does not do EVERYTHING that GROMACS-X2 can do, which includes:

1) Internal coordinate systems 2) 'Sampling correction' (deprecated, since it doesn't seem to work) 3) Analytic derivatives

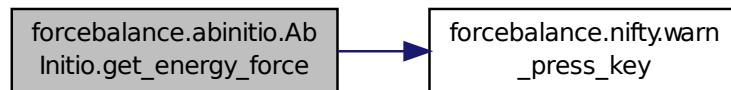
In the previous code (ForTune) this subroutine used analytic first derivatives of the energy and force to build the derivatives of the objective function. Here I will take a simplified approach, because building the derivatives are cumbersome. For now we will return the objective function ONLY. A two-point central difference should give us the first and diagonal second derivative anyhow.

Todo Parallelization over snapshots is not implemented yet

```
@param[in] mvals Mathematical parameter values
@param[in] AGrad Switch to turn on analytic gradient
@param[in] AHess Switch to turn on analytic Hessian
@return Answer Contribution to the objective function
```

Definition at line 588 of file abinitio.py.

Here is the call graph for this function:



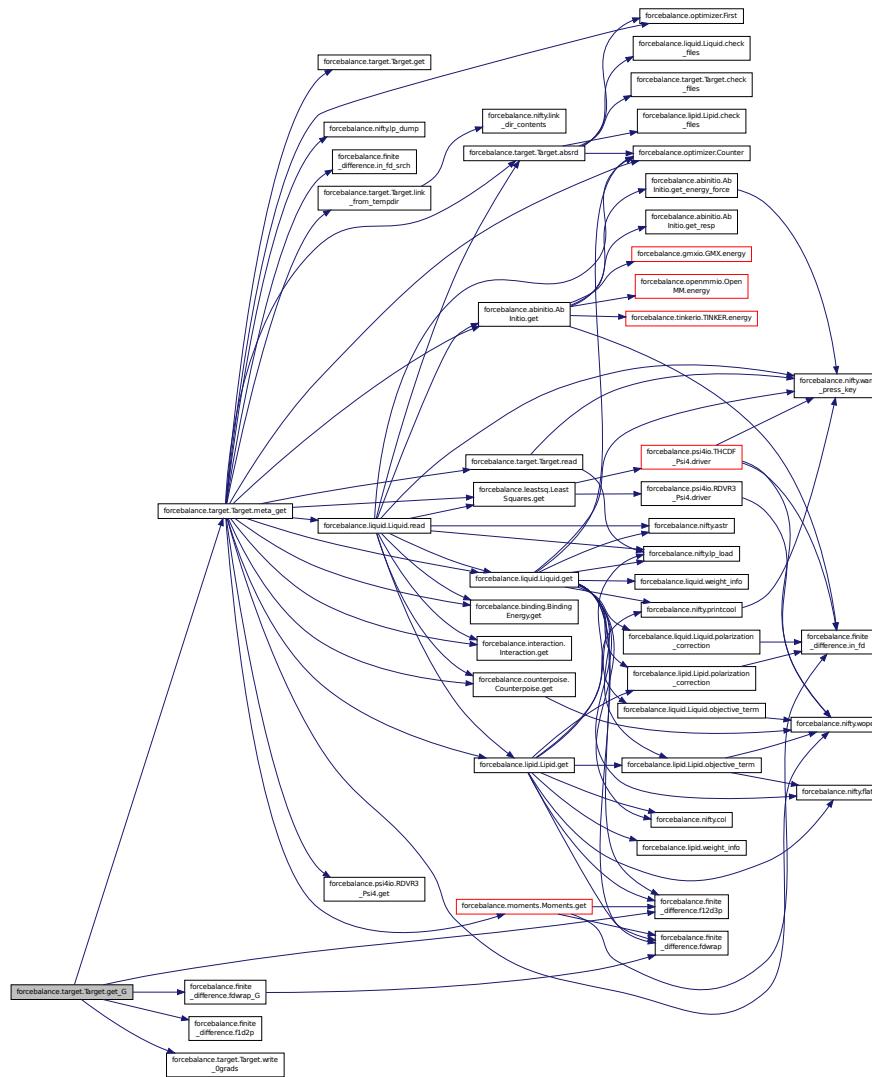
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



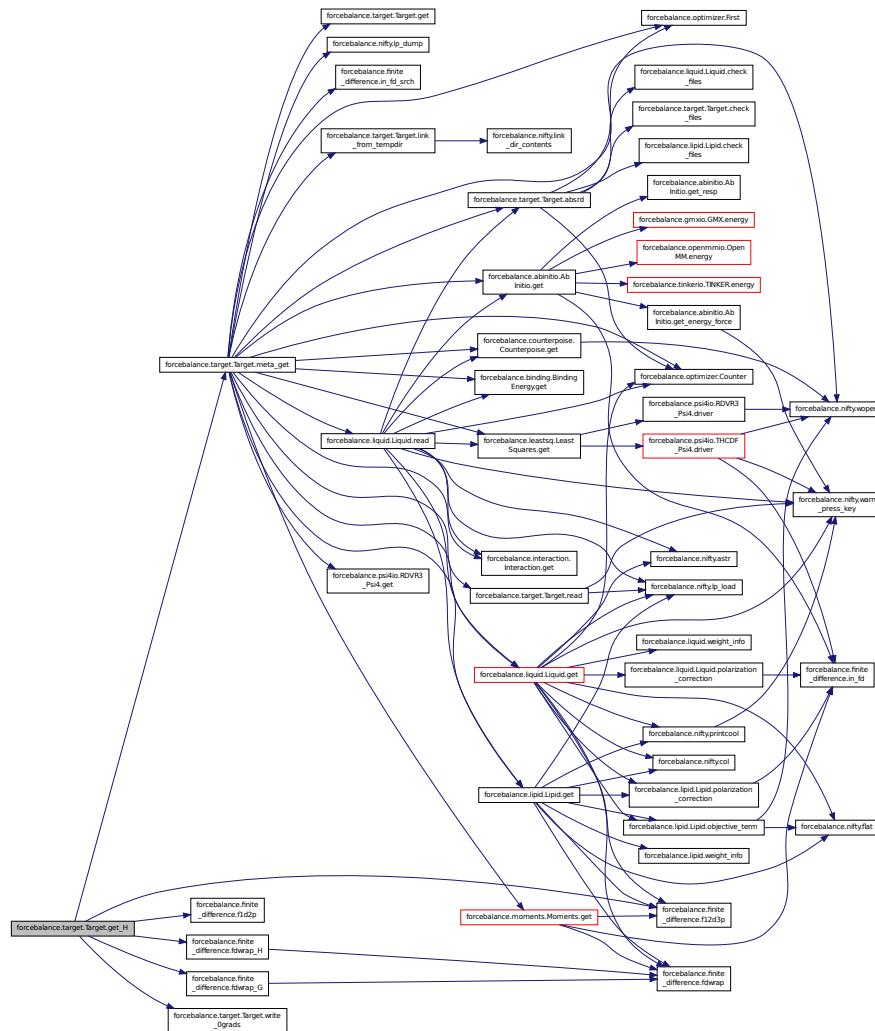
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.get_resp ( self, mvals, AGrad = False, AHess = False )
[inherited] Electrostatic potential fitting.
```

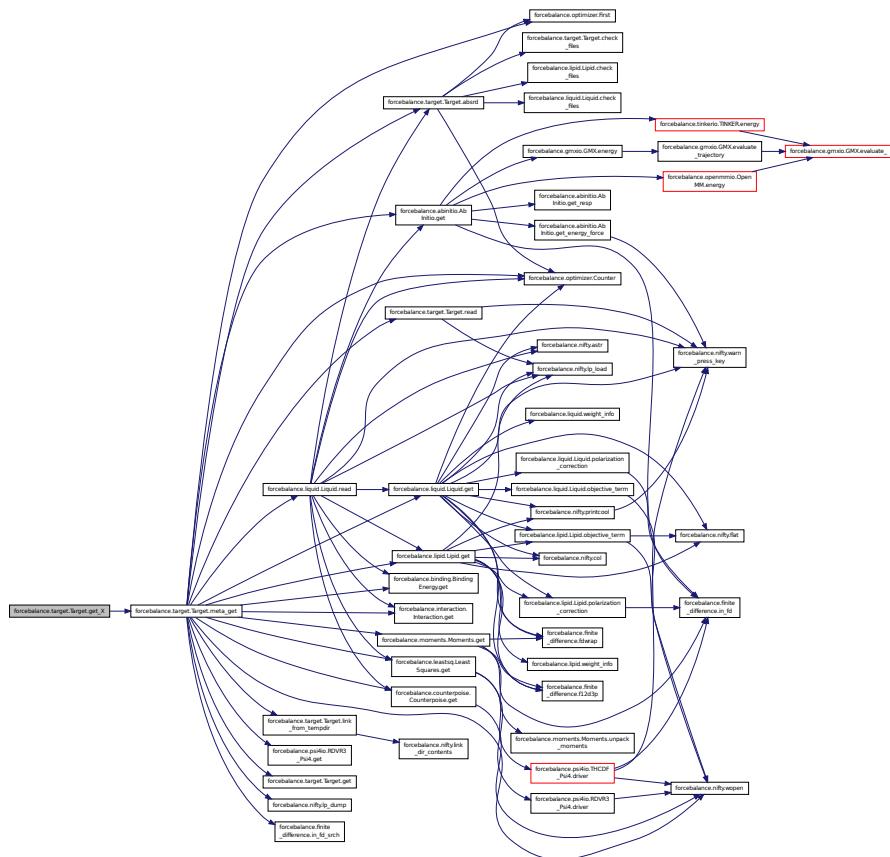
Implements the RESP objective function. (In Python so obviously not optimized.) This function takes the mathematical parameter values and returns the charges on the ATOMS (fancy mapping going on)

Definition at line 1053 of file abinitio.py.

```
def forcebalance.target.Target.get_X ( self, mvals = None ) [inherited] Computes the objective function contribution without any parametric derivatives.
```

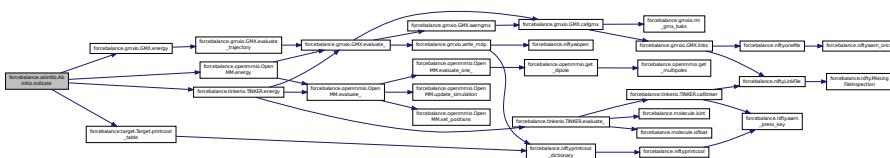
Definition at line 184 of file target.py.

Here is the call graph for this function:



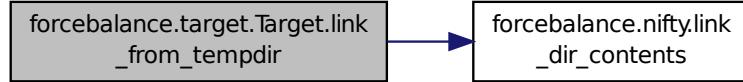
def forcebalance.abinitio.ABInitio.indicate (self) [inherited] Definition at line 448 of file abinitio.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.link_from_tempdir( self, absdestdir ) [inherited] Definition at line 315 of file target.py.
```

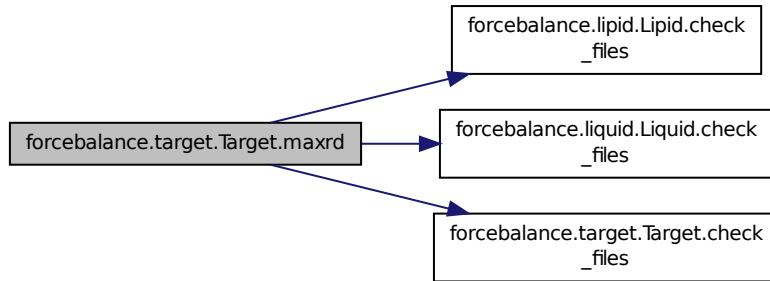
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

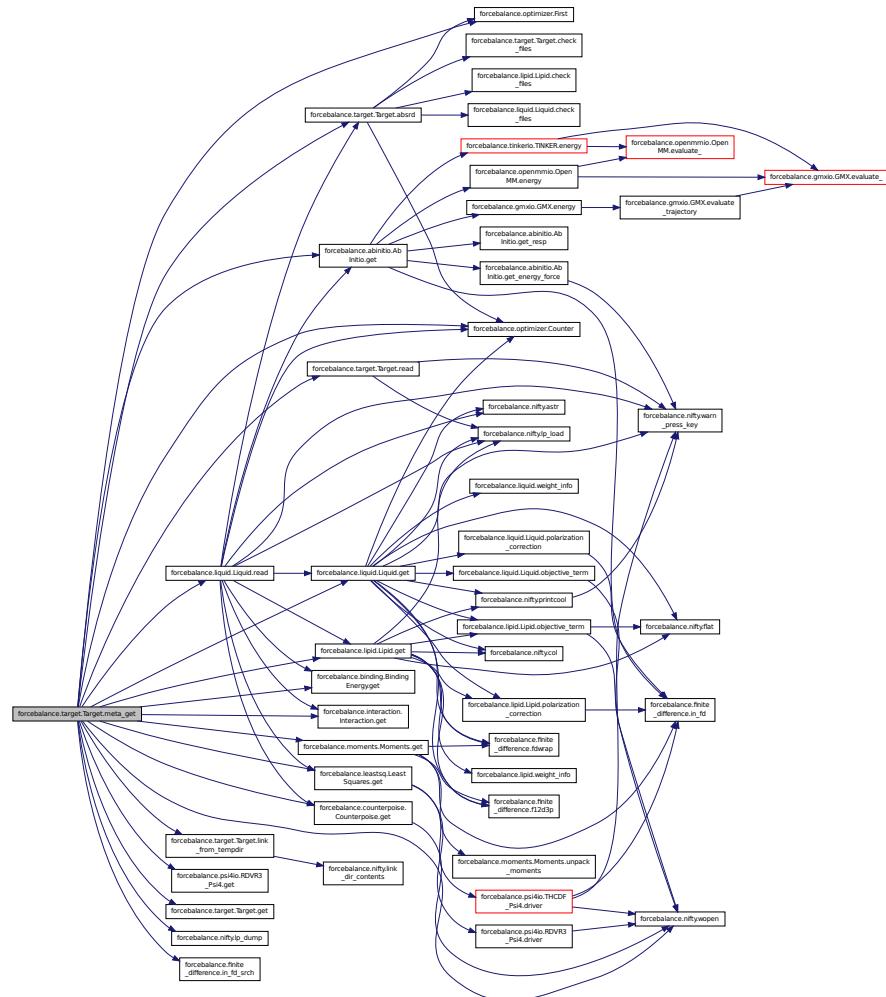


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

Here is the call graph for this function:

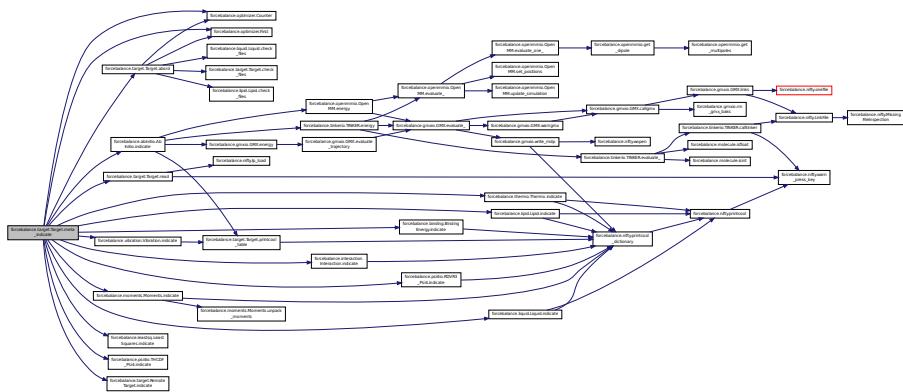


def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.

Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

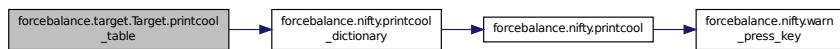
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

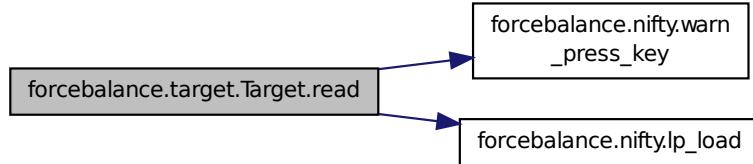
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.abinitio.AblInitio.read_reference_data (self) [inherited] Read the reference ab initio data from a file such as qdata.txt.

Todo Add an option for picking any slice out of qdata.txt, helpful for cross-validation

Todo Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

After reading in the information from qdata.txt, it is converted into the GROMACS energy units (kind of an arbitrary choice); forces (kind of a misnomer in qdata.txt) are multiplied by -1 to convert gradients to forces.

We also subtract out the mean energies of all energy arrays because energy/force matching does not account for zero-point energy differences between MM and QM (i.e. energy of electrons in core orbitals).

The configurations in force/energy matching typically come from a the thermodynamic ensemble of the MM force field at some temperature (by running MD, for example), and for many reasons it is helpful to introduce non-Boltzmann weights in front of these configurations. There are two options: WHAM Boltzmann weights (for combining the weights of several simulations together) and QM Boltzmann weights (for converting MM weights into QM weights). Note that the two sets of weights 'stack'; i.e. they can be used at the same time.

A 'hybrid' ensemble is possible where we use 50% MM and 50% QM weights. Please read more in LPW and Troy Van Voorhis, JCP Vol. 133, Pg. 231101 (2010), doi:10.1063/1.3519043.

Todo The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Finally, note that using non-Boltzmann weights degrades the statistical information content of the snapshots. This problem will generally become worse if the ensemble to which we're reweighting is dramatically different from the one we're sampling from. We end up with a set of Boltzmann weights like [1e-9, 1e-9, 1.0, 1e-9, 1e-9 ...] and this is essentially just one snapshot. I believe Troy is working on something to cure this problem.

Here, we have a measure for the information content of our snapshots, which comes easily from the definition of information entropy:

```
S = -1*Sum_i(P_i*log(P_i))
InfoContent = exp(-S)
```

With uniform weights, InfoContent is equal to the number of snapshots; with horrible weights, InfoContent is closer to one.

Definition at line 329 of file abinitio.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

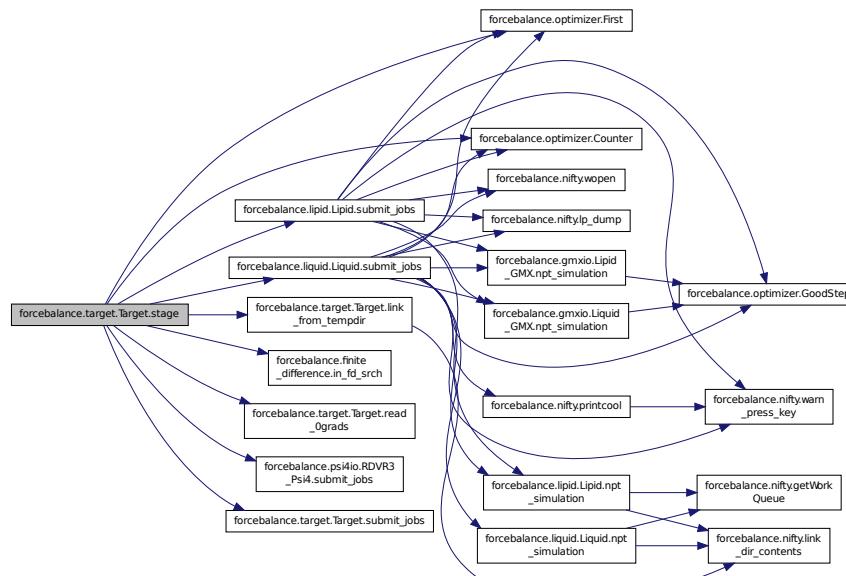
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

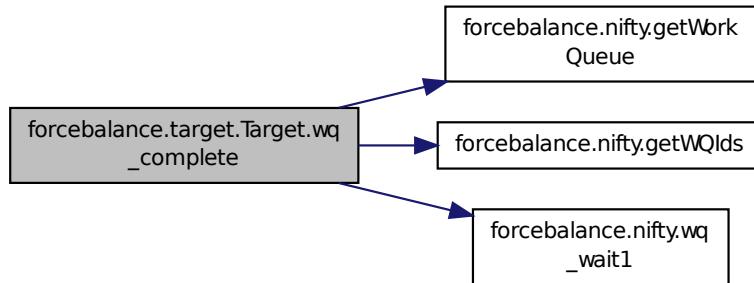


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work  
Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_Ograds ( self, Ans ) [inherited] Write a file to the target directory  
containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.4.4 Member Data Documentation

```
forcebalance.abinitio.AblInitio.AtomLists [inherited] Lists of atoms to do net force/torque fitting and excluding virtual sites.
```

Definition at line 160 of file abinitio.py.

```
forcebalance.abinitio.AblInitio.AtomMask [inherited] Definition at line 161 of file abinitio.py.
```

```
forcebalance.abinitio.AblInitio.boltz_wts [inherited] Initialize the base class.
```

Number of snapshots Whether to use WHAM Boltzmann weights Whether to use the Sampling Correction Whether to match Absolute Energies (make sure you know what you're doing) Whether to use the Covariance Matrix Whether to use QM Boltzmann weights The temperature for QM Boltzmann weights Number of atoms that we are fitting Whether to fit Energies. Whether to fit Forces. Whether to fit Electrostatic Potential. Weights for the three components. Option for how much data to write to disk. Whether to do energy and force calculations for the whole trajectory, or to do one calculation per snapshot. OpenMM-only option - whether to run the energies and forces internally. Whether we have virtual sites (set at the global option level) Attenuate the weights as a function of energy What is the energy denominator? (Valid for 'attenuate') Set upper cutoff energy WHAM Boltzmann weights

Definition at line 116 of file abinitio.py.

```
forcebalance.abinitio_internal.AblInitio_Internal.coords Name of the trajectory, we need this BEFORE initializing  
the SuperClass.
```

Definition at line 42 of file abinitio_internal.py.

forcebalance.abinitio.AbInitio.e_err [inherited] Qualitative Indicator: average energy error (in kJ/mol)
Definition at line 134 of file abinitio.py.

forcebalance.abinitio.AbInitio.e_err_pct [inherited] Definition at line 135 of file abinitio.py.

forcebalance.abinitio.AbInitio.e_ref [inherited] Definition at line 1030 of file abinitio.py.

forcebalance.abinitio.AbInitio.emd0 [inherited] Energies of the sampling simulation.
Definition at line 122 of file abinitio.py.

forcebalance.abinitio.AbInitio.engine [inherited] Build keyword dictionaries to pass to engine.
Create engine object.
Definition at line 158 of file abinitio.py.

forcebalance.abinitio.AbInitio.eqm [inherited] Reference (QM) energies.
Definition at line 120 of file abinitio.py.

forcebalance.abinitio.AbInitio.esp_err [inherited] Qualitative Indicator: "relative RMS" for electrostatic potential.
Definition at line 140 of file abinitio.py.

forcebalance.abinitio.AbInitio.espval [inherited] ESP values.
Definition at line 128 of file abinitio.py.

forcebalance.abinitio.AbInitio.espxyz [inherited] ESP grid points.
Definition at line 126 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err [inherited] Qualitative Indicator: average force error (fractional)
Definition at line 137 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err_pct [inherited] Definition at line 138 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_ref [inherited] Definition at line 1034 of file abinitio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.abinitio.AbInitio.fitatoms [inherited] Definition at line 366 of file abinitio.py.

forcebalance.abinitio.AbInitio.force [inherited] Definition at line 361 of file abinitio.py.

forcebalance.abinitio.AbInitio.force_map [inherited] Definition at line 209 of file abinitio.py.

forcebalance.abinitio.AbInitio.fqm [inherited] Reference (QM) forces.
Definition at line 124 of file abinitio.py.

forcebalance.abinitio.AbInitio.fref [inherited] Definition at line 442 of file abinitio.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.abinitio.ABInitio.invdists [inherited] Definition at line 1061 of file abinitio.py.

forcebalance.abinitio.ABInitio.mol [inherited] Definition at line 148 of file abinitio.py.

forcebalance.abinitio.ABInitio.nesp [inherited] Definition at line 363 of file abinitio.py.

forcebalance.abinitio.ABInitio.new_vsites [inherited] Read in the reference data.

The below two options are related to whether we want to rebuild virtual site positions. Rebuild the distance matrix if virtual site positions have changed

Definition at line 166 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err [inherited] Definition at line 141 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err_pct [inherited] Definition at line 142 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_ref [inherited] Definition at line 1038 of file abinitio.py.

forcebalance.abinitio.ABInitio.nftqm [inherited] Definition at line 438 of file abinitio.py.

forcebalance.abinitio.ABInitio.nnf [inherited] Definition at line 267 of file abinitio.py.

forcebalance.abinitio.ABInitio.nparticles [inherited] The number of (atoms + drude particles + virtual sites)
Definition at line 153 of file abinitio.py.

forcebalance.abinitio.ABInitio.ns [inherited] Read in the trajectory file.
Definition at line 147 of file abinitio.py.

forcebalance.abinitio.ABInitio.ntq [inherited] Definition at line 268 of file abinitio.py.

forcebalance.abinitio.ABInitio.objective [inherited] Definition at line 1172 of file abinitio.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.
Dictionary of whether to call the derivatives.
Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.abinitio.ABInitio.qfnm [inherited] The qdata.txt file that contains the QM energies and forces.
Definition at line 130 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmatoms [inherited] The number of atoms in the QM calculation (Irrelevant if not fitting forces)
Definition at line 132 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmboltz_wts [inherited] QM Boltzmann weights.

Definition at line 118 of file abinitio.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.abinitio.ABInitio.respterm [inherited] Definition at line 1140 of file abinitio.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number. The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.abinitio.ABInitio.save_mvvals [inherited] Save the mvvals from the last time we updated the vsites.

Definition at line 168 of file abinitio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.abinitio.ABInitio.tq_err [inherited] Definition at line 1042 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_err_pct [inherited] Definition at line 143 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_ref [inherited] Definition at line 1041 of file abinitio.py.

forcebalance.abinitio.ABInitio.use_nft [inherited] Whether to compute net forces and torques, or not.

Definition at line 145 of file abinitio.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.abinitio.ABInitio.w.energy [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w.force [inherited] Definition at line 362 of file abinitio.py.

forcebalance.abinitio.ABInitio.w.netforce [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w.resp [inherited] Definition at line 1054 of file abinitio.py.

forcebalance.abinitio.ABInitio.w.torque [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.whamboltz [inherited] Definition at line 382 of file abinitio.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

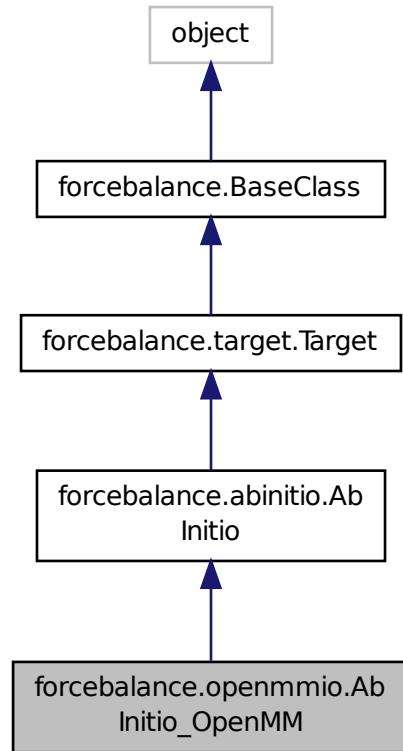
The documentation for this class was generated from the following file:

- [abinitio_internal.py](#)

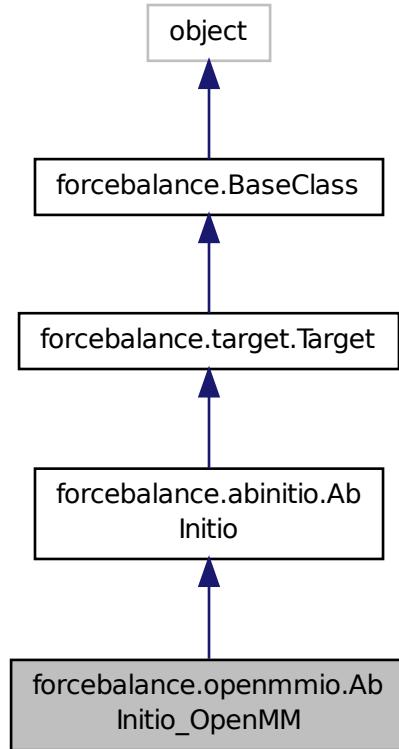
8.5 forcebalance.openmmio.ABInitio_OpenMM Class Reference

Force and energy matching using [OpenMM](#).

Inheritance diagram for forcebalance.openmmio.AbInitio_OpenMM:



Collaboration diagram for forcebalance.openmmio.AbInitio_OpenMM:



Public Member Functions

- def `_init_`
- def `build_invdist`
- def `compute_netforce_torque`
- def `read_reference_data`

Read the reference ab initio data from a file such as qdata.txt.
- def `indicate`
- def `energy_all`
- def `energy_force_all`
- def `energy_force_transform`
- def `energy_one`
- def `energy_force_one`
- def `energy_force_transform_one`
- def `get_energy_force`

LPW 06-30-2013.
- def `get_resp`

Electrostatic potential fitting.

- def `get`
 Computes the objective function contribution without any parametric derivatives.
- def `get_X`
 Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `read_0grads`
 Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`
 Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
 Computes the objective function contribution and its gradient.
- def `get_H`
 Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
 Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
 Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
 Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
 Supply the correct directory specified by user's "read" option.
- def `maxrd`
 Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
 Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
 Wrapper around the get function.
- def `submit_jobs`
- def `stage`
 Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
 This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
 Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
 Default file names for coordinates and key file.
- `boltz_wts`
 Initialize the base class.
- `qmboltz_wts`
 QM Boltzmann weights.
- `eqm`
 Reference (QM) energies.
- `emd0`
 Energies of the sampling simulation.

- **fqm**
Reference (QM) forces.
- **espxyz**
ESP grid points.
- **espval**
ESP values.
- **qfnm**
The qdata.txt file that contains the QM energies and forces.
- **qatoms**
The number of atoms in the QM calculation (Irrelevant if not fitting forces)
- **e_err**
Qualitative Indicator: average energy error (in kJ/mol)
- **e_err_pct**
- **f_err**
Qualitative Indicator: average force error (fractional)
- **f_err_pct**
- **esp_err**
Qualitative Indicator: "relative RMS" for electrostatic potential.
- **nf_err**
- **nf_err_pct**
- **tq_err_pct**
- **use_nft**
Whether to compute net forces and torques, or not.
- **ns**
Read in the trajectory file.
- **mol**
- **nparticles**
The number of (atoms + drude particles + virtual sites)
- **engine**
Build keyword dictionaries to pass to engine.
- **AtomLists**
Lists of atoms to do net force/torque fitting and excluding virtual sites.
- **AtomMask**
- **new_vsites**
Read in the reference data.
- **save_vmvabs**
Save the mvabs from the last time we updated the vsites.
- **force_map**
- **nnf**
- **ntq**
- **force**
- **w_force**
- **nesp**
- **fitatoms**
- **whamboltz**
- **nftqm**
- **fref**
- **w_energy**

- `w_netforce`
- `w_torque`
- `e_ref`
- `f_ref`
- `nf_ref`
- `tq_ref`
- `tq_err`
- `w_resp`
- `invdists`
- `respterm`
- `objective`
- `rd`

Root directory of the whole project.
- `pgrad`

Iteration where we turn on zero-gradient skipping.
- `tempbase`

Relative directory of target.
- `tempdir`
- `rundir`

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- `FF`

Need the forcefield (here for now)
- `xct`

Counts how often the objective function was computed.
- `gct`

Counts how often the gradient was computed.
- `hct`

Counts how often the Hessian was computed.
- `read_indicate`

Whether to read indicate.log from file when restarting an aborted run.
- `write_indicate`

Whether to write indicate.log at every iteration (true for all but remote.)
- `read_objective`

Whether to read objective.p from file when restarting an aborted run.
- `write_objective`

Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.5.1 Detailed Description

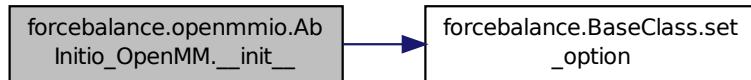
Force and energy matching using [OpenMM](#).

Definition at line 1166 of file openmmio.py.

8.5.2 Constructor & Destructor Documentation

```
def forcebalance.openmmio.ABInitio_OpenMM.__init__( self, options, tgt_opts, forcefield ) Definition at line 1167 of file openmmio.py.
```

Here is the call graph for this function:



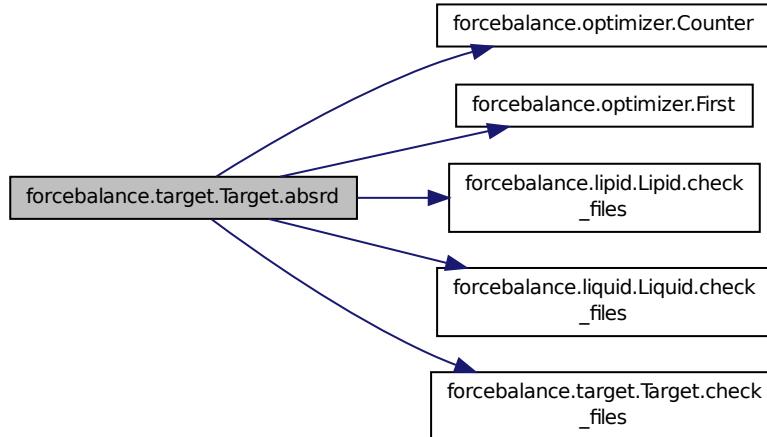
8.5.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.ABInitio.build_invdist( self, mvals ) [inherited] Definition at line 171 of file abinitio.py.
```

```
def forcebalance.target.Target.check_files( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.abinitio.AbInitio.compute_netforce_torque ( self, xyz, force, QM = False )  
[inherited] Definition at line 200 of file abinitio.py.
```

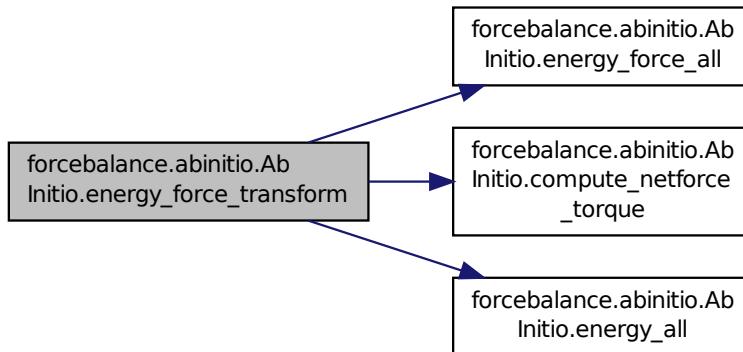
```
def forcebalance.abinitio.AbInitio.energy_all ( self ) [inherited] Definition at line 472 of file abinitio.py.
```

```
def forcebalance.abinitio.AbInitio.energy_force_all ( self ) [inherited] Definition at line 478 of file abinitio.py.
```

```
def forcebalance.abinitio.AbInitio.energy_force_one ( self, i ) [inherited] Definition at line 507 of file abinitio.py.
```

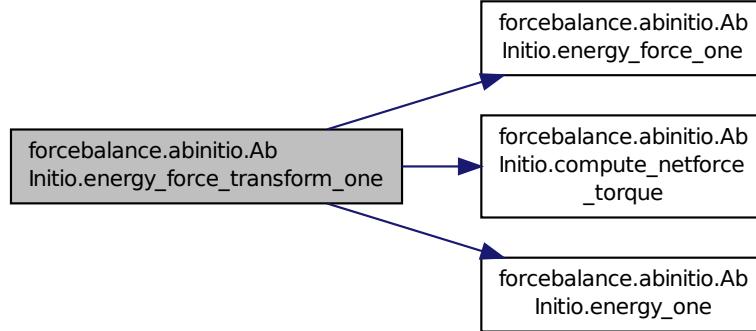
```
def forcebalance.abinitio.AbInitio.energy_force_transform ( self ) [inherited] Definition at line 484 of file abinitio.py.
```

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.energy_force_transform_one ( self, i ) [inherited] Definition at line 513 of file abinitio.py.
```

Here is the call graph for this function:

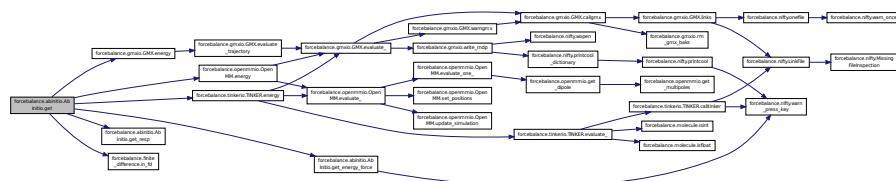


def forcebalance.abinitio.AbInitio.energy_one (self, i) [inherited] Definition at line 501 of file abinitio.py.

def forcebalance.abinitio.AbInitio.get (self, mvals, AGrad = False, AHess = False) [inherited]

Definition at line 1152 of file abinitio.py.

Here is the call graph for this function:



def forcebalance.abinitio.AbInitio.get_energy_force (self, mvals, AGrad = False, AHess = False) [inherited] LPW 06-30-2013.

This subroutine builds the objective function (and optionally its derivatives) from a general simulation software. This is in contrast to using GROMACS-X2, which computes the objective function and prints it out; then 'get' only needs to call GROMACS and read it in.

This subroutine interfaces with simulation software 'drivers'. The driver is only expected to give the energy and forces.

Now this subroutine may sound trivial since the objective function is simply a least-squares quantity $(M-Q)^2$ - but there are a number of nontrivial considerations. I will list them here.

0) Polytensor formulation: Because there may exist covariance between different components of the force (or covariance between the energy and the force), we build the objective function by taking outer products of vectors that have the form $[E \ F_{1x} \ F_{1y} \ F_{1z} \ F_{2x} \ F_{2y} \dots]$, and then we trace it with the inverse of the covariance matrix to get the objective function.

This version implements both the polytensor formulation and the standard formulation.

1) Boltzmann weights and normalization: Each snapshot has its own Boltzmann weight, which may or may not be normalized. This subroutine does the normalization automatically.

2) Subtracting out the mean energy gap: The zero-point energy difference between reference data and simulation is meaningless. This subroutine subtracts it out.

3) Hybrid ensembles: This program builds a combined objective function from both MM and QM ensembles, which is rigorously better than using a single ensemble.

Note that this subroutine does not do EVERYTHING that GROMACS-X2 can do, which includes:

1) Internal coordinate systems 2) 'Sampling correction' (deprecated, since it doesn't seem to work) 3) Analytic derivatives

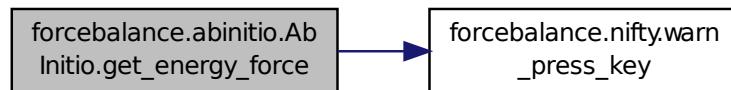
In the previous code (ForTune) this subroutine used analytic first derivatives of the energy and force to build the derivatives of the objective function. Here I will take a simplified approach, because building the derivatives are cumbersome. For now we will return the objective function ONLY. A two-point central difference should give us the first and diagonal second derivative anyhow.

Todo Parallelization over snapshots is not implemented yet

```
@param[in] mvals Mathematical parameter values
@param[in] AGrad Switch to turn on analytic gradient
@param[in] AHess Switch to turn on analytic Hessian
@return Answer Contribution to the objective function
```

Definition at line 588 of file abinitio.py.

Here is the call graph for this function:



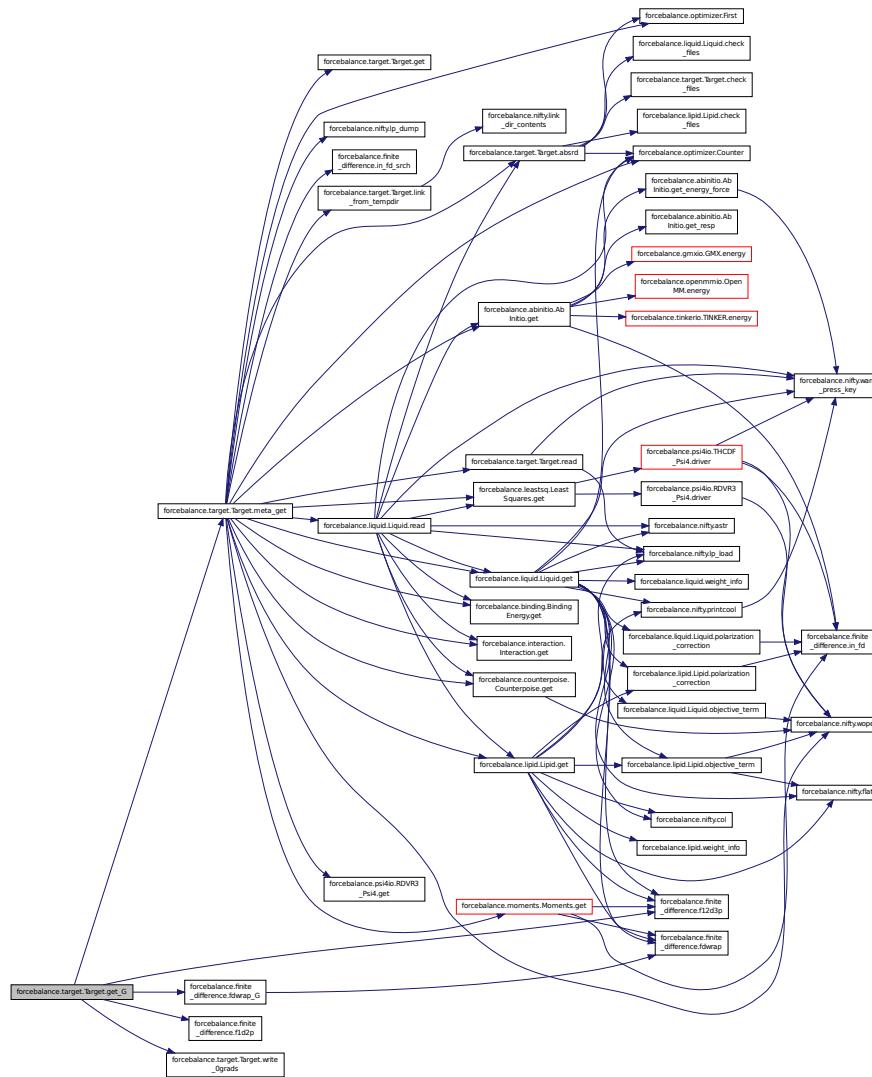
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



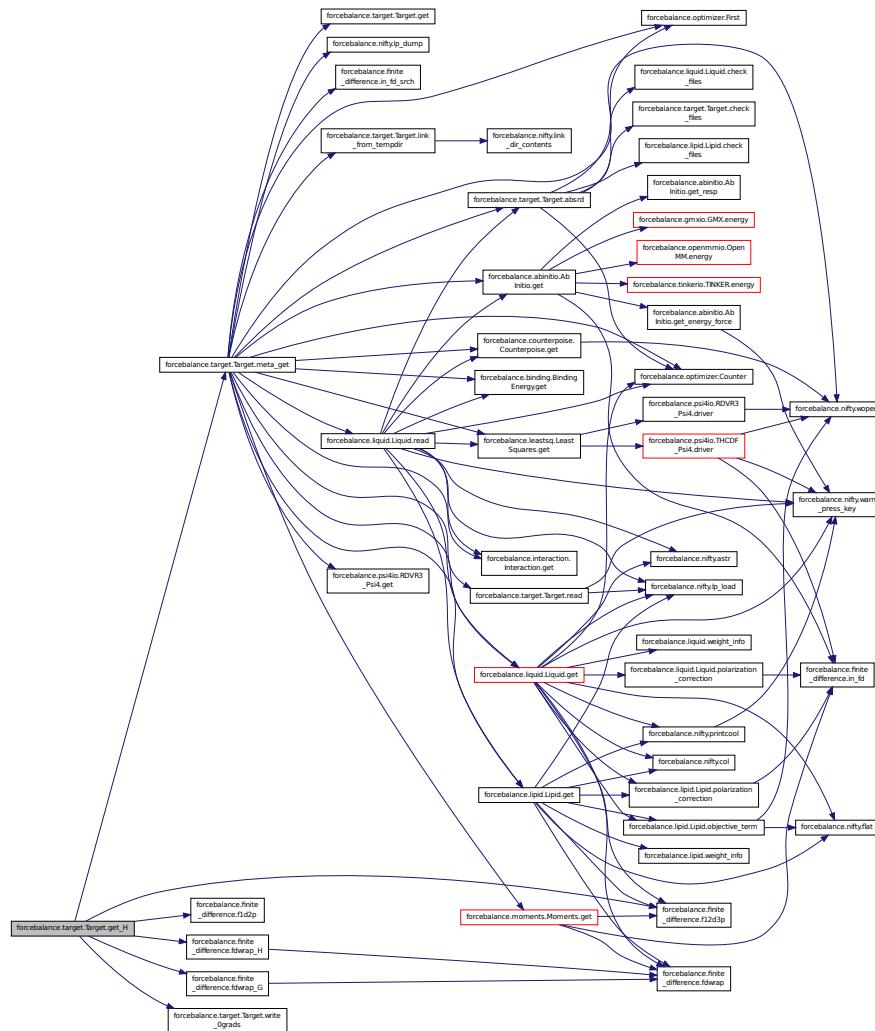
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.get_resp ( self, mvals, AGrad = False, AHess = False )
[inherited] Electrostatic potential fitting.
```

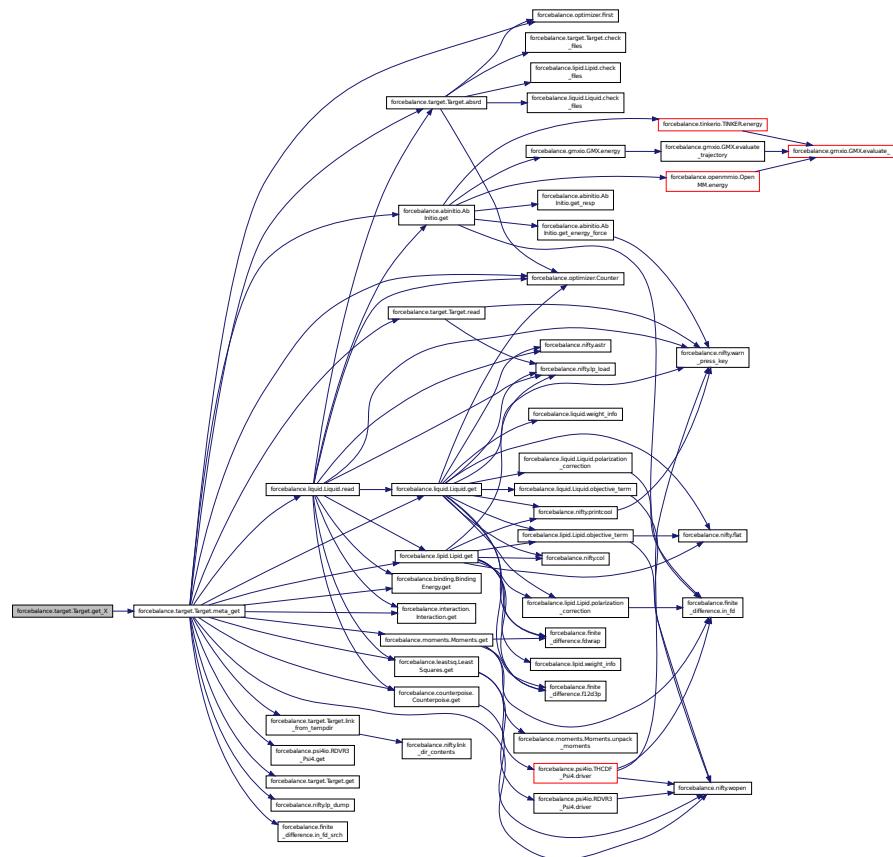
Implements the RESP objective function. (In Python so obviously not optimized.) This function takes the mathematical parameter values and returns the charges on the ATOMS (fancy mapping going on)

Definition at line 1053 of file abinitio.py.

```
def forcebalance.target.Target.get_X ( self, mvals = None ) [inherited] Computes the objective function contribution without any parametric derivatives.
```

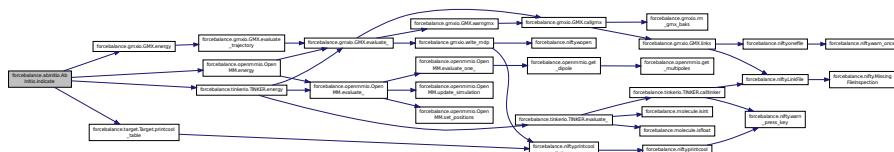
Definition at line 184 of file target.py.

Here is the call graph for this function:



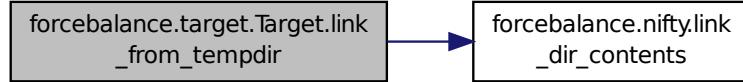
def forcebalance.abinitio.AblInitio.indicate (self) [inherited] Definition at line 448 of file abinitio.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

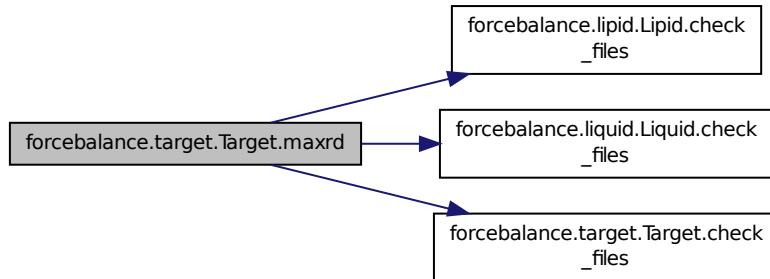
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

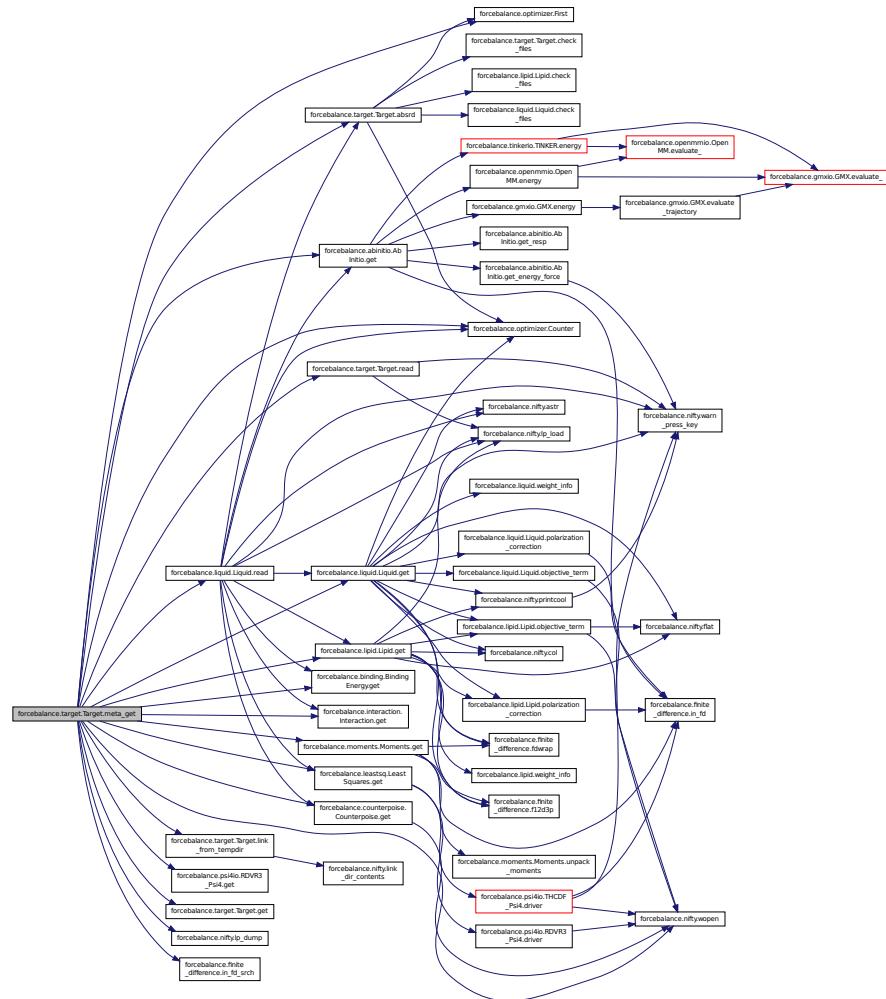


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

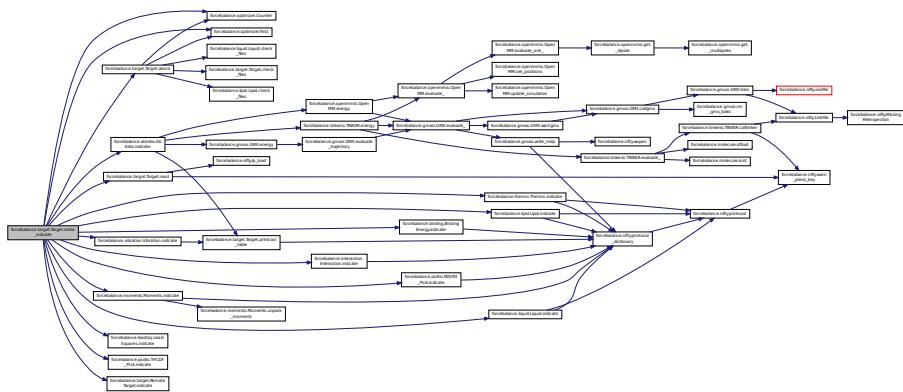
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

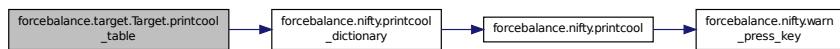
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

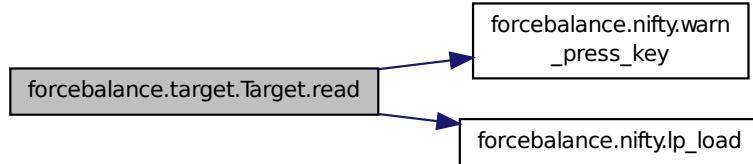
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.abinitio.AblInitio.read_reference_data (self) [inherited] Read the reference ab initio data from a file such as qdata.txt.

Todo Add an option for picking any slice out of qdata.txt, helpful for cross-validation

Todo Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

After reading in the information from qdata.txt, it is converted into the GROMACS energy units (kind of an arbitrary choice); forces (kind of a misnomer in qdata.txt) are multiplied by -1 to convert gradients to forces.

We also subtract out the mean energies of all energy arrays because energy/force matching does not account for zero-point energy differences between MM and QM (i.e. energy of electrons in core orbitals).

The configurations in force/energy matching typically come from a the thermodynamic ensemble of the MM force field at some temperature (by running MD, for example), and for many reasons it is helpful to introduce non-Boltzmann weights in front of these configurations. There are two options: WHAM Boltzmann weights (for combining the weights of several simulations together) and QM Boltzmann weights (for converting MM weights into QM weights). Note that the two sets of weights 'stack'; i.e. they can be used at the same time.

A 'hybrid' ensemble is possible where we use 50% MM and 50% QM weights. Please read more in LPW and Troy Van Voorhis, JCP Vol. 133, Pg. 231101 (2010), doi:10.1063/1.3519043.

Todo The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Finally, note that using non-Boltzmann weights degrades the statistical information content of the snapshots. This problem will generally become worse if the ensemble to which we're reweighting is dramatically different from the one we're sampling from. We end up with a set of Boltzmann weights like [1e-9, 1e-9, 1.0, 1e-9, 1e-9 ...] and this is essentially just one snapshot. I believe Troy is working on something to cure this problem.

Here, we have a measure for the information content of our snapshots, which comes easily from the definition of information entropy:

```
S = -1*Sum_i(P_i*log(P_i))
InfoContent = exp(-S)
```

With uniform weights, InfoContent is equal to the number of snapshots; with horrible weights, InfoContent is closer to one.

Definition at line 329 of file abinitio.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

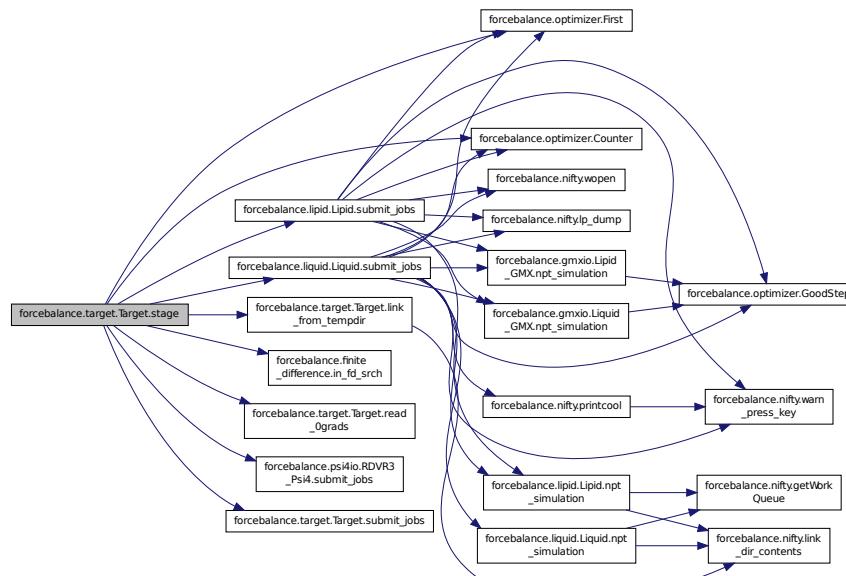
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

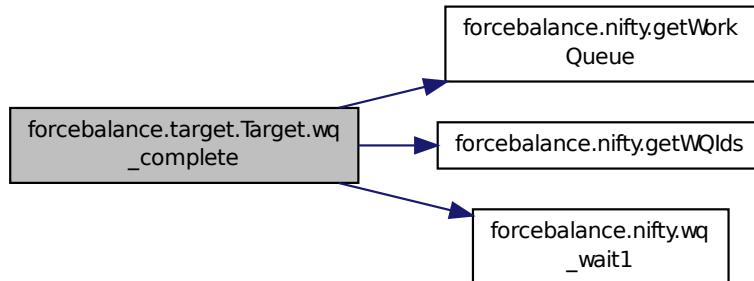


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work  
Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_Ograds ( self, Ans ) [inherited] Write a file to the target directory  
containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.5.4 Member Data Documentation

```
forcebalance.abinitio.ABInitio.AtomLists [inherited] Lists of atoms to do net force/torque fitting and excluding virtual sites.
```

Definition at line 160 of file abinitio.py.

```
forcebalance.abinitio.ABInitio.AtomMask [inherited] Definition at line 161 of file abinitio.py.
```

```
forcebalance.abinitio.ABInitio.boltz_wts [inherited] Initialize the base class.
```

Number of snapshots Whether to use WHAM Boltzmann weights Whether to use the Sampling Correction Whether to match Absolute Energies (make sure you know what you're doing) Whether to use the Covariance Matrix Whether to use QM Boltzmann weights The temperature for QM Boltzmann weights Number of atoms that we are fitting Whether to fit Energies. Whether to fit Forces. Whether to fit Electrostatic Potential. Weights for the three components. Option for how much data to write to disk. Whether to do energy and force calculations for the whole trajectory, or to do one calculation per snapshot. OpenMM-only option - whether to run the energies and forces internally. Whether we have virtual sites (set at the global option level) Attenuate the weights as a function of energy What is the energy denominator? (Valid for 'attenuate') Set upper cutoff energy WHAM Boltzmann weights

Definition at line 116 of file abinitio.py.

```
forcebalance.abinitio.ABInitio.e_err [inherited] Qualitative Indicator: average energy error (in kJ/mol)
```

Definition at line 134 of file abinitio.py.

```
forcebalance.abinitio.ABInitio.e_err_pct [inherited] Definition at line 135 of file abinitio.py.
```

forcebalance.abinitio.AbInitio.e.ref [inherited] Definition at line 1030 of file abinitio.py.

forcebalance.abinitio.AbInitio.emd0 [inherited] Energies of the sampling simulation.
Definition at line 122 of file abinitio.py.

forcebalance.abinitio.AbInitio.engine [inherited] Build keyword dictionaries to pass to engine.
Create engine object.
Definition at line 158 of file abinitio.py.

forcebalance.openmmio.AbInitio_OpenMM.engine Default file names for coordinates and key file.
Definition at line 1173 of file openmmio.py.

forcebalance.abinitio.AbInitio.eqm [inherited] Reference (QM) energies.
Definition at line 120 of file abinitio.py.

forcebalance.abinitio.AbInitio.esp_err [inherited] Qualitative Indicator: "relative RMS" for electrostatic potential.
Definition at line 140 of file abinitio.py.

forcebalance.abinitio.AbInitio.espval [inherited] ESP values.
Definition at line 128 of file abinitio.py.

forcebalance.abinitio.AbInitio.espxyz [inherited] ESP grid points.
Definition at line 126 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err [inherited] Qualitative Indicator: average force error (fractional)
Definition at line 137 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err_pct [inherited] Definition at line 138 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_ref [inherited] Definition at line 1034 of file abinitio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.abinitio.AbInitio.fitatoms [inherited] Definition at line 366 of file abinitio.py.

forcebalance.abinitio.AbInitio.force [inherited] Definition at line 361 of file abinitio.py.

forcebalance.abinitio.AbInitio.force_map [inherited] Definition at line 209 of file abinitio.py.

forcebalance.abinitio.AbInitio.fqm [inherited] Reference (QM) forces.
Definition at line 124 of file abinitio.py.

forcebalance.abinitio.AbInitio.fref [inherited] Definition at line 442 of file abinitio.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.abinitio.ABInitio.invdist [inherited] Definition at line 1061 of file abinitio.py.

forcebalance.abinitio.ABInitio.mol [inherited] Definition at line 148 of file abinitio.py.

forcebalance.abinitio.ABInitio.nesp [inherited] Definition at line 363 of file abinitio.py.

forcebalance.abinitio.ABInitio.new_vsites [inherited] Read in the reference data.

The below two options are related to whether we want to rebuild virtual site positions. Rebuild the distance matrix if virtual site positions have changed

Definition at line 166 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err [inherited] Definition at line 141 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err_pct [inherited] Definition at line 142 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_ref [inherited] Definition at line 1038 of file abinitio.py.

forcebalance.abinitio.ABInitio.nftqm [inherited] Definition at line 438 of file abinitio.py.

forcebalance.abinitio.ABInitio.nnf [inherited] Definition at line 267 of file abinitio.py.

forcebalance.abinitio.ABInitio.nparticles [inherited] The number of (atoms + drude particles + virtual sites)
Definition at line 153 of file abinitio.py.

forcebalance.abinitio.ABInitio.ns [inherited] Read in the trajectory file.

Definition at line 147 of file abinitio.py.

forcebalance.abinitio.ABInitio.ntq [inherited] Definition at line 268 of file abinitio.py.

forcebalance.abinitio.ABInitio.objective [inherited] Definition at line 1172 of file abinitio.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.abinitio.ABInitio.qfnm [inherited] The qdata.txt file that contains the QM energies and forces.
Definition at line 130 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmatoms [inherited] The number of atoms in the QM calculation (Irrelevant if not fitting forces)

Definition at line 132 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmboltz_wts [inherited] QM Boltzmann weights.

Definition at line 118 of file abinitio.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.abinitio.ABInitio.respterm [inherited] Definition at line 1140 of file abinitio.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.abinitio.ABInitio.save_vmvales [inherited] Save the mvales from the last time we updated the vsites.

Definition at line 168 of file abinitio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.abinitio.ABInitio.tq_err [inherited] Definition at line 1042 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_err_pct [inherited] Definition at line 143 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_ref [inherited] Definition at line 1041 of file abinitio.py.

forcebalance.abinitio.ABInitio.use_nft [inherited] Whether to compute net forces and torques, or not.

Definition at line 145 of file abinitio.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.abinitio.ABInitio.w_energy [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_force [inherited] Definition at line 362 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_netforce [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_resp [inherited] Definition at line 1054 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_torque [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.whamboltz [inherited] Definition at line 382 of file abinitio.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

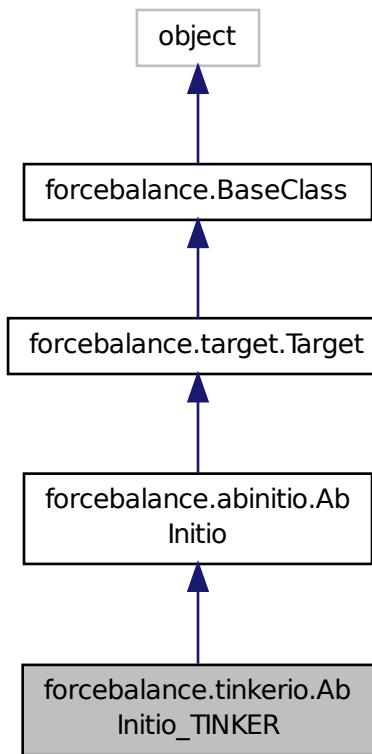
The documentation for this class was generated from the following file:

- [openmmio.py](#)

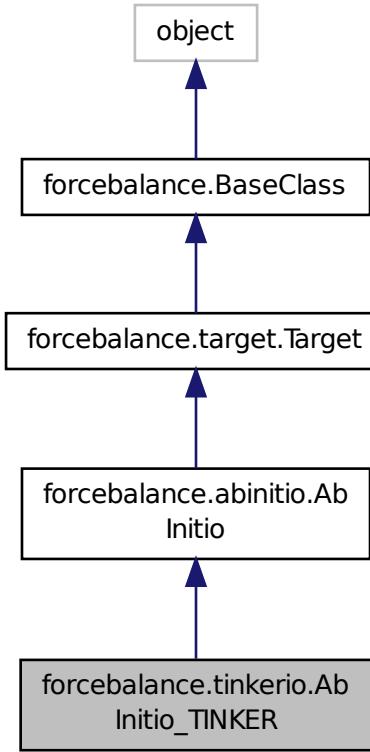
8.6 forcebalance.tinkerio.ABInitio_TINKER Class Reference

Subclass of Target for force and energy matching using [TINKER](#).

Inheritance diagram for forcebalance.tinkerio.AbInitio_TINKER:



Collaboration diagram for forcebalance.tinkerio.AbInitio_TINKER:



Public Member Functions

- def `_init_`
- def `build_invdist`
- def `compute_netforce_torque`
- def `read_reference_data`

Read the reference ab initio data from a file such as qdata.txt.
- def `indicate`
- def `energy_all`
- def `energy_force_all`
- def `energy_force_transform`
- def `energy_one`
- def `energy_force_one`
- def `energy_force_transform_one`
- def `get_energy_force`

LPW 06-30-2013.
- def `get_resp`

Electrostatic potential fitting.

- def `get`
 Computes the objective function contribution without any parametric derivatives.
- def `get_X`
 Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `read_0grads`
 Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`
 Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
 Computes the objective function contribution and its gradient.
- def `get_H`
 Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
 Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
 Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
 Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
 Supply the correct directory specified by user's "read" option.
- def `maxrd`
 Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
 Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
 Wrapper around the get function.
- def `submit_jobs`
- def `stage`
 Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
 This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
 Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
 Default file names for coordinates and key file.
- `boltz_wts`
 Initialize the base class.
- `qmboltz_wts`
 QM Boltzmann weights.
- `eqm`
 Reference (QM) energies.
- `emd0`
 Energies of the sampling simulation.

- **fqm**
Reference (QM) forces.
- **espxyz**
ESP grid points.
- **espval**
ESP values.
- **qfnm**
The qdata.txt file that contains the QM energies and forces.
- **qmatoms**
The number of atoms in the QM calculation (Irrelevant if not fitting forces)
- **e_err**
Qualitative Indicator: average energy error (in kJ/mol)
- **e_err_pct**
- **f_err**
Qualitative Indicator: average force error (fractional)
- **f_err_pct**
- **esp_err**
Qualitative Indicator: "relative RMS" for electrostatic potential.
- **nf_err**
- **nf_err_pct**
- **tq_err_pct**
- **use_nft**
Whether to compute net forces and torques, or not.
- **ns**
Read in the trajectory file.
- **mol**
- **nparticles**
The number of (atoms + drude particles + virtual sites)
- **engine**
Build keyword dictionaries to pass to engine.
- **AtomLists**
Lists of atoms to do net force/torque fitting and excluding virtual sites.
- **AtomMask**
- **new_vsites**
Read in the reference data.
- **save_vmvalls**
Save the mvalls from the last time we updated the vsites.
- **force_map**
- **nnf**
- **ntq**
- **force**
- **w_force**
- **nesp**
- **fitatoms**
- **whamboltz**
- **nftqm**
- **fref**
- **w_energy**

- `w_netforce`
- `w_torque`
- `e_ref`
- `f_ref`
- `nf_ref`
- `tq_ref`
- `tq_err`
- `w_resp`
- `invdists`
- `respterm`
- `objective`
- `rd`

Root directory of the whole project.
- `pgrad`

Iteration where we turn on zero-gradient skipping.
- `tempbase`

Relative directory of target.
- `tempdir`
- `rundir`

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- `FF`

Need the forcefield (here for now)
- `xct`

Counts how often the objective function was computed.
- `gct`

Counts how often the gradient was computed.
- `hct`

Counts how often the Hessian was computed.
- `read_indicate`

Whether to read indicate.log from file when restarting an aborted run.
- `write_indicate`

Whether to write indicate.log at every iteration (true for all but remote.)
- `read_objective`

Whether to read objective.p from file when restarting an aborted run.
- `write_objective`

Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

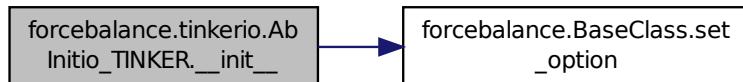
8.6.1 Detailed Description

Subclass of Target for force and energy matching using [TINKER](#).
 Definition at line 1067 of file `tinkerio.py`.

8.6.2 Constructor & Destructor Documentation

```
def forcebalance.tinkerio.AbInitio_TINKER.__init__ ( self, options, tgt_opts, forcefield ) Definition at line 1068 of file tinkerio.py.
```

Here is the call graph for this function:



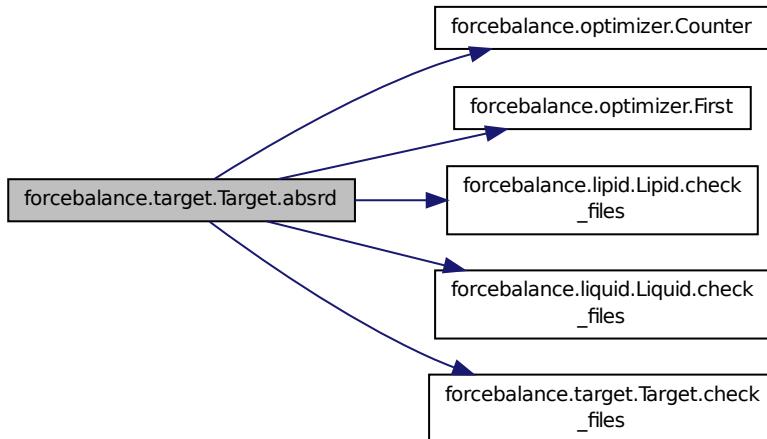
8.6.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.build_invdist ( self, mvals ) [inherited] Definition at line 171 of file abinitio.py.
```

```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.abinitio.AbInitio.compute_netforce_torque ( self, xyz, force, QM = False )  
[inherited] Definition at line 200 of file abinitio.py.
```

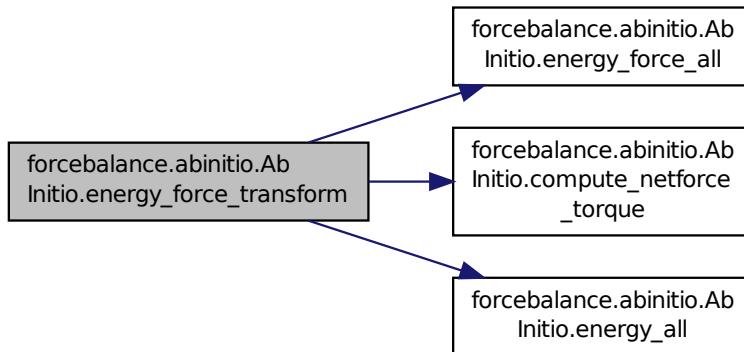
```
def forcebalance.abinitio.AbInitio.energy_all ( self ) [inherited] Definition at line 472 of file abinitio.py.
```

```
def forcebalance.abinitio.AbInitio.energy_force_all ( self ) [inherited] Definition at line 478 of file abinitio.py.
```

```
def forcebalance.abinitio.AbInitio.energy_force_one ( self, i ) [inherited] Definition at line 507 of file abinitio.py.
```

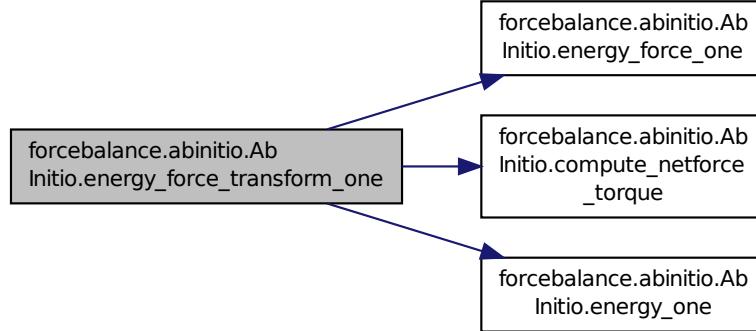
```
def forcebalance.abinitio.AbInitio.energy_force_transform ( self ) [inherited] Definition at line 484 of file abinitio.py.
```

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.energy_force_transform_one ( self, i ) [inherited] Definition at line 513 of file abinitio.py.
```

Here is the call graph for this function:

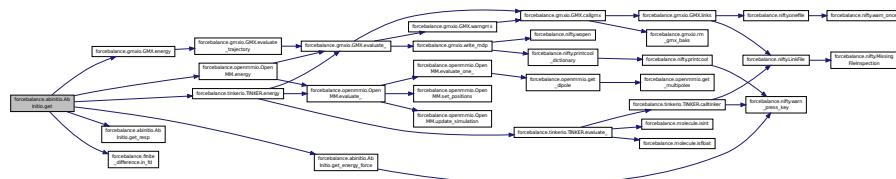


def forcebalance.abinitio.AbInitio.energy_one (self, i) [inherited] Definition at line 501 of file abinitio.py.

def forcebalance.abinitio.AbInitio.get (self, mvals, AGrad = False, AHess = False) [inherited]

Definition at line 1152 of file abinitio.py.

Here is the call graph for this function:



def forcebalance.abinitio.AbInitio.get_energy_force (self, mvals, AGrad = False, AHess = False) [inherited] LPW 06-30-2013.

This subroutine builds the objective function (and optionally its derivatives) from a general simulation software. This is in contrast to using GROMACS-X2, which computes the objective function and prints it out; then 'get' only needs to call GROMACS and read it in.

This subroutine interfaces with simulation software 'drivers'. The driver is only expected to give the energy and forces.

Now this subroutine may sound trivial since the objective function is simply a least-squares quantity $(M-Q)^2$ - but there are a number of nontrivial considerations. I will list them here.

0) Polytensor formulation: Because there may exist covariance between different components of the force (or covariance between the energy and the force), we build the objective function by taking outer products of vectors that have the form $[E \ F_{1x} \ F_{1y} \ F_{1z} \ F_{2x} \ F_{2y} \dots]$, and then we trace it with the inverse of the covariance matrix to get the objective function.

This version implements both the polytensor formulation and the standard formulation.

1) Boltzmann weights and normalization: Each snapshot has its own Boltzmann weight, which may or may not be normalized. This subroutine does the normalization automatically.

2) Subtracting out the mean energy gap: The zero-point energy difference between reference data and simulation is meaningless. This subroutine subtracts it out.

3) Hybrid ensembles: This program builds a combined objective function from both MM and QM ensembles, which is rigorously better than using a single ensemble.

Note that this subroutine does not do EVERYTHING that GROMACS-X2 can do, which includes:

1) Internal coordinate systems 2) 'Sampling correction' (deprecated, since it doesn't seem to work) 3) Analytic derivatives

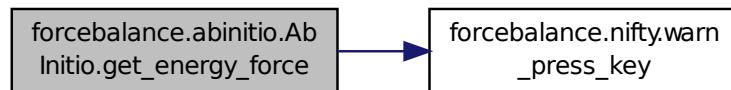
In the previous code (ForTune) this subroutine used analytic first derivatives of the energy and force to build the derivatives of the objective function. Here I will take a simplified approach, because building the derivatives are cumbersome. For now we will return the objective function ONLY. A two-point central difference should give us the first and diagonal second derivative anyhow.

Todo Parallelization over snapshots is not implemented yet

```
@param[in] mvals Mathematical parameter values
@param[in] AGrad Switch to turn on analytic gradient
@param[in] AHess Switch to turn on analytic Hessian
@return Answer Contribution to the objective function
```

Definition at line 588 of file abinitio.py.

Here is the call graph for this function:



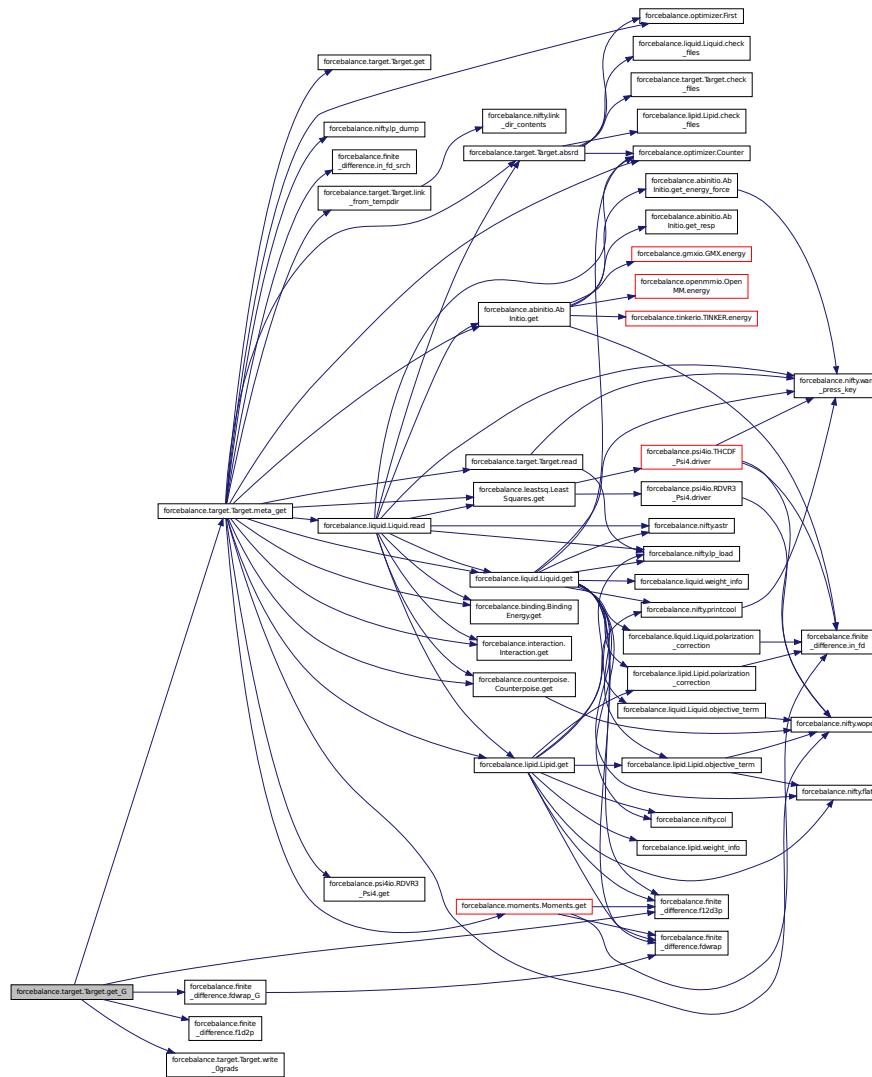
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



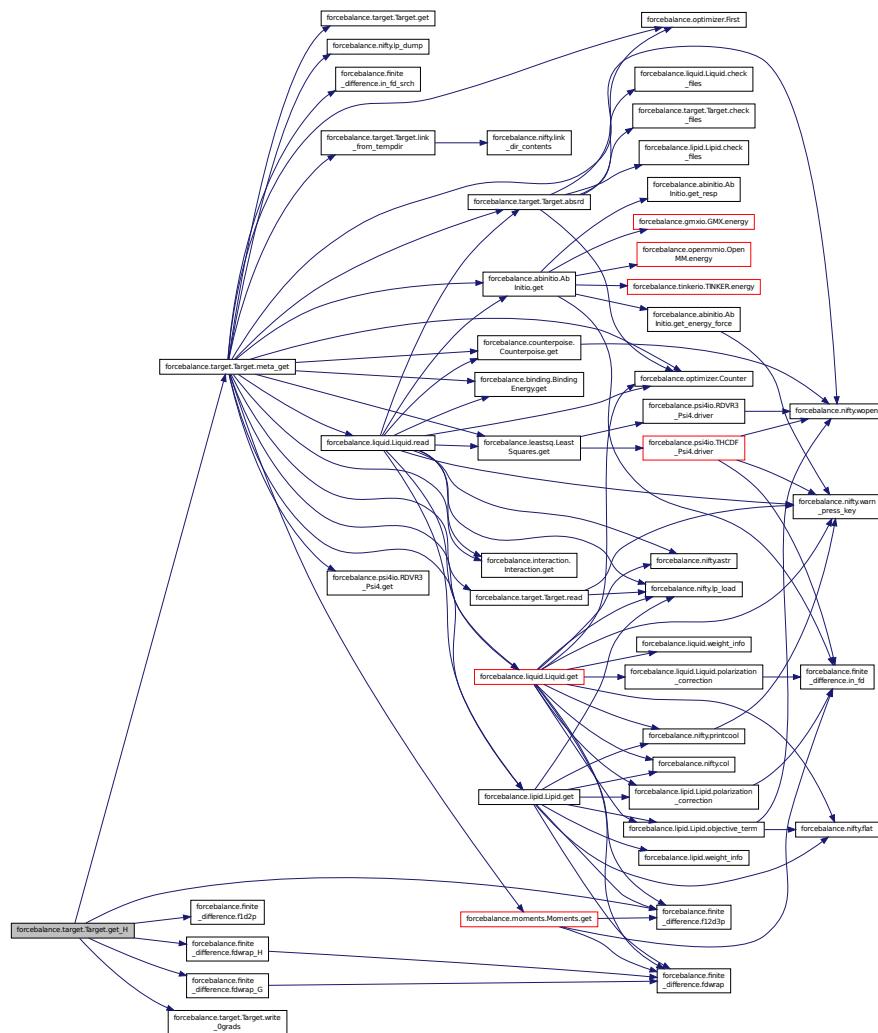
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

Here is the call graph for this function:



```
def forcebalance.abinitio.AbInitio.get_resp ( self, mvals, AGrad = False, AHess = False )  
[inherited] Electrostatic potential fitting.
```

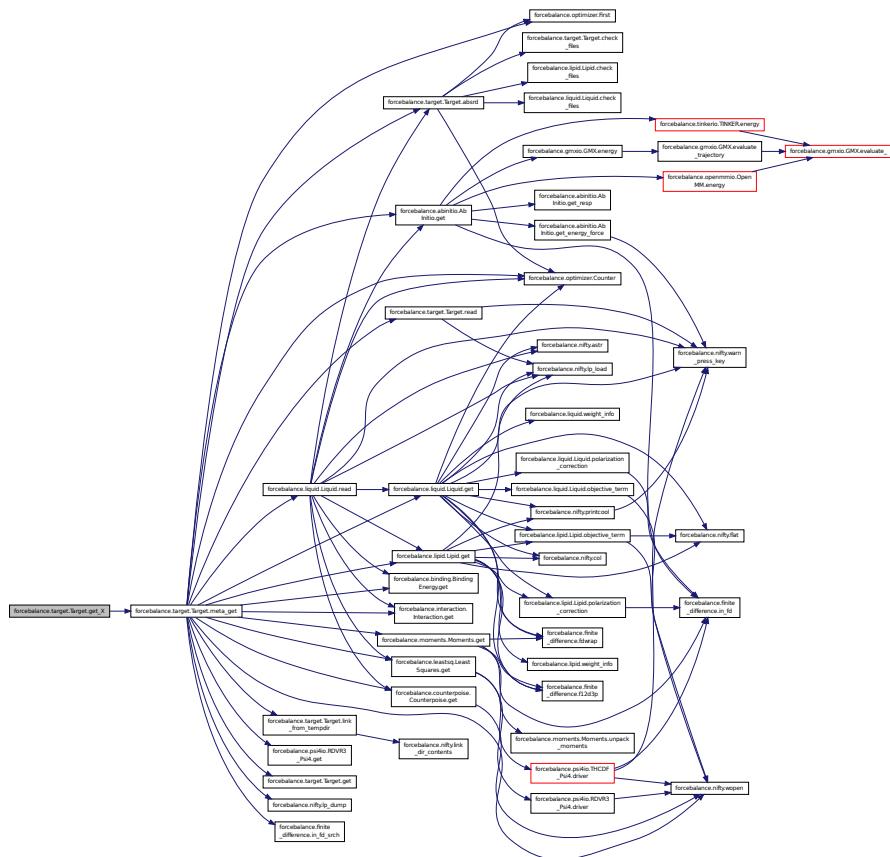
Implements the RESP objective function. (In Python so obviously not optimized.) This function takes the mathematical parameter values and returns the charges on the ATOMS (fancy mapping going on)

Definition at line 1053 of file abinitio.py.

def forcebalance.target.Target.get_X(self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

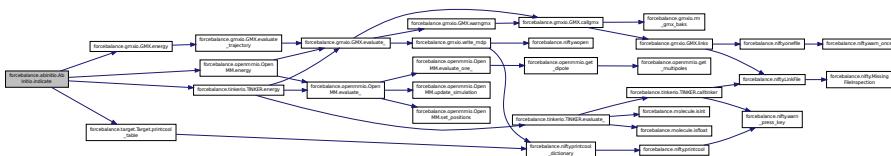
Definition at line 184 of file target.py.

Here is the call graph for this function:



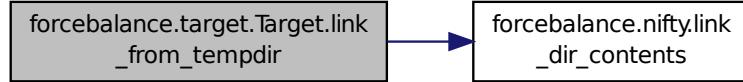
def forcebalance.abinitio.ABInitio.indicate (self) [inherited] Definition at line 448 of file abinitio.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

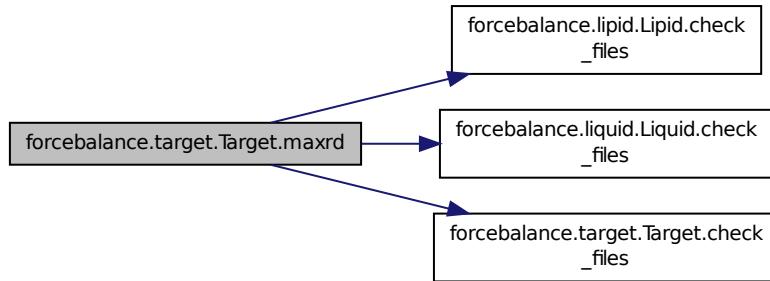
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

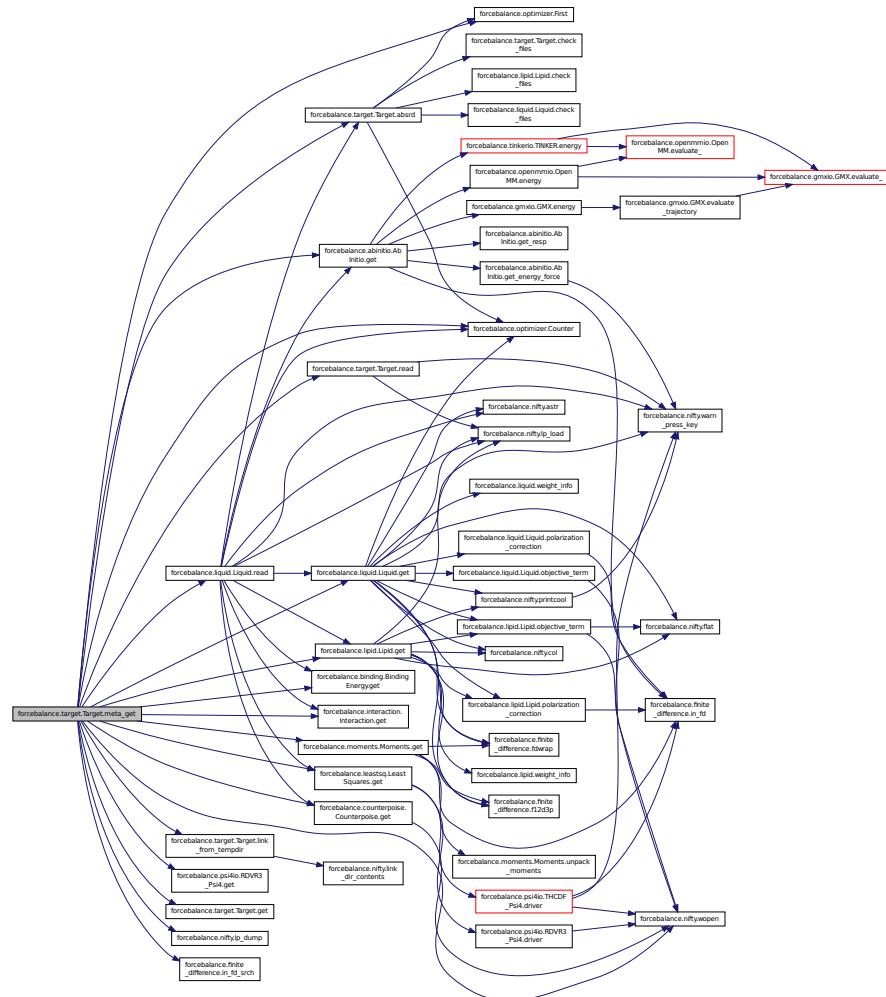


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

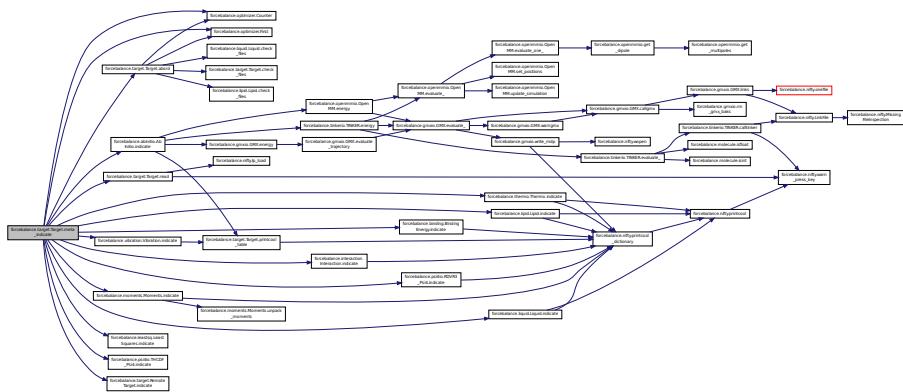
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

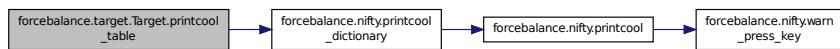
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

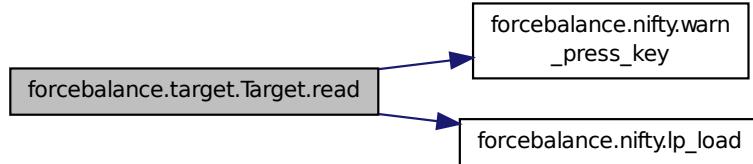
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.abinitio.AblInitio.read_reference_data (self) [inherited] Read the reference ab initio data from a file such as qdata.txt.

Todo Add an option for picking any slice out of qdata.txt, helpful for cross-validation

Todo Closer integration of reference data with program - leave behind the qdata.txt format? (For now, I like the readability of qdata.txt)

After reading in the information from qdata.txt, it is converted into the GROMACS energy units (kind of an arbitrary choice); forces (kind of a misnomer in qdata.txt) are multiplied by -1 to convert gradients to forces.

We also subtract out the mean energies of all energy arrays because energy/force matching does not account for zero-point energy differences between MM and QM (i.e. energy of electrons in core orbitals).

The configurations in force/energy matching typically come from a the thermodynamic ensemble of the MM force field at some temperature (by running MD, for example), and for many reasons it is helpful to introduce non-Boltzmann weights in front of these configurations. There are two options: WHAM Boltzmann weights (for combining the weights of several simulations together) and QM Boltzmann weights (for converting MM weights into QM weights). Note that the two sets of weights 'stack'; i.e. they can be used at the same time.

A 'hybrid' ensemble is possible where we use 50% MM and 50% QM weights. Please read more in LPW and Troy Van Voorhis, JCP Vol. 133, Pg. 231101 (2010), doi:10.1063/1.3519043.

Todo The WHAM Boltzmann weights are generated by external scripts (wanalyze.py and make-wham-data.sh) and passed in; perhaps these scripts can be added to the ForceBalance distribution or integrated more tightly.

Finally, note that using non-Boltzmann weights degrades the statistical information content of the snapshots. This problem will generally become worse if the ensemble to which we're reweighting is dramatically different from the one we're sampling from. We end up with a set of Boltzmann weights like [1e-9, 1e-9, 1.0, 1e-9, 1e-9 ...] and this is essentially just one snapshot. I believe Troy is working on something to cure this problem.

Here, we have a measure for the information content of our snapshots, which comes easily from the definition of information entropy:

```
S = -1*Sum_i(P_i*log(P_i))
InfoContent = exp(-S)
```

With uniform weights, InfoContent is equal to the number of snapshots; with horrible weights, InfoContent is closer to one.

Definition at line 329 of file abinitio.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

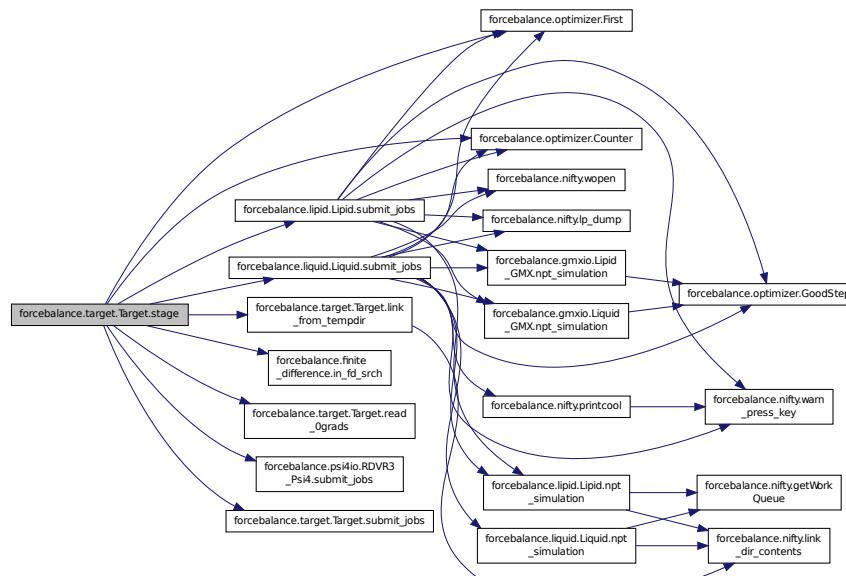
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

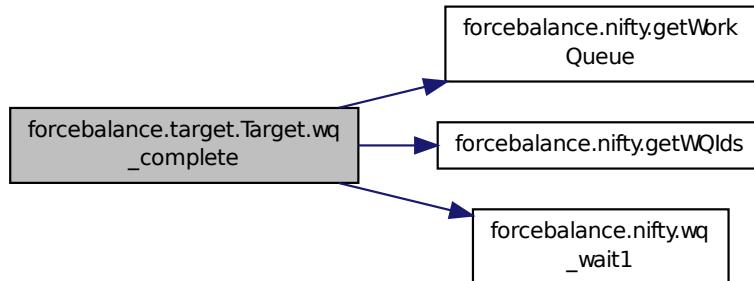


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work  
Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_Ograds ( self, Ans ) [inherited] Write a file to the target directory  
containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.6.4 Member Data Documentation

```
forcebalance.abinitio.ABInitio.AtomLists [inherited] Lists of atoms to do net force/torque fitting and excluding virtual sites.
```

Definition at line 160 of file abinitio.py.

```
forcebalance.abinitio.ABInitio.AtomMask [inherited] Definition at line 161 of file abinitio.py.
```

```
forcebalance.abinitio.ABInitio.boltz_wts [inherited] Initialize the base class.
```

Number of snapshots Whether to use WHAM Boltzmann weights Whether to use the Sampling Correction Whether to match Absolute Energies (make sure you know what you're doing) Whether to use the Covariance Matrix Whether to use QM Boltzmann weights The temperature for QM Boltzmann weights Number of atoms that we are fitting Whether to fit Energies. Whether to fit Forces. Whether to fit Electrostatic Potential. Weights for the three components. Option for how much data to write to disk. Whether to do energy and force calculations for the whole trajectory, or to do one calculation per snapshot. OpenMM-only option - whether to run the energies and forces internally. Whether we have virtual sites (set at the global option level) Attenuate the weights as a function of energy What is the energy denominator? (Valid for 'attenuate') Set upper cutoff energy WHAM Boltzmann weights

Definition at line 116 of file abinitio.py.

```
forcebalance.abinitio.ABInitio.e_err [inherited] Qualitative Indicator: average energy error (in kJ/mol)
```

Definition at line 134 of file abinitio.py.

```
forcebalance.abinitio.ABInitio.e_err_pct [inherited] Definition at line 135 of file abinitio.py.
```

forcebalance.abinitio.AbInitio.e.ref [inherited] Definition at line 1030 of file abinitio.py.

forcebalance.abinitio.AbInitio.emd0 [inherited] Energies of the sampling simulation.
Definition at line 122 of file abinitio.py.

forcebalance.abinitio.AbInitio.engine [inherited] Build keyword dictionaries to pass to engine.
Create engine object.
Definition at line 158 of file abinitio.py.

forcebalance.tinkerio.AbInitio_TINKER.engine Default file names for coordinates and key file.
Definition at line 1072 of file tinkerio.py.

forcebalance.abinitio.AbInitio.eqm [inherited] Reference (QM) energies.
Definition at line 120 of file abinitio.py.

forcebalance.abinitio.AbInitio.esp_err [inherited] Qualitative Indicator: "relative RMS" for electrostatic potential.
Definition at line 140 of file abinitio.py.

forcebalance.abinitio.AbInitio.espval [inherited] ESP values.
Definition at line 128 of file abinitio.py.

forcebalance.abinitio.AbInitio.espxyz [inherited] ESP grid points.
Definition at line 126 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err [inherited] Qualitative Indicator: average force error (fractional)
Definition at line 137 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_err_pct [inherited] Definition at line 138 of file abinitio.py.

forcebalance.abinitio.AbInitio.f_ref [inherited] Definition at line 1034 of file abinitio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.abinitio.AbInitio.fitatoms [inherited] Definition at line 366 of file abinitio.py.

forcebalance.abinitio.AbInitio.force [inherited] Definition at line 361 of file abinitio.py.

forcebalance.abinitio.AbInitio.force_map [inherited] Definition at line 209 of file abinitio.py.

forcebalance.abinitio.AbInitio.fqm [inherited] Reference (QM) forces.
Definition at line 124 of file abinitio.py.

forcebalance.abinitio.AbInitio.fref [inherited] Definition at line 442 of file abinitio.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.abinitio.ABInitio.invdist [inherited] Definition at line 1061 of file abinitio.py.

forcebalance.abinitio.ABInitio.mol [inherited] Definition at line 148 of file abinitio.py.

forcebalance.abinitio.ABInitio.nesp [inherited] Definition at line 363 of file abinitio.py.

forcebalance.abinitio.ABInitio.new_vsites [inherited] Read in the reference data.

The below two options are related to whether we want to rebuild virtual site positions. Rebuild the distance matrix if virtual site positions have changed

Definition at line 166 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err [inherited] Definition at line 141 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_err_pct [inherited] Definition at line 142 of file abinitio.py.

forcebalance.abinitio.ABInitio.nf_ref [inherited] Definition at line 1038 of file abinitio.py.

forcebalance.abinitio.ABInitio.nftqm [inherited] Definition at line 438 of file abinitio.py.

forcebalance.abinitio.ABInitio.nnf [inherited] Definition at line 267 of file abinitio.py.

forcebalance.abinitio.ABInitio.nparticles [inherited] The number of (atoms + drude particles + virtual sites)
Definition at line 153 of file abinitio.py.

forcebalance.abinitio.ABInitio.ns [inherited] Read in the trajectory file.

Definition at line 147 of file abinitio.py.

forcebalance.abinitio.ABInitio.ntq [inherited] Definition at line 268 of file abinitio.py.

forcebalance.abinitio.ABInitio.objective [inherited] Definition at line 1172 of file abinitio.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.abinitio.ABInitio.qfnm [inherited] The qdata.txt file that contains the QM energies and forces.
Definition at line 130 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmatoms [inherited] The number of atoms in the QM calculation (Irrelevant if not fitting forces)

Definition at line 132 of file abinitio.py.

forcebalance.abinitio.ABInitio.qmboltz_wts [inherited] QM Boltzmann weights.

Definition at line 118 of file abinitio.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.abinitio.ABInitio.respterm [inherited] Definition at line 1140 of file abinitio.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.abinitio.ABInitio.save_vmvales [inherited] Save the mvales from the last time we updated the vsites.

Definition at line 168 of file abinitio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.abinitio.ABInitio.tq_err [inherited] Definition at line 1042 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_err_pct [inherited] Definition at line 143 of file abinitio.py.

forcebalance.abinitio.ABInitio.tq_ref [inherited] Definition at line 1041 of file abinitio.py.

forcebalance.abinitio.ABInitio.use_nft [inherited] Whether to compute net forces and torques, or not.

Definition at line 145 of file abinitio.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.abinitio.ABInitio.w_energy [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_force [inherited] Definition at line 362 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_netforce [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_resp [inherited] Definition at line 1054 of file abinitio.py.

forcebalance.abinitio.ABInitio.w_torque [inherited] Definition at line 630 of file abinitio.py.

forcebalance.abinitio.ABInitio.whamboltz [inherited] Definition at line 382 of file abinitio.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

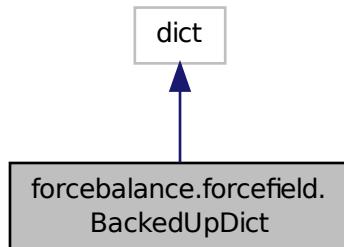
Definition at line 162 of file target.py.

The documentation for this class was generated from the following file:

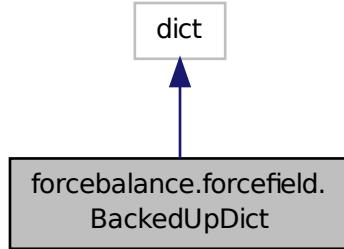
- [tinkerio.py](#)

8.7 forcebalance.forcefield.BackedUpDict Class Reference

Inheritance diagram for forcebalance.forcefield.BackedUpDict:



Collaboration diagram for forcebalance.forcefield.BackedUpDict:



Public Member Functions

- def [__init__](#)
- def [__missing__](#)

Public Attributes

- [backup_dict](#)

8.7.1 Detailed Description

Definition at line 176 of file forcefield.py.

8.7.2 Constructor & Destructor Documentation

def forcebalance.forcefield.BackedUpDict.__init__ (self, backup_dict) Definition at line 177 of file forcefield.py.

8.7.3 Member Function Documentation

def forcebalance.forcefield.BackedUpDict.__missing__ (self, key) Definition at line 180 of file forcefield.py.

8.7.4 Member Data Documentation

forcebalance.forcefield.BackedUpDict.backup_dict Definition at line 179 of file forcefield.py.

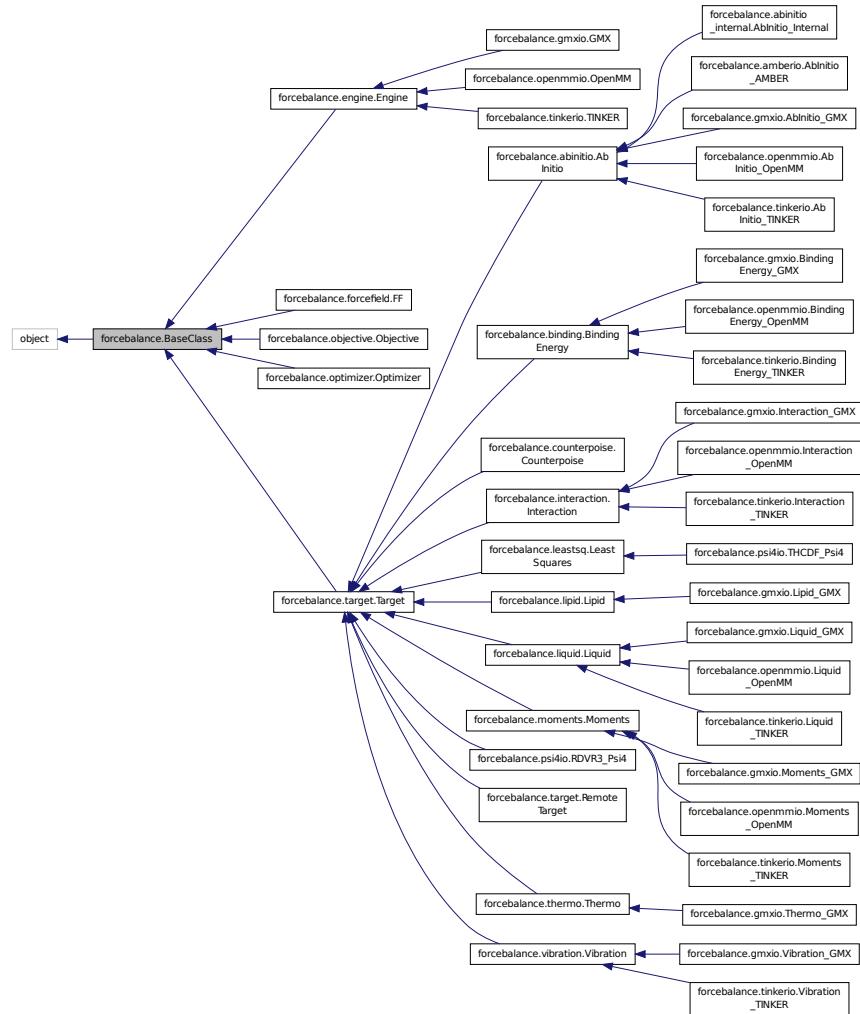
The documentation for this class was generated from the following file:

- [forcefield.py](#)

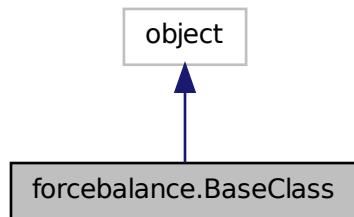
8.8 forcebalance.BaseClass Class Reference

Provides some nifty functions that are common to all ForceBalance classes.

Inheritance diagram for forcebalance.BaseClass:



Collaboration diagram for forcebalance.BaseClass:



Public Member Functions

- def `__setattr__`
- def `__init__`
- def `set_option`

Public Attributes

- `verbose_options`
- `PrintOptionDict`

8.8.1 Detailed Description

Provides some nifty functions that are common to all ForceBalance classes.

Definition at line 26 of file `__init__.py`.

8.8.2 Constructor & Destructor Documentation

`def forcebalance.BaseClass.__init__(self, options)` Definition at line 39 of file `__init__.py`.

8.8.3 Member Function Documentation

`def forcebalance.BaseClass.__setattr__(self, key, value)` Definition at line 28 of file `__init__.py`.

`def forcebalance.BaseClass.set_option(self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False)` Definition at line 42 of file `__init__.py`.

8.8.4 Member Data Documentation

`forcebalance.BaseClass.PrintOptionDict` Definition at line 44 of file `__init__.py`.

`forcebalance.BaseClass.verbose_options` Definition at line 40 of file `__init__.py`.

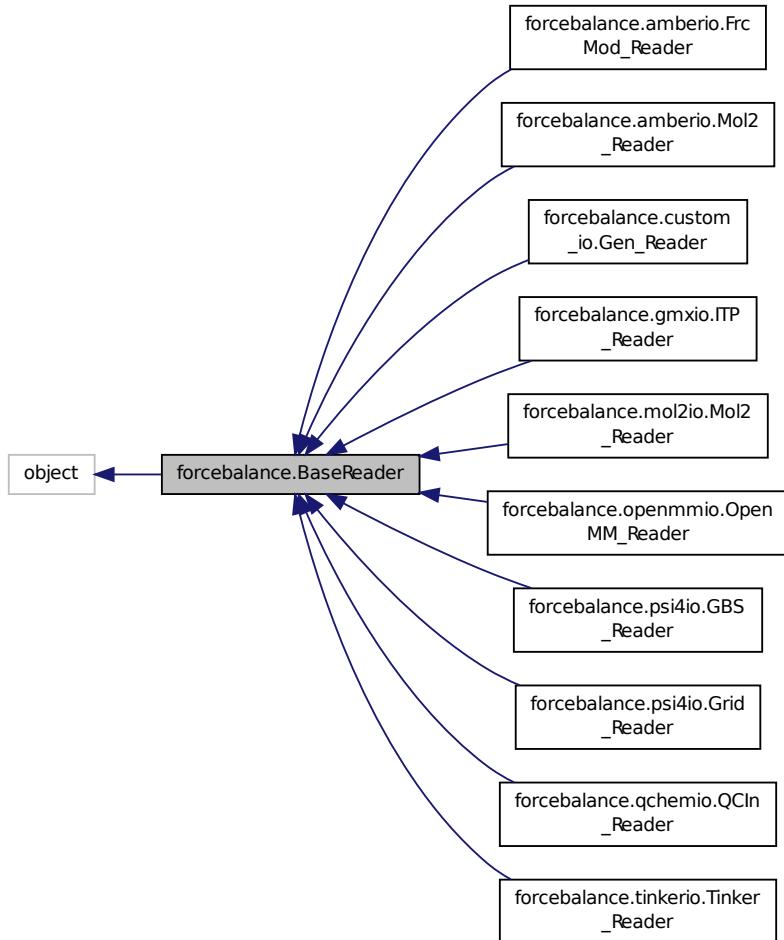
The documentation for this class was generated from the following file:

- `__init__.py`

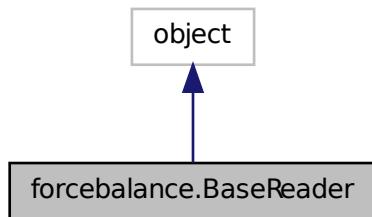
8.9 forcebalance.BaseReader Class Reference

The 'reader' class.

Inheritance diagram for forcebalance.BaseReader:



Collaboration diagram for forcebalance.BaseReader:



Public Member Functions

- def `_init_`
- def `Split`
- def `Whites`
- def `feed`
- def `build_pid`

Returns the parameter type (e.g.

Public Attributes

- `In`
- `itype`
- `suffix`
- `pdict`
- `adict`

The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.
- `molatom`

The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.
- `Molecules`
- `AtomTypes`

8.9.1 Detailed Description

The 'reader' class.

It serves two main functions:

- 1) When parsing a text force field file, the 'feed' method is called once for every line. Calling the 'feed' method stores the internal variables that are needed for making the unique parameter identifier.
- 2) The 'reader' also stores the 'pdict' dictionary, which is needed for building the matrix of rescaling factors. This is not needed for the XML force fields, so in XML force fields pdict is replaced with a string called "XML_Override".

Definition at line 81 of file `__init__.py`.

8.9.2 Constructor & Destructor Documentation

`def forcebalance.BaseReader.__init__(self, fnm)` Definition at line 83 of file `__init__.py`.

8.9.3 Member Function Documentation

`def forcebalance.BaseReader.build_pid(self, pfd)` Returns the parameter type (e.g.

K in BONDSK) based on the current interaction type.

Both the 'pdict' dictionary (see `gmlio.pdict`) and the interaction type 'state' (here, BONDS) are needed to get the parameter type.

If, however, 'pdict' does not contain the ptype value, a suitable substitute is simply the field number.

Note that if the interaction type state is not set, then it defaults to the file name, so a generic parameter ID is 'filename.line_num.field_num'

Definition at line 124 of file `__init__.py`.

`def forcebalance.BaseReader.feed(self, line)` Definition at line 105 of file `__init__.py`.

`def forcebalance.BaseReader.Split(self, line)` Definition at line 99 of file `__init__.py`.

`def forcebalance.BaseReader.Whites(self, line)` Definition at line 102 of file `__init__.py`.

8.9.4 Member Data Documentation

forcebalance.BaseReader.adict The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

Definition at line 89 of file __init__.py.

forcebalance.BaseReader.AtomTypes Definition at line 97 of file __init__.py.

forcebalance.BaseReader.itype Definition at line 85 of file __init__.py.

forcebalance.BaseReader.In Definition at line 84 of file __init__.py.

forcebalance.BaseReader.molatom The mapping of (molecule name) to a dictionary of of atom types for the atoms in that residue.

self.moleculerdict = OrderedDict() The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.

Definition at line 94 of file __init__.py.

forcebalance.BaseReader.Molecules Definition at line 96 of file __init__.py.

forcebalance.BaseReader.pdict Definition at line 87 of file __init__.py.

forcebalance.BaseReader.suffix Definition at line 86 of file __init__.py.

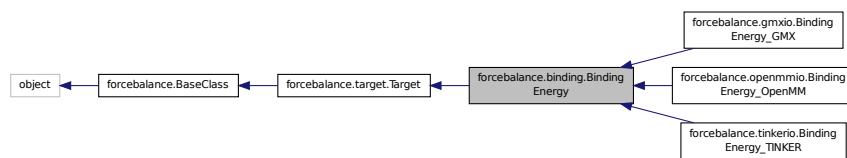
The documentation for this class was generated from the following file:

- [__init__.py](#)

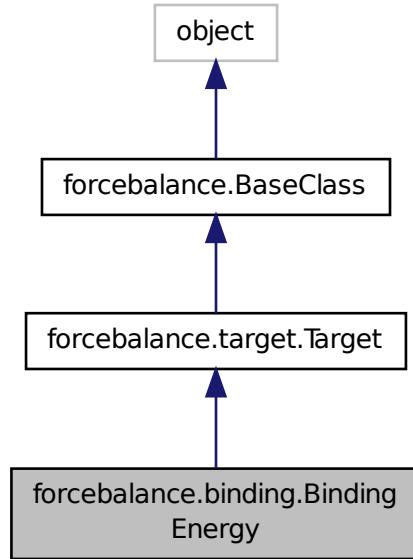
8.10 forcebalance.binding.BindingEnergy Class Reference

Improved subclass of Target for fitting force fields to binding energies.

Inheritance diagram for forcebalance.binding.BindingEnergy:



Collaboration diagram for forcebalance.binding.BindingEnergy:



Public Member Functions

- def `__init__`
- def `system_driver`
- def `indicate`
- def `get`
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`

Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`

Check this directory for the presence of readable files when the 'read' option is set.
- def `read`

Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

- def **absrd**
Supply the correct directory specified by user's "read" option.
- def **maxrd**
Supply the latest existing temp-directory containing valid data.
- def **meta._indicate**
Wrap around the indicate function, so it can print to screen and also to a file.
- def **meta.get**
Wrapper around the get function.
- def **submit_jobs**
- def **stage**
Stages the directory for the target, and then launches Work Queue processes if any.
- def **wq.complete**
This method determines whether the Work Queue tasks for the current target have completed.
- def **printcool.table**
Print target information in an organized table format.
- def **__setattr__**
- def **set_option**

Public Attributes

- **inter_opts**
engines
Build keyword dictionaries to pass to engine.
- **PrintDict**
- **RMSDDict**
- **rmsd_part**
- **energy_part**
- **objective**
- **rd**
Root directory of the whole project.
- **pgrad**
Iteration where we turn on zero-gradient skipping.
- **tempbase**
Relative directory of target.
- **tempdir**
- **rundir**
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**

Whether to write indicate.log at every iteration (true for all but remote.)

- [read_objective](#)

Whether to read objective.p from file when restarting an aborted run.

- [write_objective](#)

Whether to write objective.p at every iteration (true for all but remote.)

- [verbose_options](#)
- [PrintOptionDict](#)

8.10.1 Detailed Description

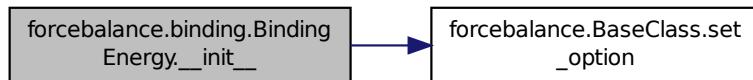
Improved subclass of Target for fitting force fields to binding energies.

Definition at line 122 of file binding.py.

8.10.2 Constructor & Destructor Documentation

def forcebalance.binding.BindingEnergy.__init__ (self, options, tgt_opts, forcefield) Definition at line 125 of file binding.py.

Here is the call graph for this function:



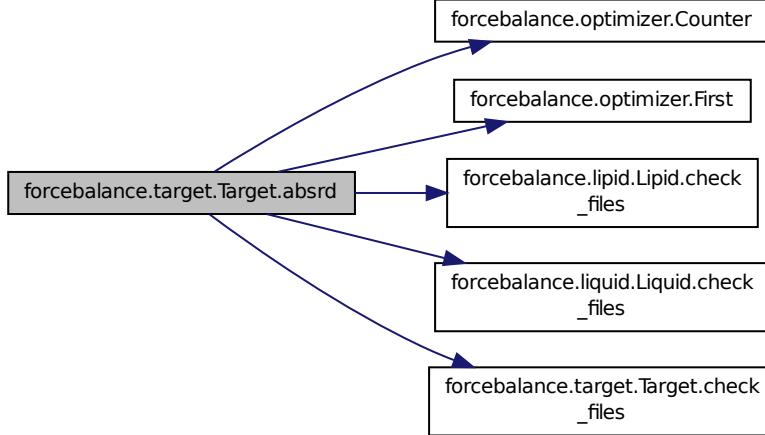
8.10.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited] Definition at line 28 of file __init__.py.

def forcebalance.target.Target.absrd (self, inum = None) [inherited] Supply the correct directory specified by user's "read" option.

Definition at line 393 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.check_files(self, there) [inherited] Check this directory for the presence of readable files when the 'read' option is set.

Definition at line 364 of file target.py.

def forcebalance.binding.BindingEnergy.get(self, mvals, AGrad = False, AHess = False) Definition at line 184 of file binding.py.

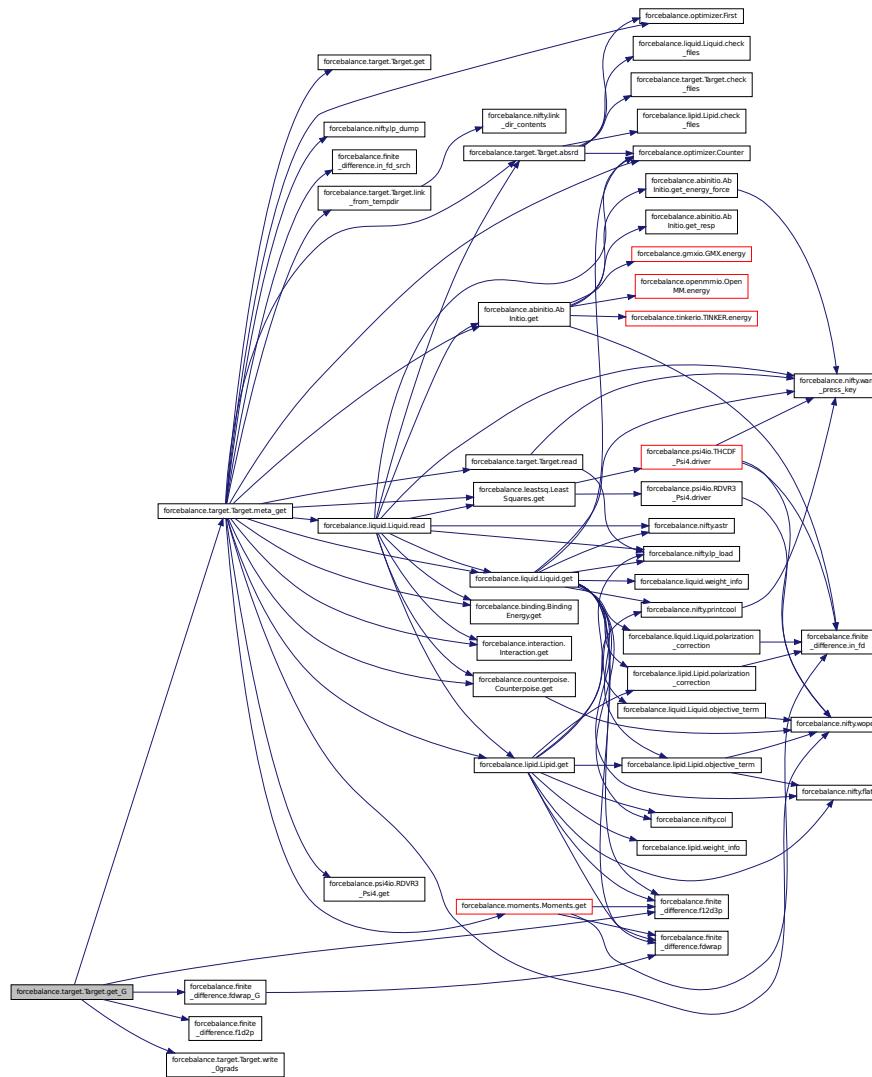
def forcebalance.target.Target.get_G(self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



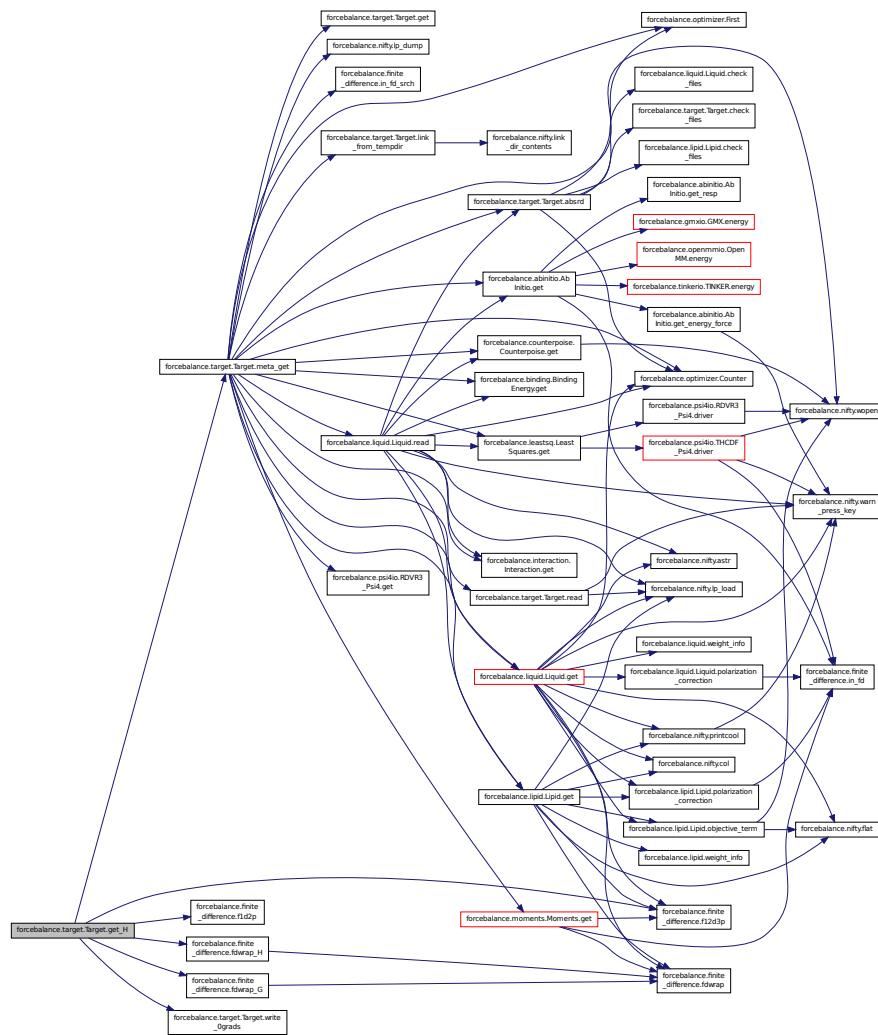
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

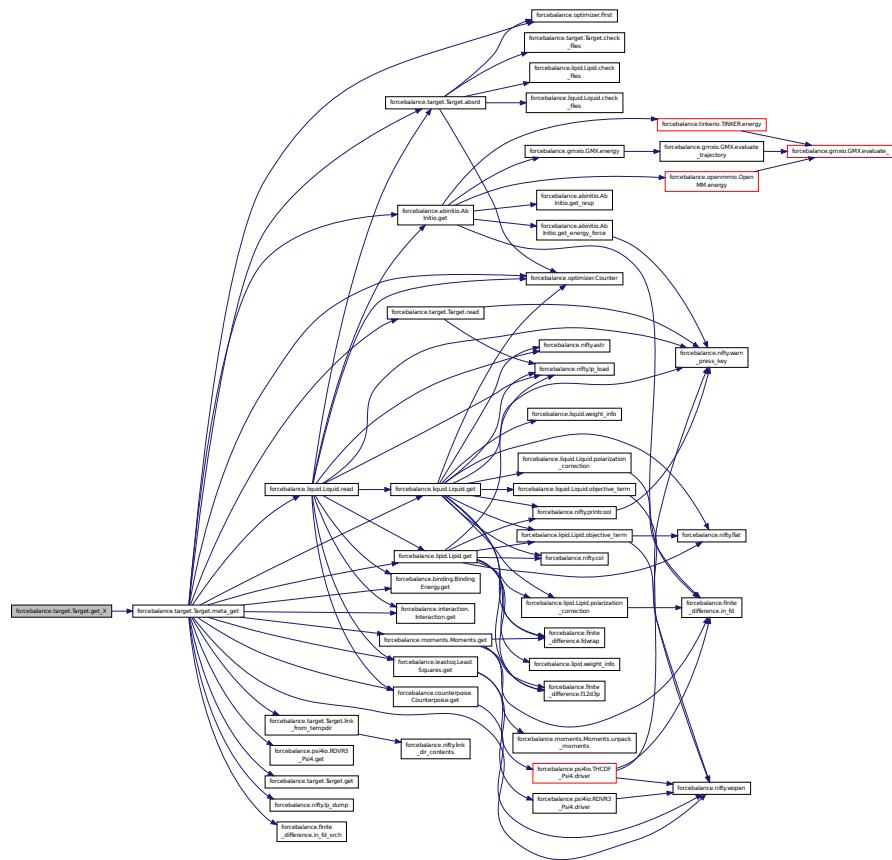
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

Here is the call graph for this function:



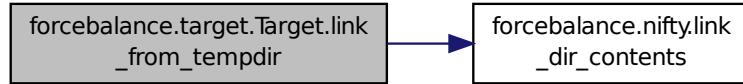
def forcebalance.binding.BindingEnergy.indicate (self) Definition at line 178 of file binding.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

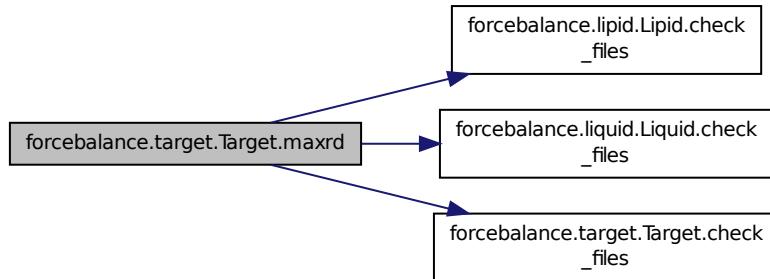
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

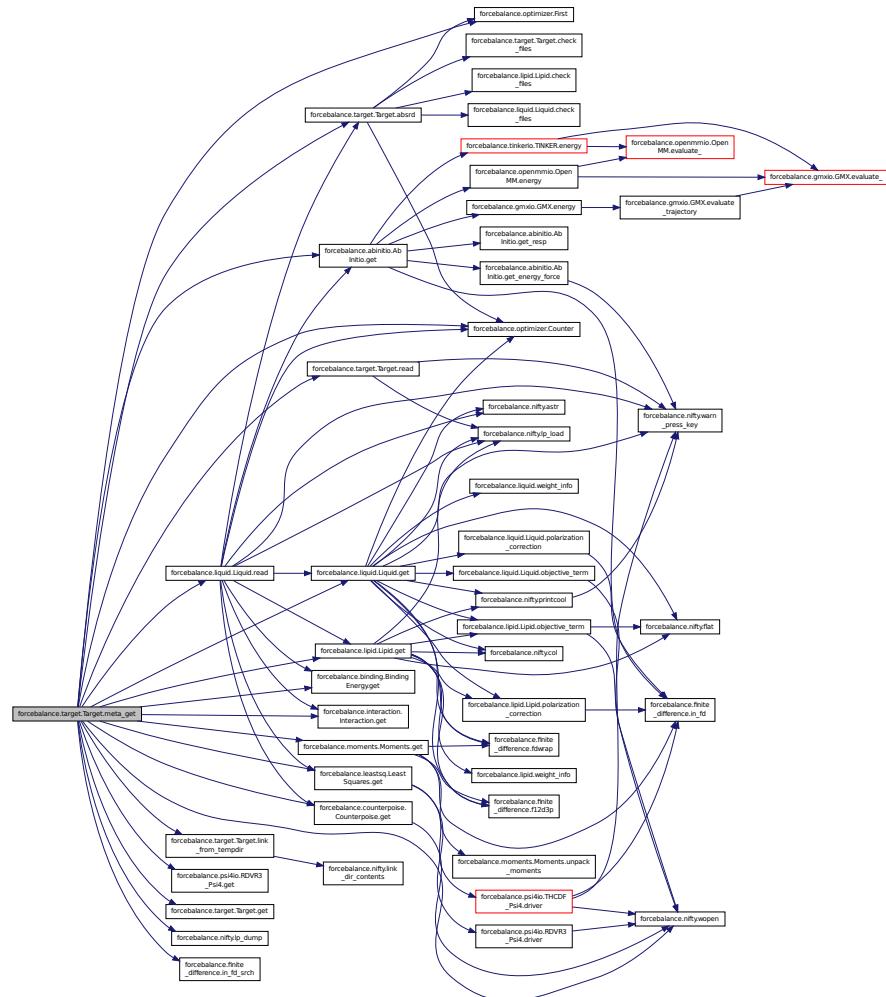


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

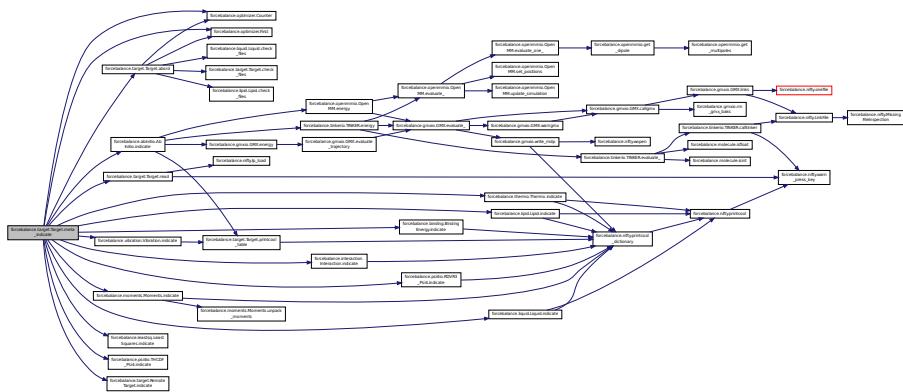
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

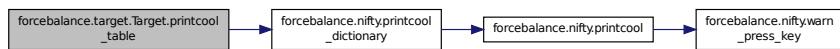
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

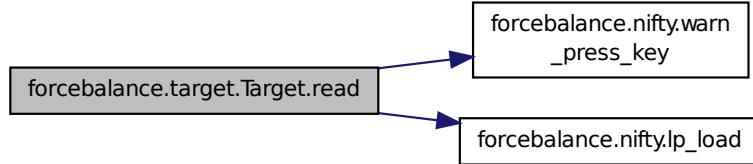
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

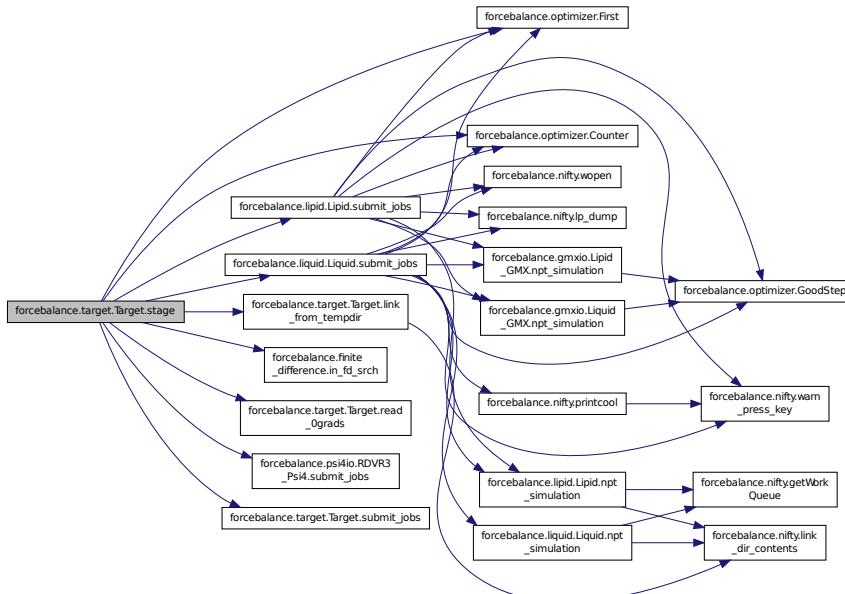
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



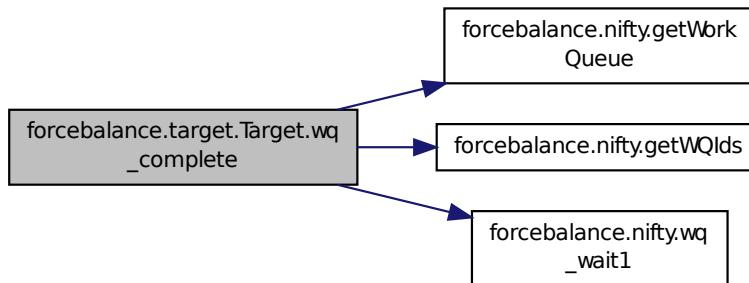
```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.binding.BindingEnergy.system_driver( self, sysname ) Definition at line 174 of file binding.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.10.4 Member Data Documentation

forcebalance.binding.BindingEnergy.energy_part Definition at line 228 of file binding.py.

forcebalance.binding.BindingEnergy.engines Build keyword dictionaries to pass to engine.

Create engine objects.

Definition at line 165 of file binding.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.binding.BindingEnergy.inter_opts Definition at line 128 of file binding.py.

forcebalance.binding.BindingEnergy.objective Definition at line 252 of file binding.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.binding.BindingEnergy.PrintDict Definition at line 186 of file binding.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.binding.BindingEnergy.rmsd_part Definition at line 226 of file binding.py.

forcebalance.binding.BindingEnergy.RMSDDict Definition at line 187 of file binding.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number
The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

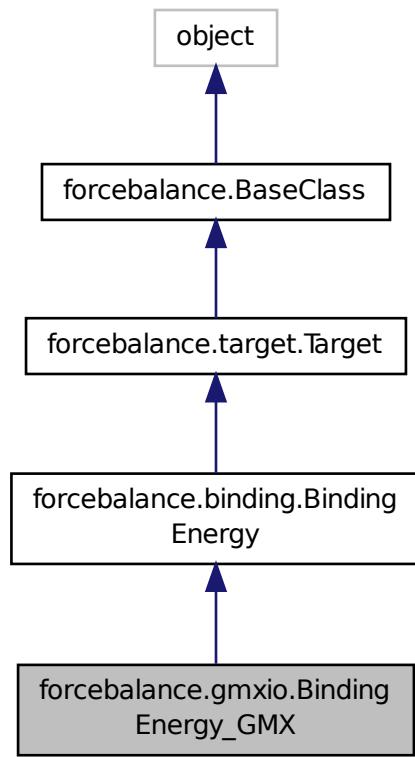
The documentation for this class was generated from the following file:

- [binding.py](#)

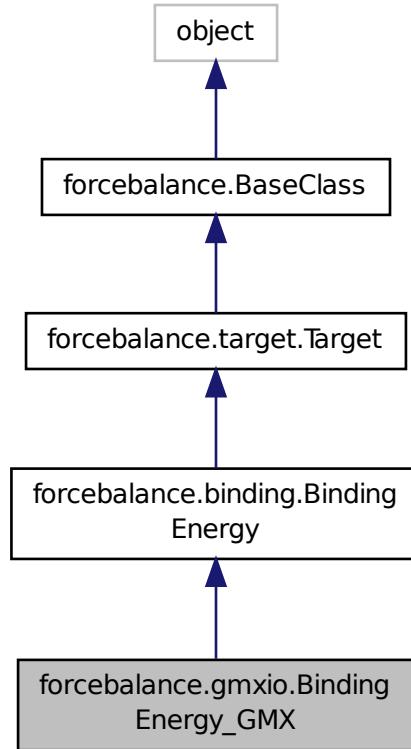
8.11 forcebalance.gmxio.BindingEnergy_GMX Class Reference

Binding energy matching using Gromacs.

Inheritance diagram for forcebalance.gmxio.BindingEnergy_GMX:



Collaboration diagram for forcebalance.gmxio.BindingEnergy_GMX:



Public Member Functions

- def `_init_`
- def `system_driver`
- def `indicate`
- def `get`
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`

Back up the temporary directory if desired, delete it and then create a new one.

- def [check_files](#)

Check this directory for the presence of readable files when the 'read' option is set.

- def [read](#)

Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

- def [absrd](#)

Supply the correct directory specified by user's "read" option.

- def [maxrd](#)

Supply the latest existing temp-directory containing valid data.

- def [meta_indicate](#)

Wrap around the indicate function, so it can print to screen and also to a file.

- def [meta_get](#)

Wrapper around the get function.

- def [submit_jobs](#)

- def [stage](#)

Stages the directory for the target, and then launches Work Queue processes if any.

- def [wq_complete](#)

This method determines whether the Work Queue tasks for the current target have completed.

- def [printcool_table](#)

Print target information in an organized table format.

- def [__setattr__](#)

- def [set_option](#)

Public Attributes

- [engine_](#)

- [inter_opts](#)

- [engines](#)

Build keyword dictionaries to pass to engine.

- [PrintDict](#)

- [RMSDDict](#)

- [rmsd_part](#)

- [energy_part](#)

- [objective](#)

- [rd](#)

Root directory of the whole project.

- [pgrad](#)

Iteration where we turn on zero-gradient skipping.

- [tempbase](#)

Relative directory of target.

- [tempdir](#)

- [rundir](#)

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

- [FF](#)

Need the forcefield (here for now)

- [xct](#)

Counts how often the objective function was computed.

- [gct](#)

- `hct`
Counts how often the gradient was computed.
- `read_indicate`
Whether to read `indicate.log` from file when restarting an aborted run.
- `write_indicate`
Whether to write `indicate.log` at every iteration (true for all but remote.)
- `read_objective`
Whether to read `objective.p` from file when restarting an aborted run.
- `write_objective`
Whether to write `objective.p` at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.11.1 Detailed Description

Binding energy matching using Gromacs.

Definition at line 1461 of file `gmxio.py`.

8.11.2 Constructor & Destructor Documentation

```
def forcebalance.gmxio.BindingEnergy_GMX.__init__ ( self, options, tgt_opts, forcefield )
```

Definition at line 1461 of file `gmxio.py`.

8.11.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited]
```

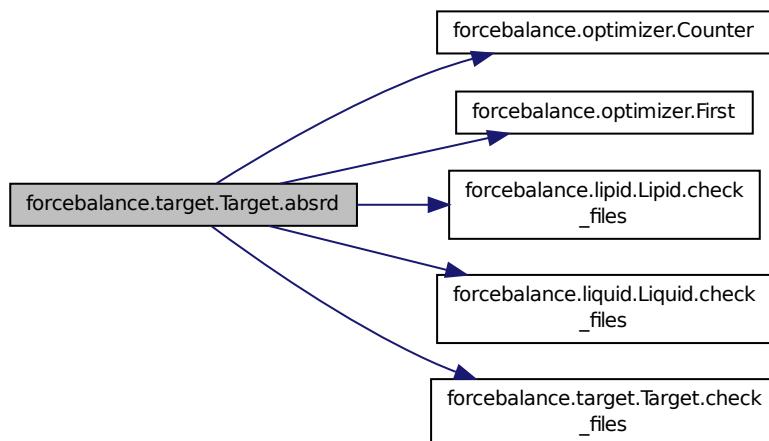
Definition at line 28 of file `__init__.py`.

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited]
```

Supply the correct directory specified by user's "read" option.

Definition at line 393 of file `target.py`.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files( self, there ) [inherited] Check this directory for the presence  
of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.binding.BindingEnergy.get ( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 184 of file binding.py.
```

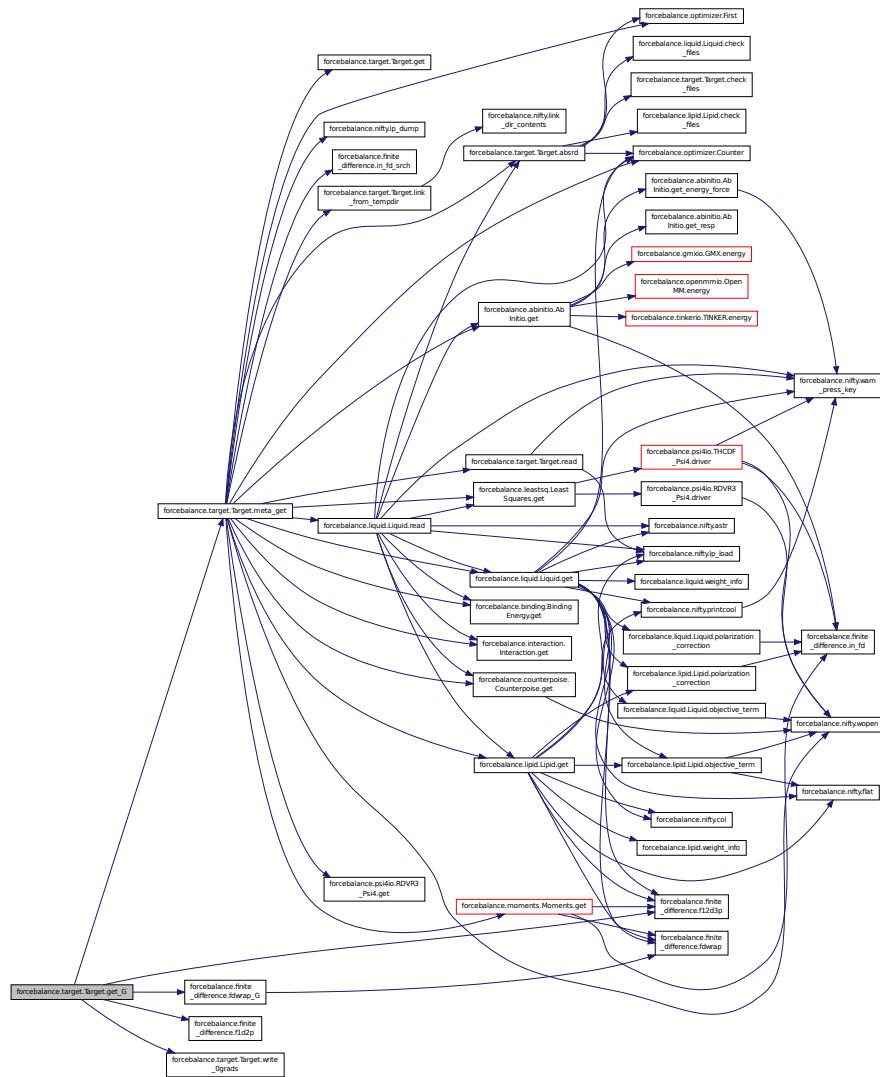
```
def forcebalance.target.Target.get_G( self, mvals = None ) [inherited] Computes the objective function  
contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1.pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



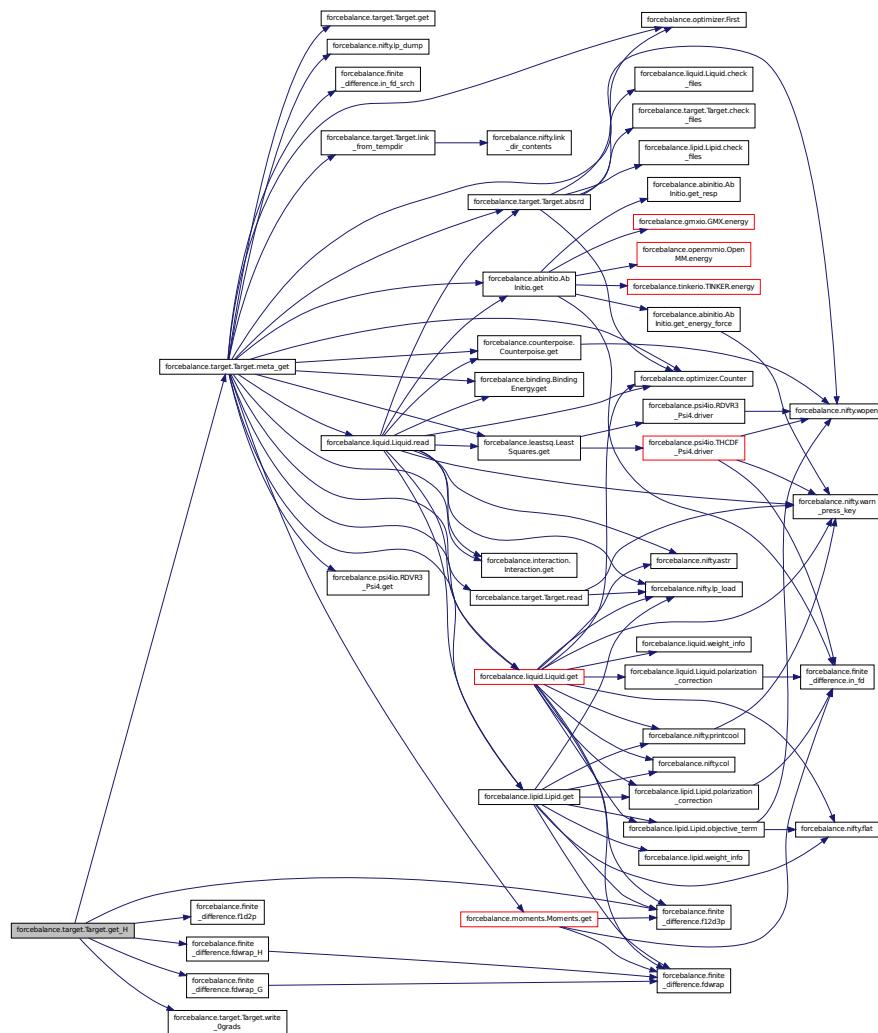
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the `fd2.pids` and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

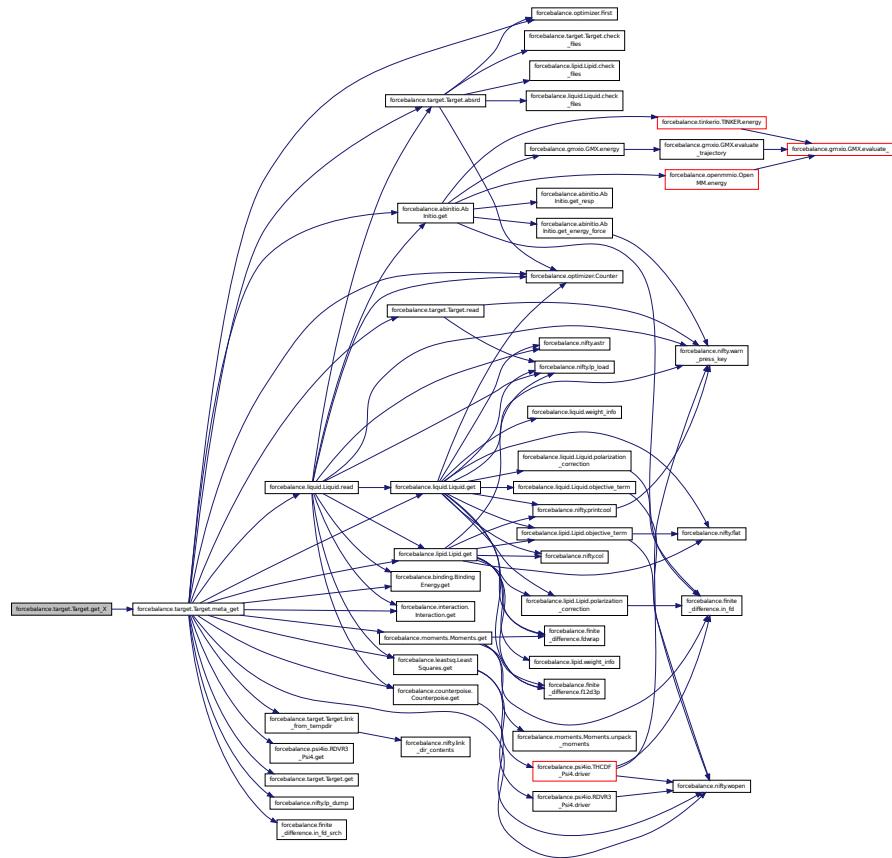
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

Here is the call graph for this function:



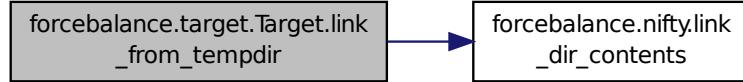
def forcebalance.binding.BindingEnergy.indicate (self) [inherited] Definition at line 178 of file binding.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

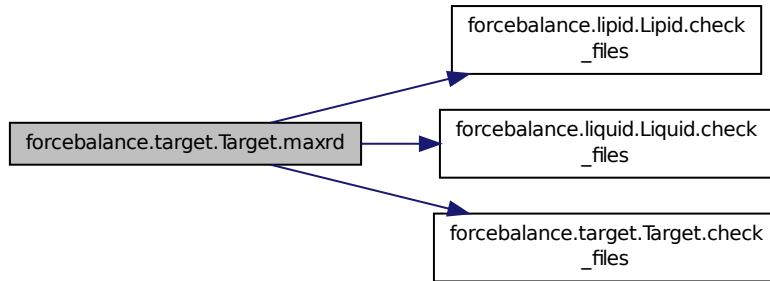
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

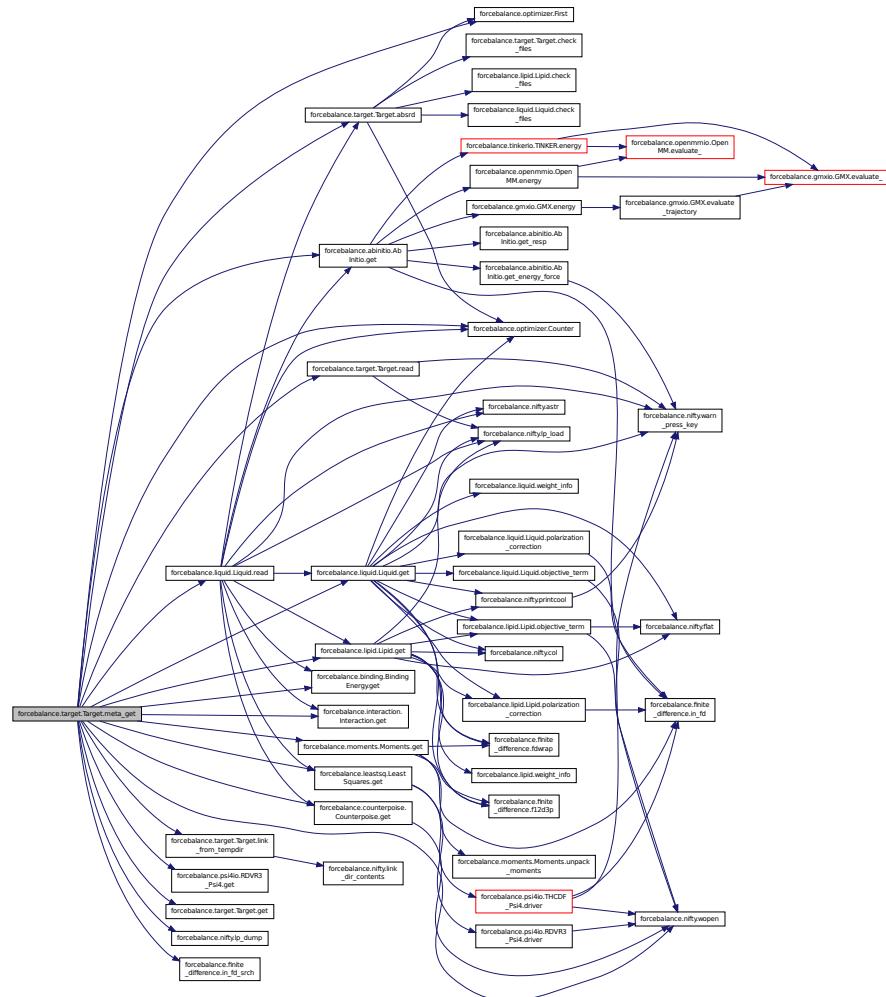


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

Here is the call graph for this function:

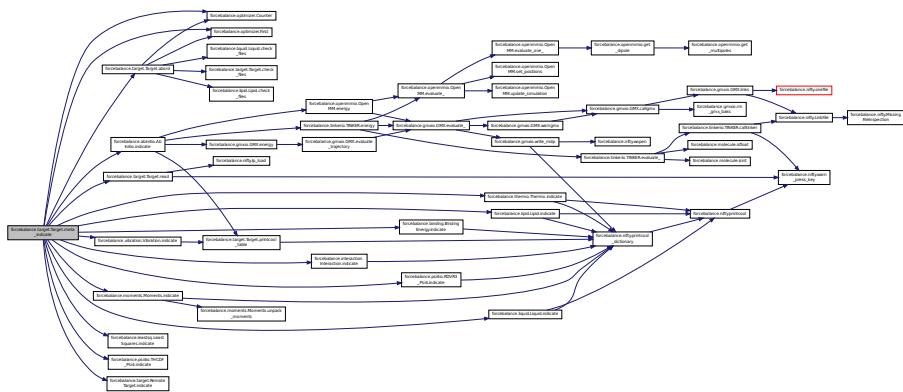


def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.

Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

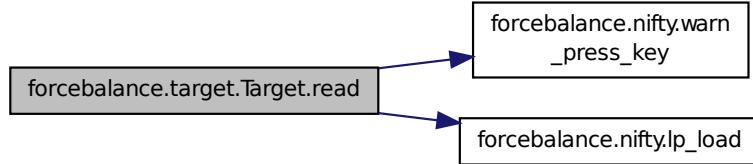
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

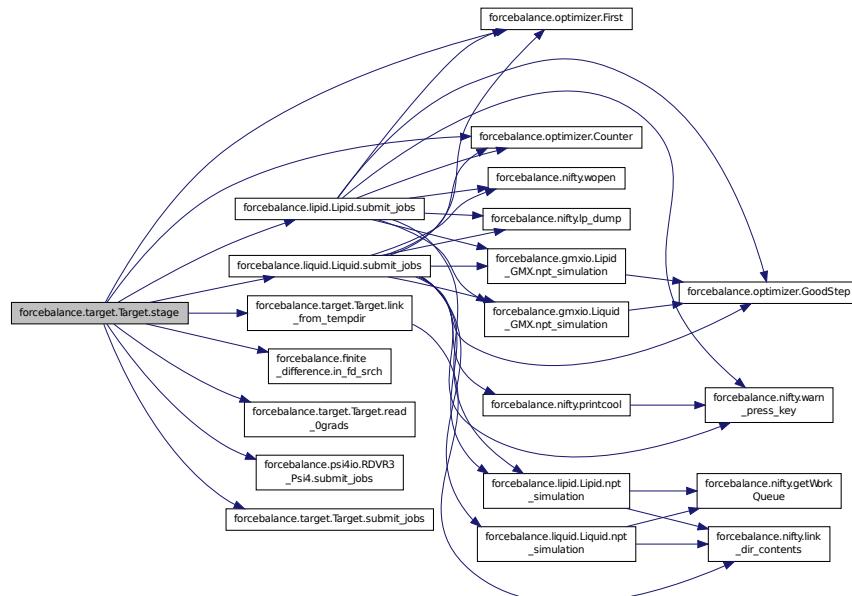
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



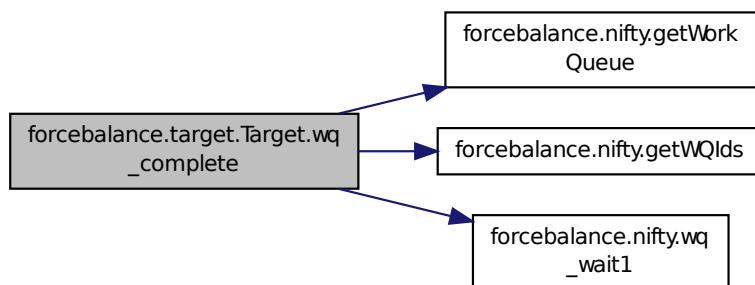
```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.binding.BindingEnergy.system_driver ( self, sysname ) [inherited] Definition at line 174 of file binding.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.11.4 Member Data Documentation

forcebalance.binding.BindingEnergy.energy_part [inherited] Definition at line 228 of file binding.py.

forcebalance.gmxio.BindingEnergy_GMX.engine_ Definition at line 1463 of file gmxio.py.

forcebalance.binding.BindingEnergy.engines [inherited] Build keyword dictionaries to pass to engine.

Create engine objects.

Definition at line 165 of file binding.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.binding.BindingEnergy.inter_opts [inherited] Definition at line 128 of file binding.py.

forcebalance.binding.BindingEnergy.objective [inherited] Definition at line 252 of file binding.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.binding.BindingEnergy.PrintDict [inherited] Definition at line 186 of file binding.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.binding.BindingEnergy.rmsd.part [inherited] Definition at line 226 of file binding.py.

forcebalance.binding.BindingEnergy.RMSDDict [inherited] Definition at line 187 of file binding.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number
The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

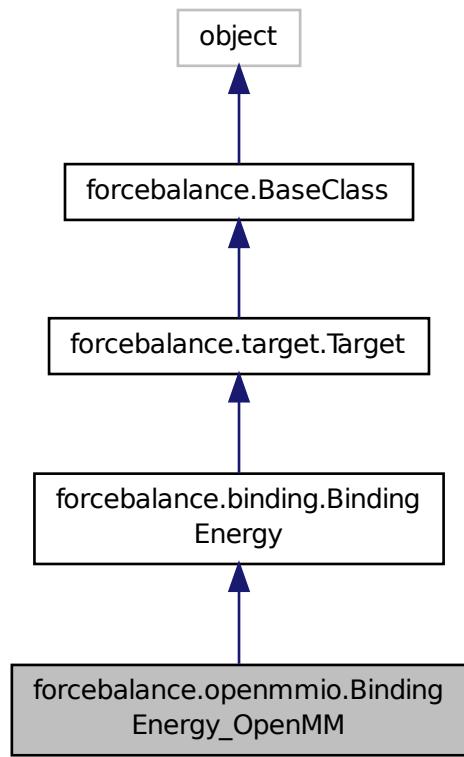
The documentation for this class was generated from the following file:

- [gmxio.py](#)

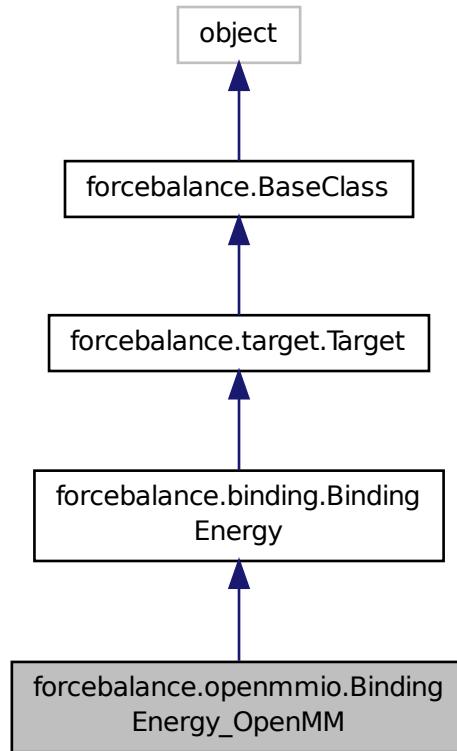
8.12 forcebalance.openmmio.BindingEnergy_OpenMM Class Reference

Binding energy matching using [OpenMM](#).

Inheritance diagram for forcebalance.openmmio.BindingEnergy_OpenMM:



Collaboration diagram for forcebalance.openmmio.BindingEnergy_OpenMM:



Public Member Functions

- def `_init_`
- def `system_driver`
- def `indicate`
- def `get`
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`

Back up the temporary directory if desired, delete it and then create a new one.

- def [check_files](#)

Check this directory for the presence of readable files when the 'read' option is set.

- def [read](#)

Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

- def [absrd](#)

Supply the correct directory specified by user's "read" option.

- def [maxrd](#)

Supply the latest existing temp-directory containing valid data.

- def [meta_indicate](#)

Wrap around the indicate function, so it can print to screen and also to a file.

- def [meta_get](#)

Wrapper around the get function.

- def [submit_jobs](#)

- def [stage](#)

Stages the directory for the target, and then launches Work Queue processes if any.

- def [wq_complete](#)

This method determines whether the Work Queue tasks for the current target have completed.

- def [printcool_table](#)

Print target information in an organized table format.

- def [__setattr__](#)

- def [set_option](#)

Public Attributes

- [engine_](#)

- [inter_opts](#)

- [engines](#)

Build keyword dictionaries to pass to engine.

- [PrintDict](#)

- [RMSDDict](#)

- [rmsd_part](#)

- [energy_part](#)

- [objective](#)

- [rd](#)

Root directory of the whole project.

- [pgrad](#)

Iteration where we turn on zero-gradient skipping.

- [tempbase](#)

Relative directory of target.

- [tempdir](#)

- [rundir](#)

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

- [FF](#)

Need the forcefield (here for now)

- [xct](#)

Counts how often the objective function was computed.

- [gct](#)

- `hct`
Counts how often the gradient was computed.
- `read_indicate`
Whether to read indicate.log from file when restarting an aborted run.
- `write_indicate`
Whether to write indicate.log at every iteration (true for all but remote.)
- `read_objective`
Whether to read objective.p from file when restarting an aborted run.
- `write_objective`
Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.12.1 Detailed Description

Binding energy matching using [OpenMM](#).

Definition at line 1179 of file openmmio.py.

8.12.2 Constructor & Destructor Documentation

`def forcebalance.openmmio.BindingEnergy_OpenMM.__init__(self, options, tgt_opts, forcefield)` Definition at line 1181 of file openmmio.py.

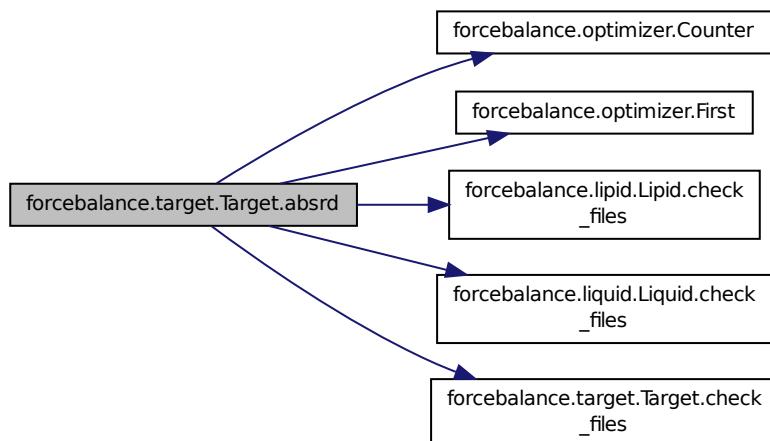
8.12.3 Member Function Documentation

`def forcebalance.BaseClass.__setattr__(self, key, value) [inherited]` Definition at line 28 of file __init__.py.

`def forcebalance.target.Target.absrd(self, inum = None) [inherited]` Supply the correct directory specified by user's "read" option.

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files( self, there ) [inherited] Check this directory for the presence  
of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.binding.BindingEnergy.get ( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 184 of file binding.py.
```

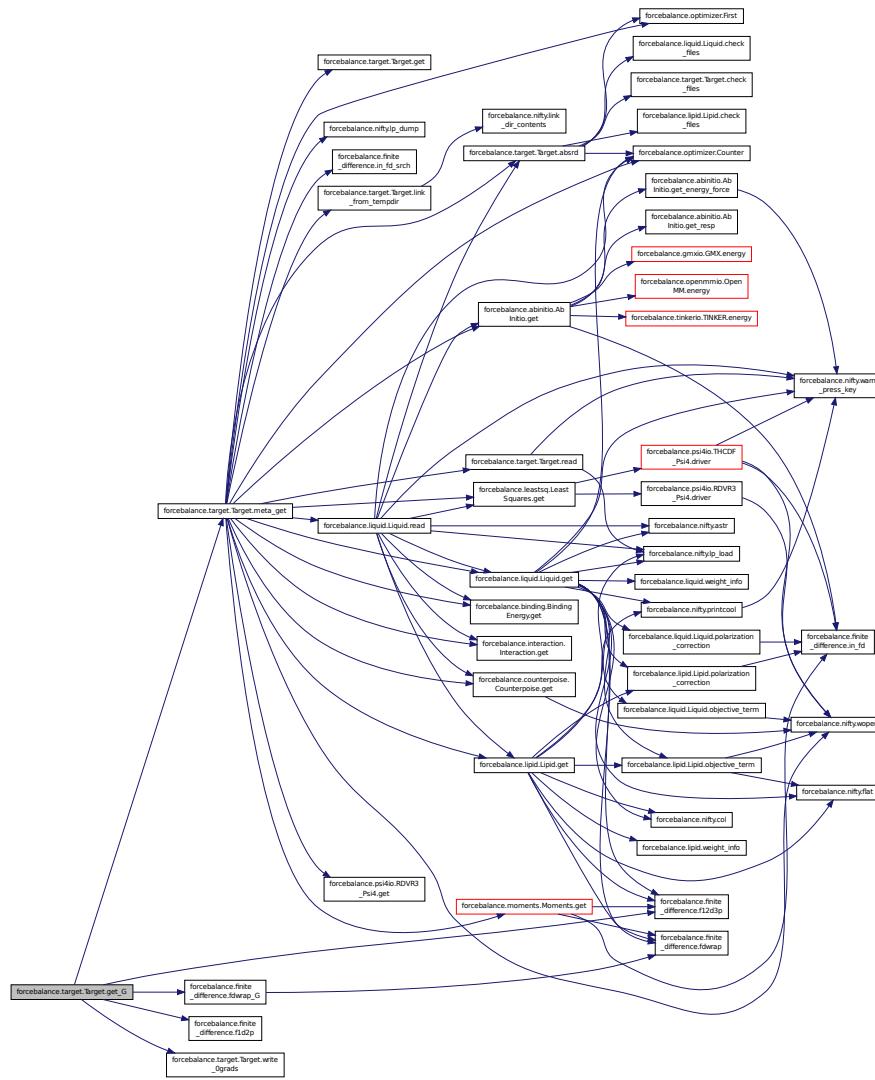
```
def forcebalance.target.Target.get_G( self, mvals = None ) [inherited] Computes the objective function  
contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1.pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



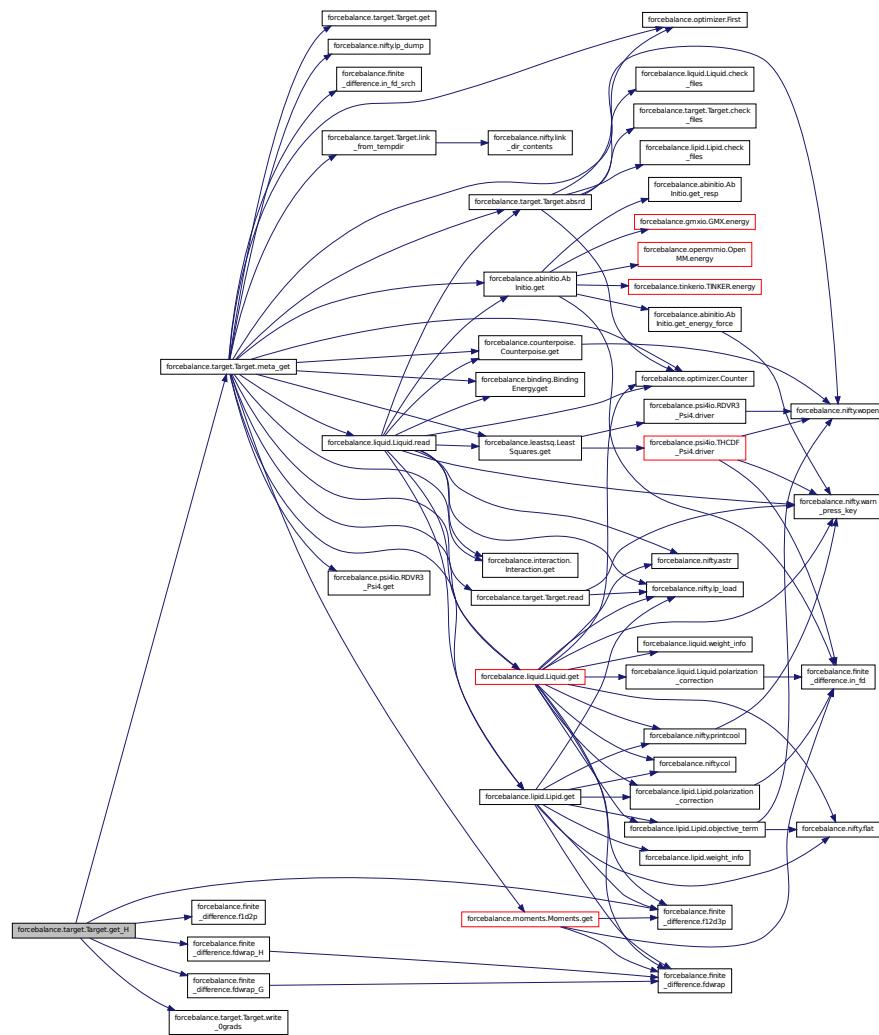
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

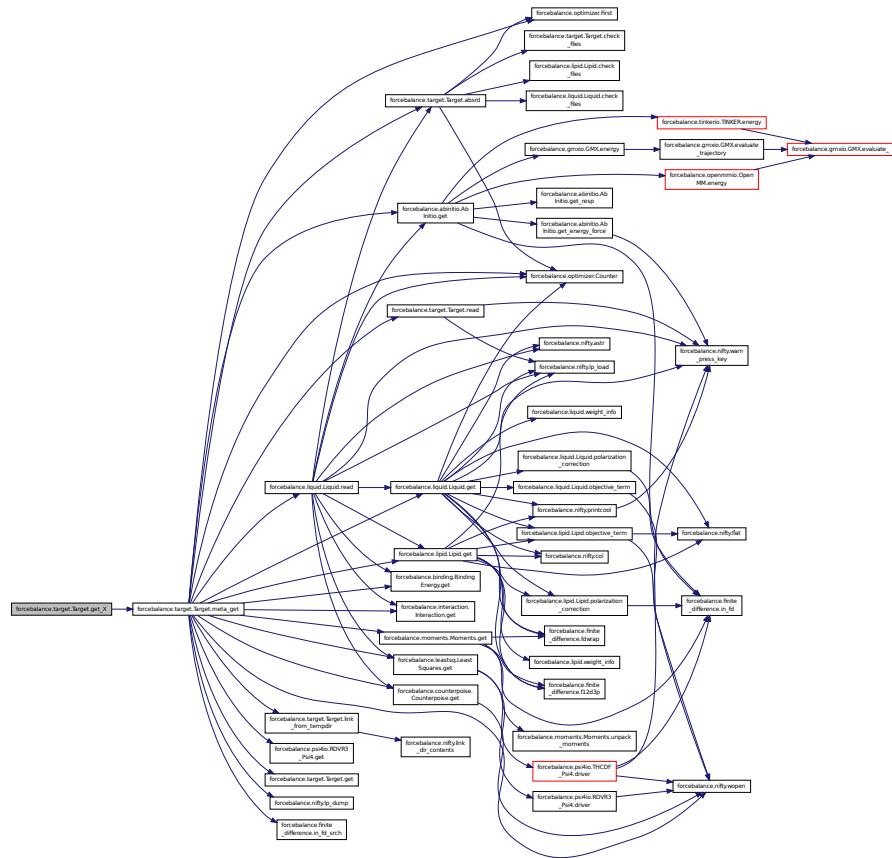
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

Here is the call graph for this function:



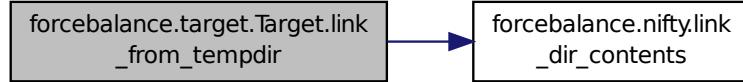
def forcebalance.binding.BindingEnergy.indicate (self) [inherited] Definition at line 178 of file binding.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

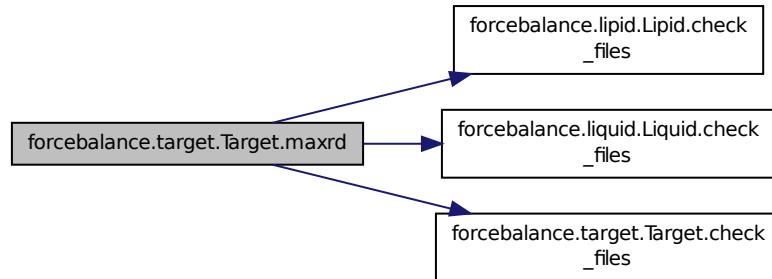
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

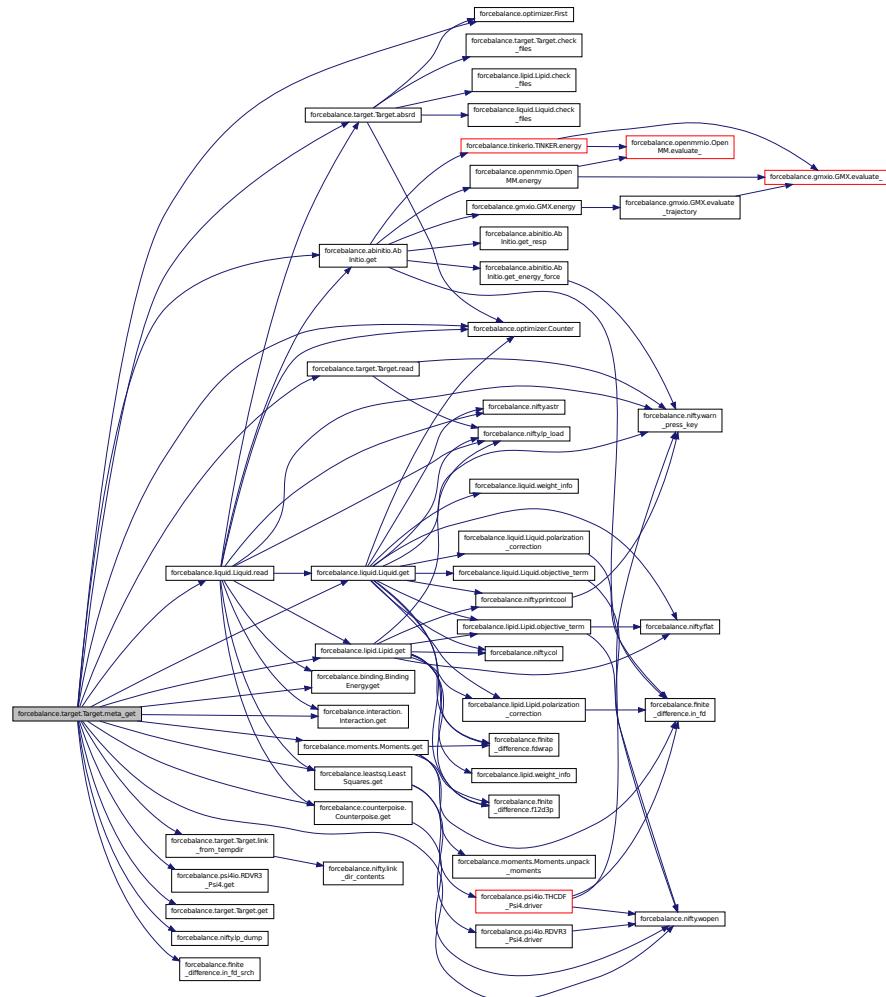


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

Here is the call graph for this function:

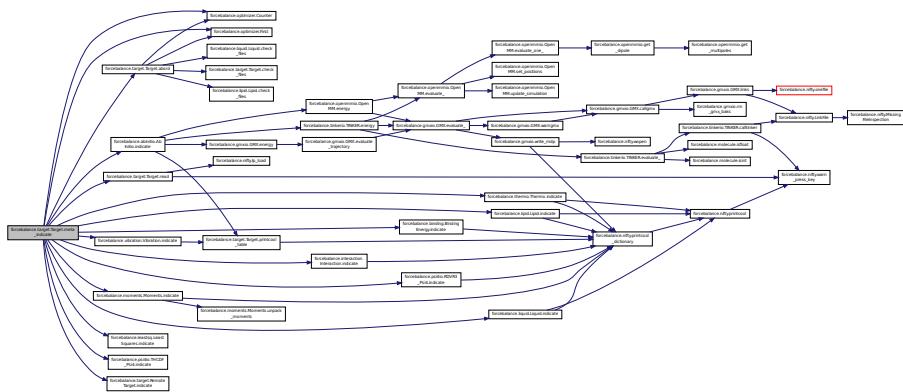


def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.

Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

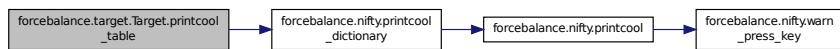
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

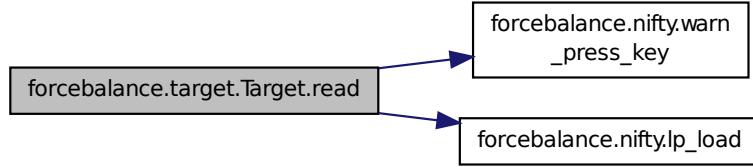
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

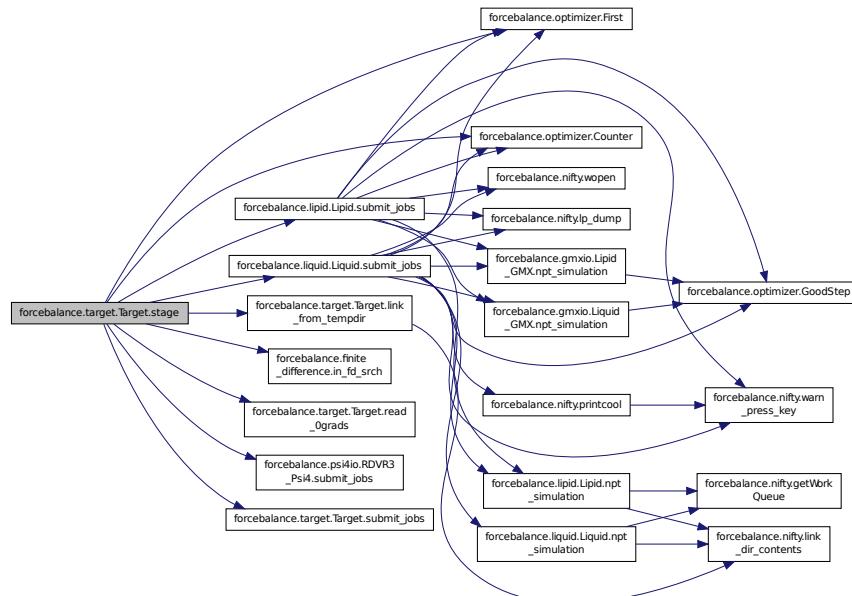
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



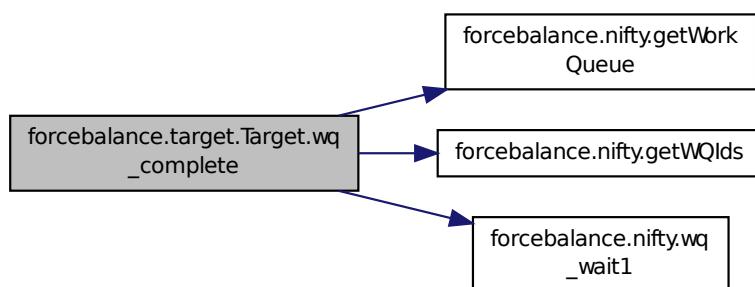
```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.binding.BindingEnergy.system_driver ( self, sysname ) [inherited] Definition at line 174 of file binding.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.12.4 Member Data Documentation

forcebalance.binding.BindingEnergy.energy_part [inherited] Definition at line 228 of file binding.py.

forcebalance.openmmio.BindingEnergy_OpenMM.engine_ Definition at line 1182 of file openmmio.py.

forcebalance.binding.BindingEnergy.engines [inherited] Build keyword dictionaries to pass to engine.

Create engine objects.

Definition at line 165 of file binding.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.binding.BindingEnergy.inter_opts [inherited] Definition at line 128 of file binding.py.

forcebalance.binding.BindingEnergy.objective [inherited] Definition at line 252 of file binding.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.binding.BindingEnergy.PrintDict [inherited] Definition at line 186 of file binding.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.binding.BindingEnergy.rmsd.part [inherited] Definition at line 226 of file binding.py.

forcebalance.binding.BindingEnergy.RMSDDict [inherited] Definition at line 187 of file binding.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number
The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

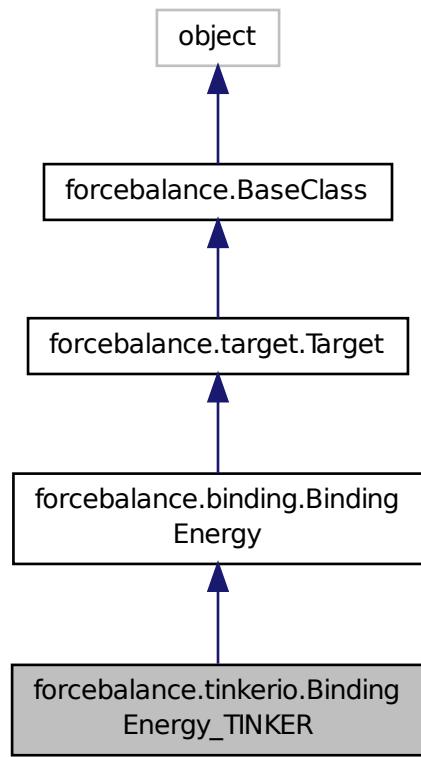
The documentation for this class was generated from the following file:

- [openmmio.py](#)

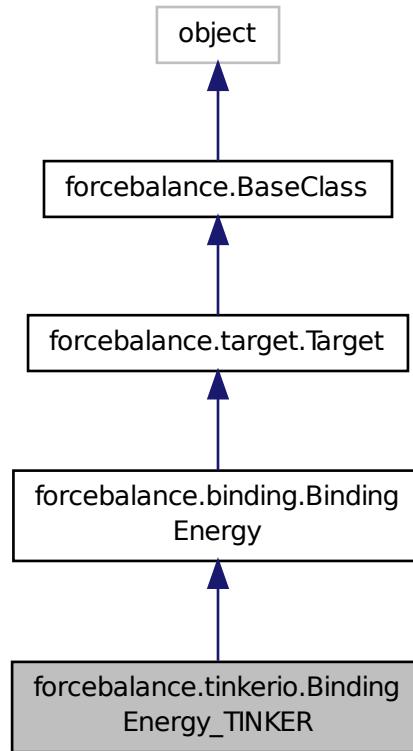
8.13 forcebalance.tinkerio.BindingEnergy_TINKER Class Reference

Binding energy matching using [TINKER](#).

Inheritance diagram for forcebalance.tinkerio.BindingEnergy_TINKER:



Collaboration diagram for forcebalance.tinkerio.BindingEnergy_TINKER:



Public Member Functions

- def `_init_`
- def `system_driver`
- def `indicate`
- def `get`
- def `get_X`

Computes the objective function contribution without any parametric derivatives.

- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.

- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.

- def `get_G`

Computes the objective function contribution and its gradient.

- def `get_H`

Computes the objective function contribution and its gradient / Hessian.

- def `link_from_tempdir`

- def `refresh_temp_directory`

Back up the temporary directory if desired, delete it and then create a new one.

- def [check_files](#)

Check this directory for the presence of readable files when the 'read' option is set.

- def [read](#)

Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

- def [absrd](#)

Supply the correct directory specified by user's "read" option.

- def [maxrd](#)

Supply the latest existing temp-directory containing valid data.

- def [meta_indicate](#)

Wrap around the indicate function, so it can print to screen and also to a file.

- def [meta_get](#)

Wrapper around the get function.

- def [submit_jobs](#)

- def [stage](#)

Stages the directory for the target, and then launches Work Queue processes if any.

- def [wq_complete](#)

This method determines whether the Work Queue tasks for the current target have completed.

- def [printcool_table](#)

Print target information in an organized table format.

- def [__setattr__](#)

- def [set_option](#)

Public Attributes

- [engine_](#)

- [inter_opts](#)

- [engines](#)

Build keyword dictionaries to pass to engine.

- [PrintDict](#)

- [RMSDDict](#)

- [rmsd_part](#)

- [energy_part](#)

- [objective](#)

- [rd](#)

Root directory of the whole project.

- [pgrad](#)

Iteration where we turn on zero-gradient skipping.

- [tempbase](#)

Relative directory of target.

- [tempdir](#)

- [rundir](#)

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

- [FF](#)

Need the forcefield (here for now)

- [xct](#)

Counts how often the objective function was computed.

- [gct](#)

- `hct`
Counts how often the gradient was computed.
- `read_indicate`
Whether to read `indicate.log` from file when restarting an aborted run.
- `write_indicate`
Whether to write `indicate.log` at every iteration (true for all but remote.)
- `read_objective`
Whether to read `objective.p` from file when restarting an aborted run.
- `write_objective`
Whether to write `objective.p` at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.13.1 Detailed Description

Binding energy matching using [TINKER](#).

Definition at line 1078 of file `tinkerio.py`.

8.13.2 Constructor & Destructor Documentation

```
def forcebalance.tinkerio.BindingEnergy_TINKER.__init__( self, options, tgt_opts, forcefield )
```

Definition at line 1079 of file `tinkerio.py`.

8.13.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited]
```

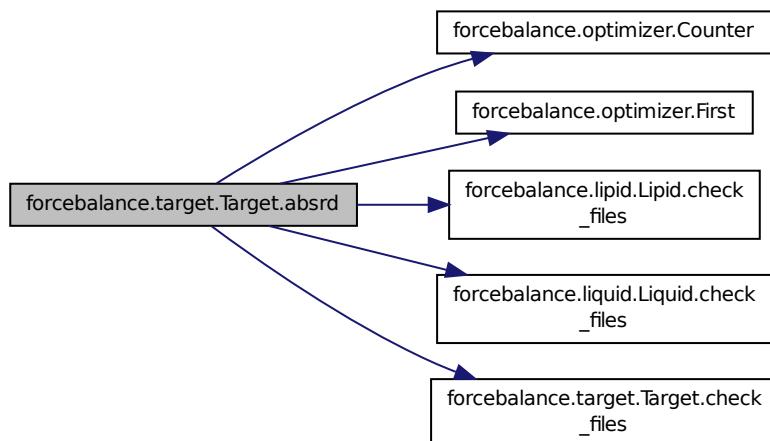
Definition at line 28 of file `__init__.py`.

```
def forcebalance.target.Target.absrd( self, inum = None ) [inherited]
```

Supply the correct directory specified by user's "read" option.

Definition at line 393 of file `target.py`.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files( self, there ) [inherited] Check this directory for the presence  
of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.binding.BindingEnergy.get ( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 184 of file binding.py.
```

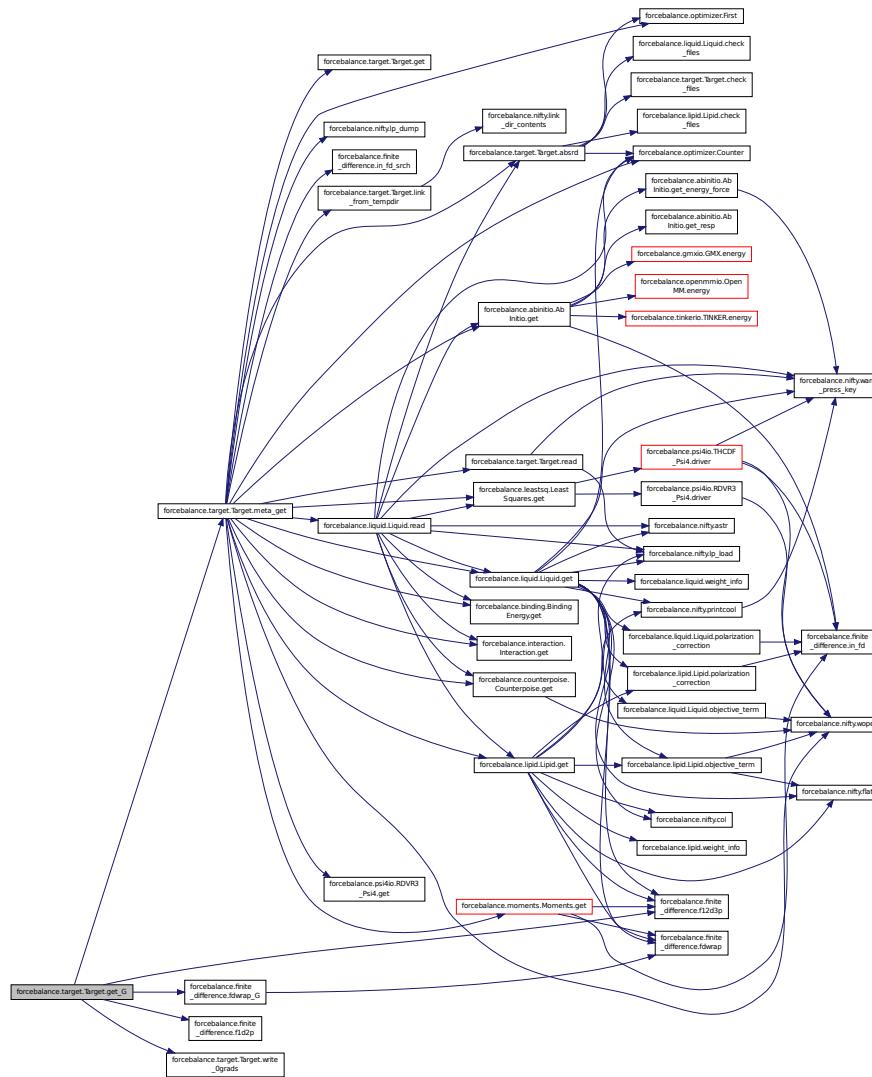
```
def forcebalance.target.Target.get_G( self, mvals = None ) [inherited] Computes the objective function  
contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1.pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



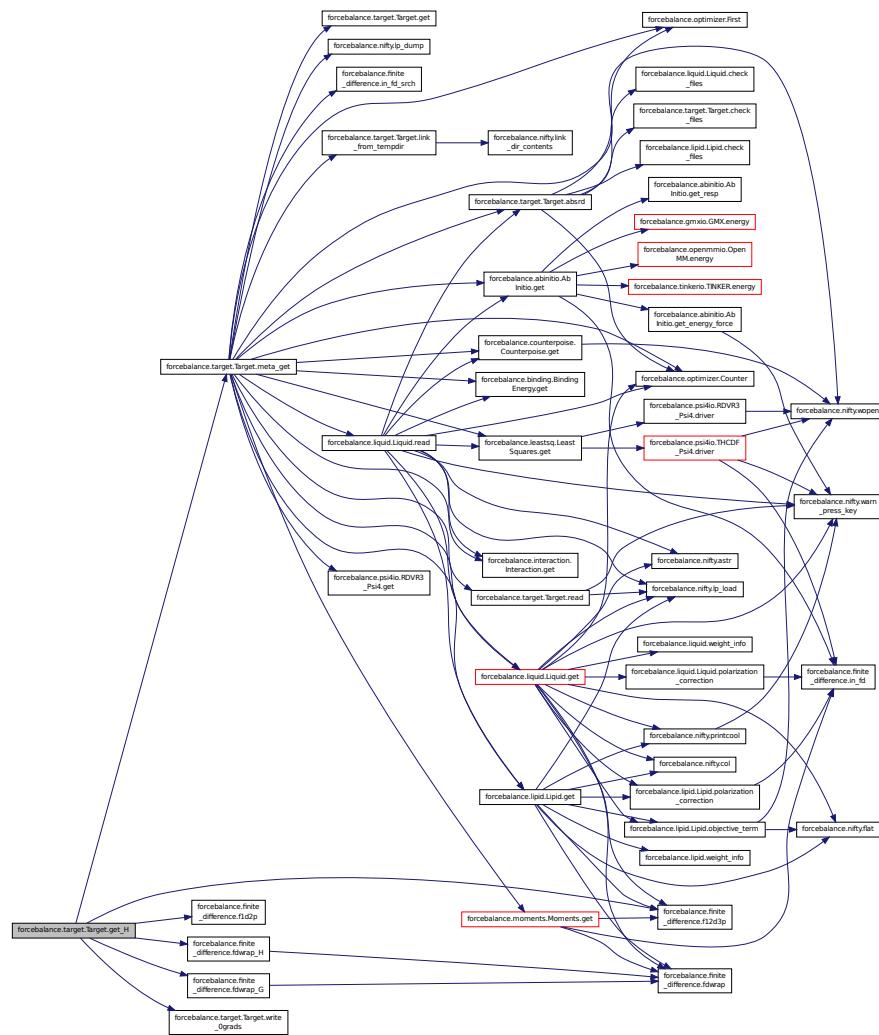
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

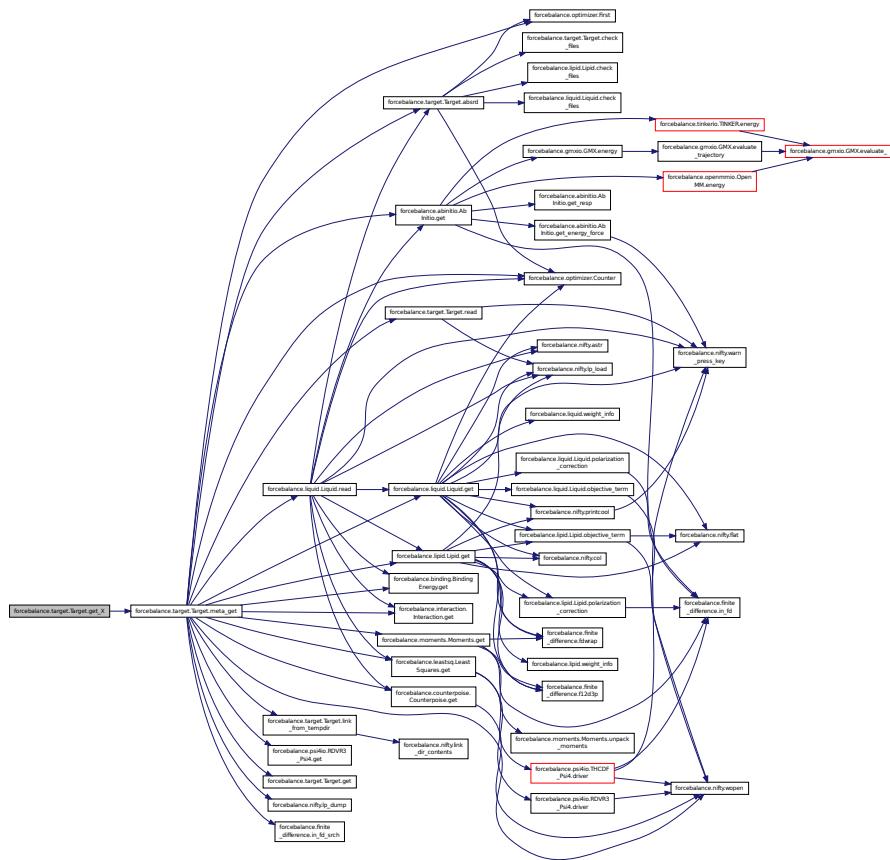
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

Here is the call graph for this function:



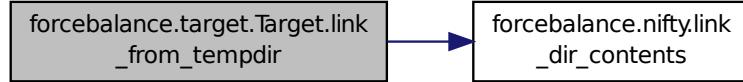
```
def forcebalance.binding.BindingEnergy.indicate( self ) [inherited] Definition at line 178 of file binding.py.
```

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

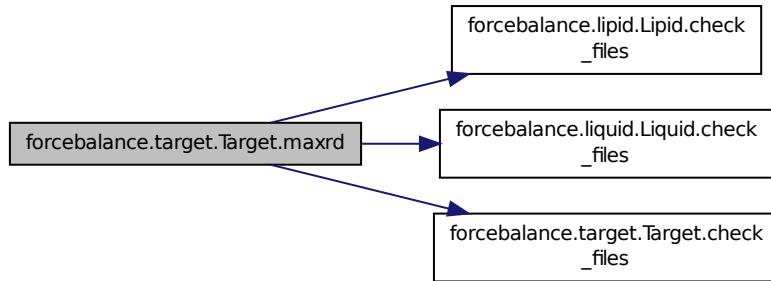
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

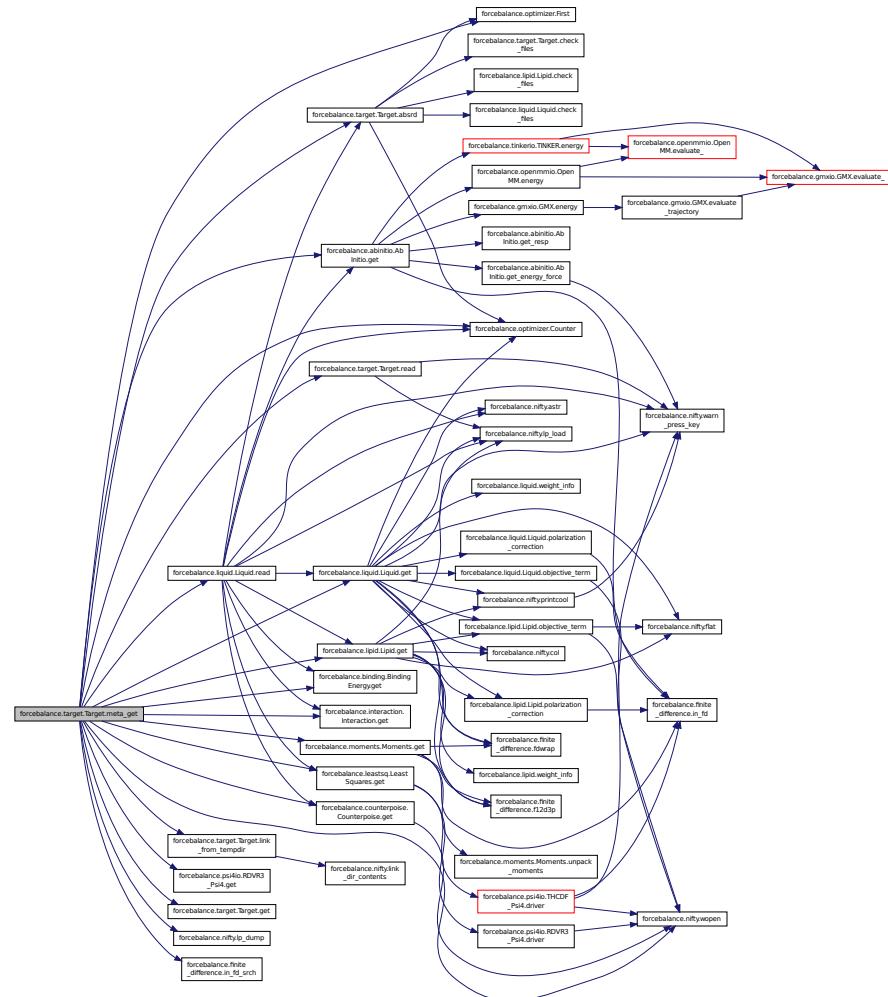


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

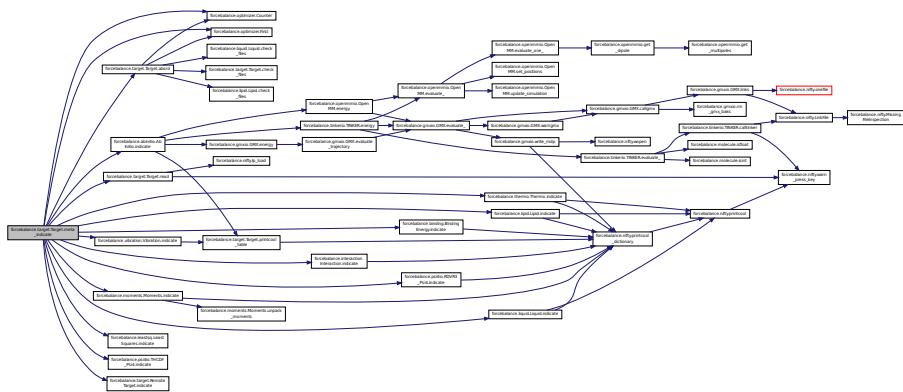
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

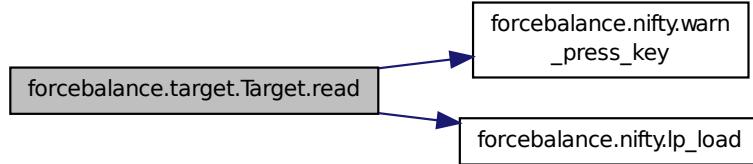
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

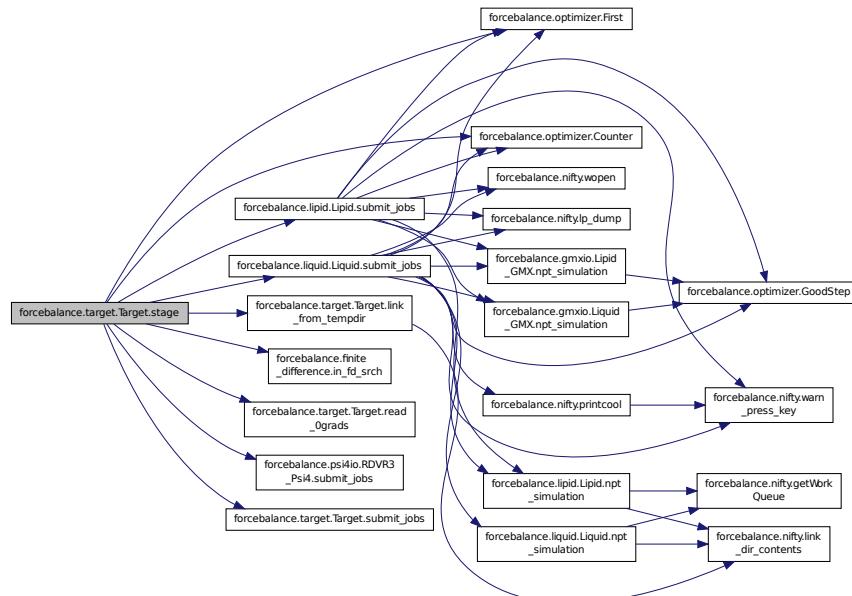
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



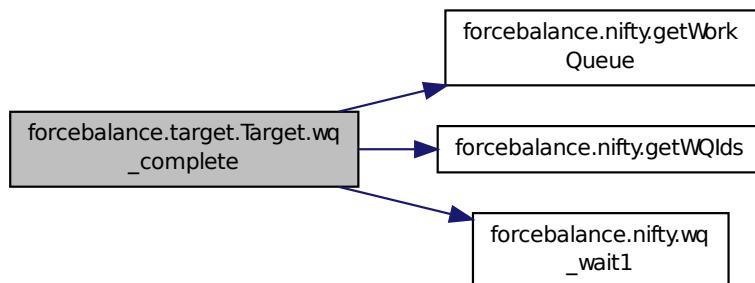
```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.binding.BindingEnergy.system_driver ( self, sysname ) [inherited] Definition at line 174 of file binding.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.13.4 Member Data Documentation

forcebalance.binding.BindingEnergy.energy_part [inherited] Definition at line 228 of file binding.py.

forcebalance.tinkerio.BindingEnergy_TINKER.engine_ Definition at line 1080 of file tinkerio.py.

forcebalance.binding.BindingEnergy.engines [inherited] Build keyword dictionaries to pass to engine.

Create engine objects.

Definition at line 165 of file binding.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.binding.BindingEnergy.inter_opts [inherited] Definition at line 128 of file binding.py.

forcebalance.binding.BindingEnergy.objective [inherited] Definition at line 252 of file binding.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.binding.BindingEnergy.PrintDict [inherited] Definition at line 186 of file binding.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.binding.BindingEnergy.rmsd.part [inherited] Definition at line 226 of file binding.py.

forcebalance.binding.BindingEnergy.RMSDDict [inherited] Definition at line 187 of file binding.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number
The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

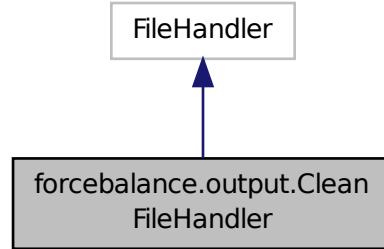
The documentation for this class was generated from the following file:

- [tinkerio.py](#)

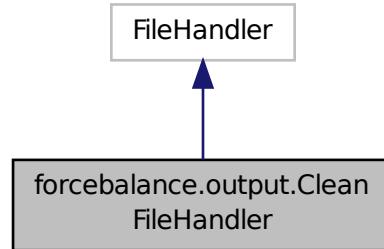
8.14 forcebalance.output.CleanFileHandler Class Reference

File handler that does not write terminal escape codes and carriage returns to files.

Inheritance diagram for forcebalance.output.CleanFileHandler:



Collaboration diagram for forcebalance.output.CleanFileHandler:



Public Member Functions

- def [emit](#)

8.14.1 Detailed Description

File handler that does not write terminal escape codes and carriage returns to files.

Use this when writing to a file that will probably not be viewed in a terminal

Definition at line 69 of file [output.py](#).

8.14.2 Member Function Documentation

def forcebalance.output.CleanFileHandler.emit (self, record) Definition at line 70 of file [output.py](#).

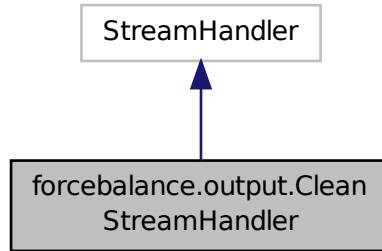
The documentation for this class was generated from the following file:

- [output.py](#)

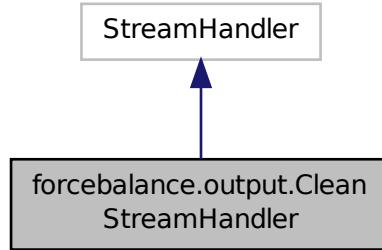
8.15 forcebalance.output.CleanStreamHandler Class Reference

Similar to [RawStreamHandler](#) except it does not write terminal escape codes.

Inheritance diagram for forcebalance.output.CleanStreamHandler:



Collaboration diagram for forcebalance.output.CleanStreamHandler:



Public Member Functions

- def `__init__`
- def `emit`

8.15.1 Detailed Description

Similar to [RawStreamHandler](#) except it does not write terminal escape codes.

Use this for 'plain' terminal output without any fancy colors or formatting

Definition at line 56 of file `output.py`.

8.15.2 Constructor & Destructor Documentation

def forcebalance.output.CleanStreamHandler.__init__ (self, stream = sys.stdout) Definition at line 57 of file `output.py`.

8.15.3 Member Function Documentation

```
def forcebalance.output.CleanStreamHandler.emit ( self, record )
```

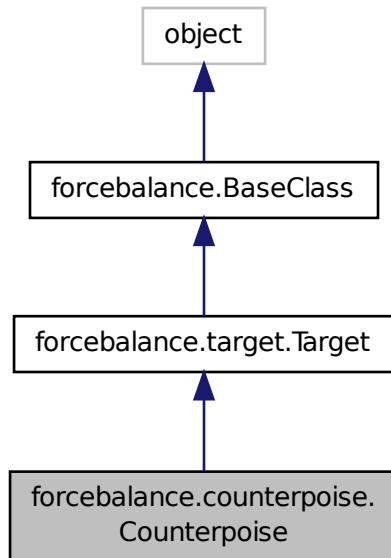
Definition at line 60 of file output.py.
The documentation for this class was generated from the following file:

- [output.py](#)

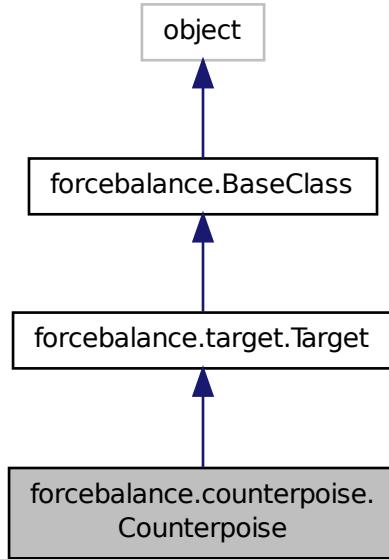
8.16 forcebalance.counterpoise.Counterpoise Class Reference

Target subclass for matching the counterpoise correction.

Inheritance diagram for forcebalance.counterpoise.Counterpoise:



Collaboration diagram for forcebalance.counterpoise.Counterpoise:



Public Member Functions

- def `__init__`
To instantiate `Counterpoise`, we read the coordinates and counterpoise data.
- def `loadxyz`
Parse an XYZ file which contains several xyz coordinates, and return their elements.
- def `load_cp`
Load in the counterpoise data, which is easy; the file consists of floating point numbers separated by newlines.
- def `get`
Gets the objective function for fitting the counterpoise correction.
- def `get_X`
Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
Computes the objective function contribution and its gradient.
- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.

- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `_setattr_`
- def `set_option`

Public Attributes

- `xyzs`
Number of snapshots.
- `cpqm`
Counterpoise correction data.
- `na`
Number of atoms.
- `ns`
- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`
Relative directory of target.
- `tempdir`
- `rundir`
`self.tempdir = os.path.join('temp',self.name)` *The directory in which the simulation is running - this can be updated.*
- `FF`
Need the forcefield (here for now)
- `xct`
Counts how often the objective function was computed.
- `gct`
Counts how often the gradient was computed.
- `hct`
Counts how often the Hessian was computed.

- `read_indicate`
Whether to read indicate.log from file when restarting an aborted run.
- `write_indicate`
Whether to write indicate.log at every iteration (true for all but remote.)
- `read_objective`
Whether to read objective.p from file when restarting an aborted run.
- `write_objective`
Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.16.1 Detailed Description

Target subclass for matching the counterpoise correction.

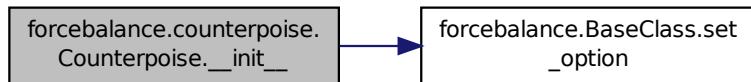
Definition at line 34 of file counterpoise.py.

8.16.2 Constructor & Destructor Documentation

`def forcebalance.counterpoise.Counterpoise.__init__ (self, options, tgt_opts, forcefield)` To instantiate Counterpoise, we read the coordinates and counterpoise data.

Definition at line 38 of file counterpoise.py.

Here is the call graph for this function:



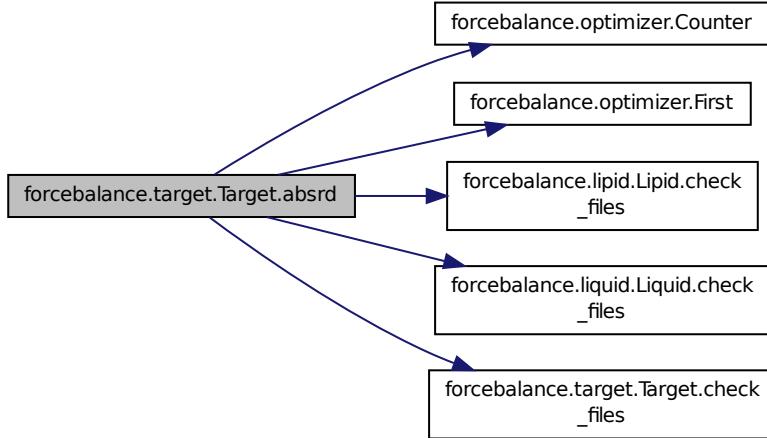
8.16.3 Member Function Documentation

`def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited]` Definition at line 28 of file __init__.py.

`def forcebalance.target.Target.absrd (self, inum = None) [inherited]` Supply the correct directory specified by user's "read" option.

Definition at line 393 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.check_files(self, there) [inherited] Check this directory for the presence of readable files when the 'read' option is set.

Definition at line 364 of file target.py.

def forcebalance.counterpoise.Counterpoise.get(self, mvals, AGrad = False, AHess = False) Gets the objective function for fitting the counterpoise correction.

As opposed to AbInitio_GMXX2, which calls an external program, this script actually computes the empirical interaction given the force field parameters.

It loops through the snapshots and atom pairs, and computes pairwise contributions to an energy term according to hard-coded functional forms.

One potential issue is that we go through all atom pairs instead of looking only at atom pairs between different fragments. This means that even for two infinitely separated fragments it will predict a finite CP correction. While it might be okay to apply such a potential in practice, there will be some issues for the fitting. Thus, we assume the last snapshot to be CP-free and subtract that value of the potential back out.

Note that forces and parametric derivatives are not implemented.

Parameters

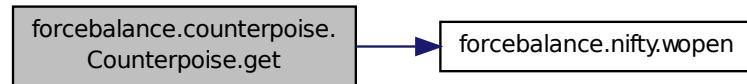
in	<i>mvals</i>	Mathematical parameter values
in	<i>AGrad</i>	Switch to turn on analytic gradient (not implemented)
in	<i>AHess</i>	Switch to turn on analytic Hessian (not implemented)

Returns

Answer Contribution to the objective function

Definition at line 125 of file counterpoise.py.

Here is the call graph for this function:



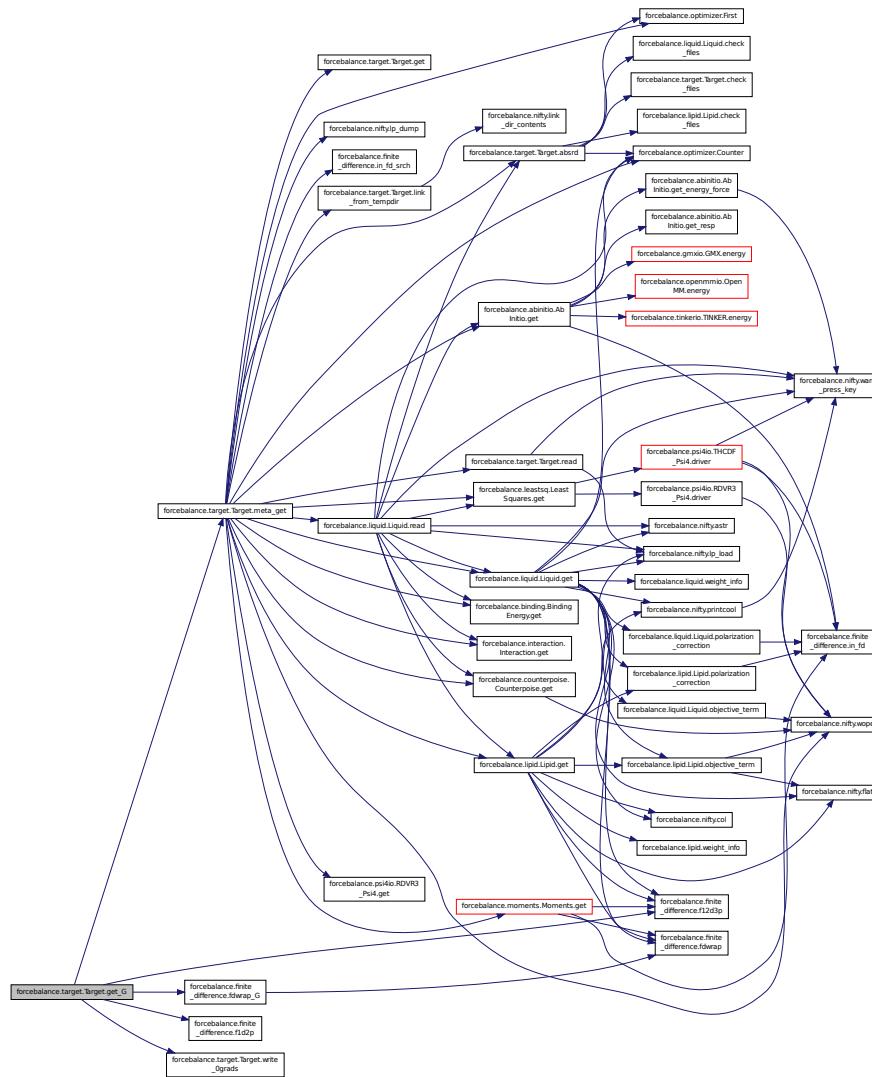
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1.pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



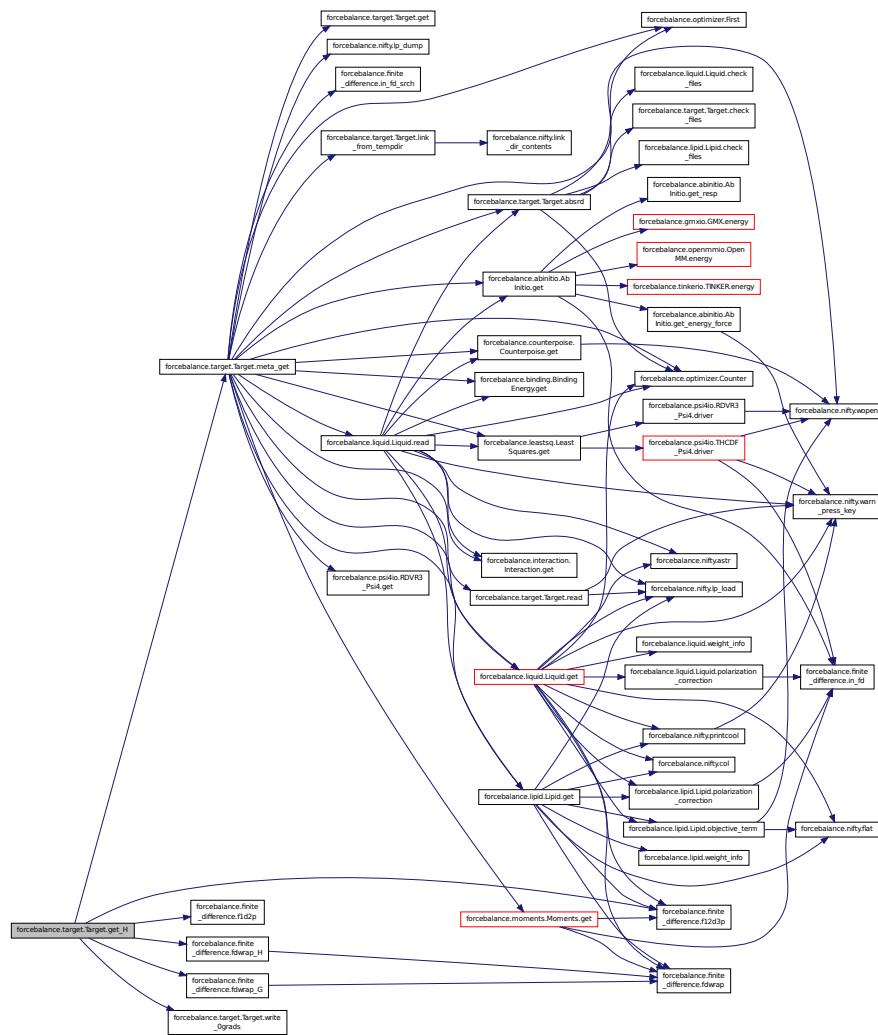
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

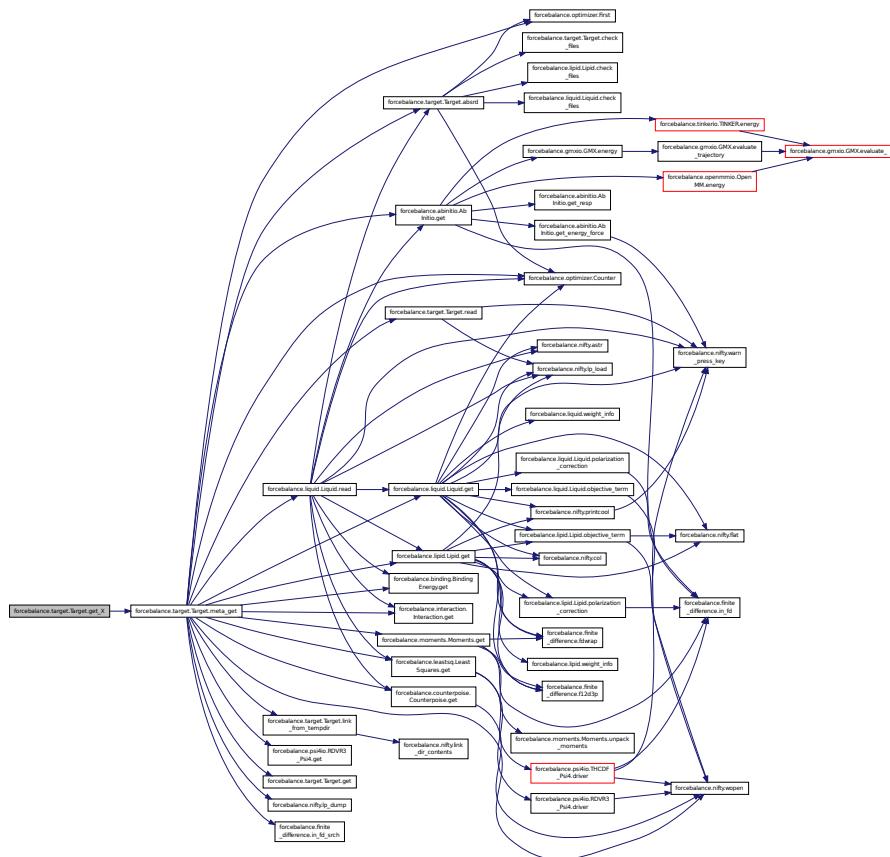
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

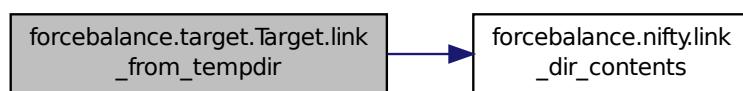
Definition at line 184 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

Here is the call graph for this function:



def forcebalance.counterpoise.Counterpoise.load_cp (self, fnm) Load in the counterpoise data, which is easy; the file consists of floating point numbers separated by newlines.

Definition at line 96 of file counterpoise.py.

```
def forcebalance.counterpoise.Counterpoise.loadxyz ( self, fnm ) Parse an XYZ file which contains several xyz coordinates, and return their elements.
```

Parameters

in	<i>fnm</i>	The input XYZ file name
----	------------	-------------------------

Returns

elem A list of chemical elements in the XYZ file
xyzs A list of XYZ coordinates (number of snapshots times number of atoms)

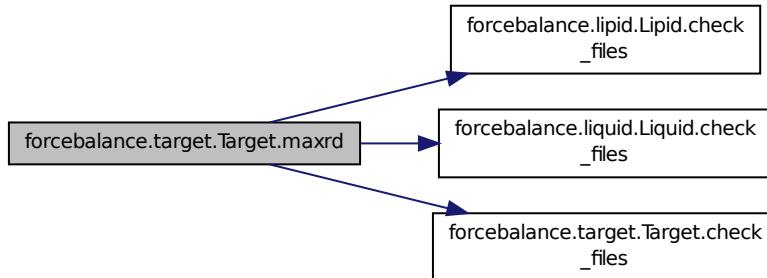
Todo I should probably put this into a more general library for reading coordinates.

Definition at line 64 of file counterpoise.py.

def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

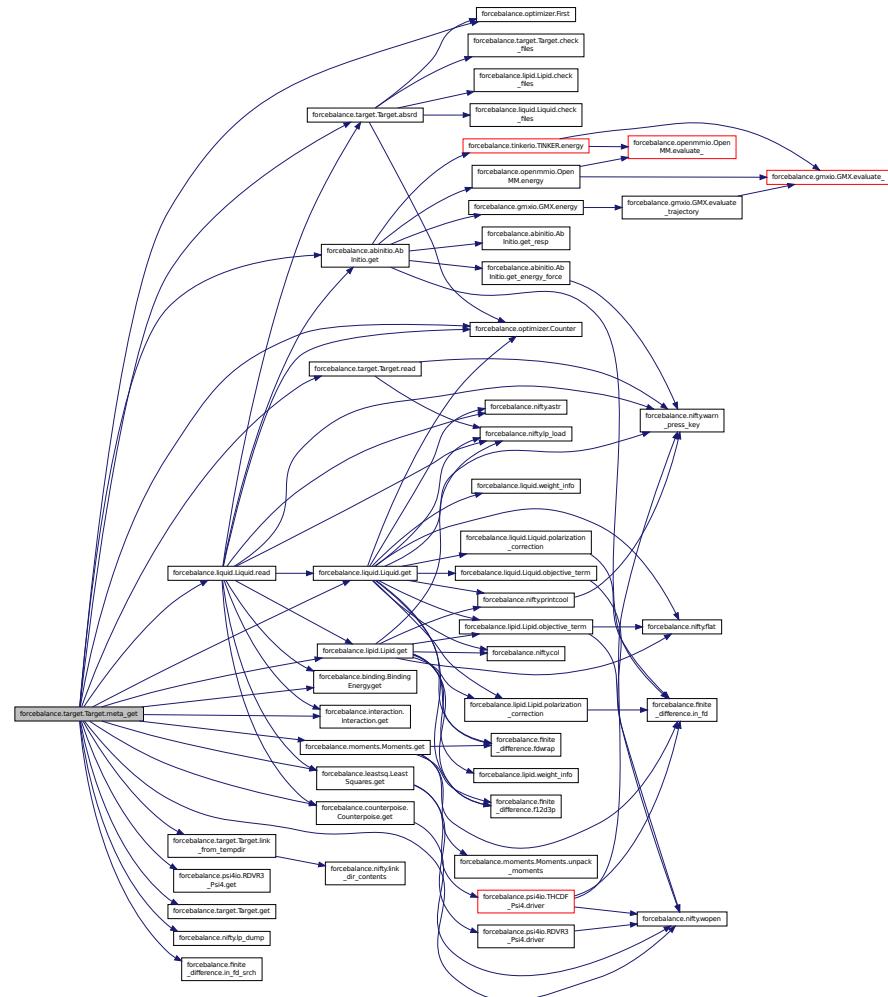


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

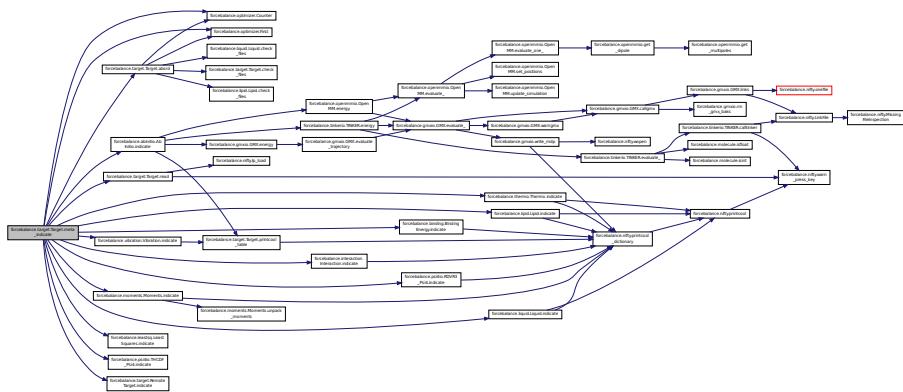
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

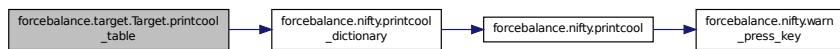
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

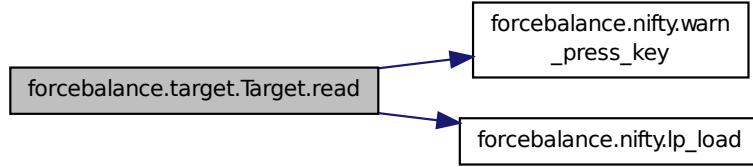
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

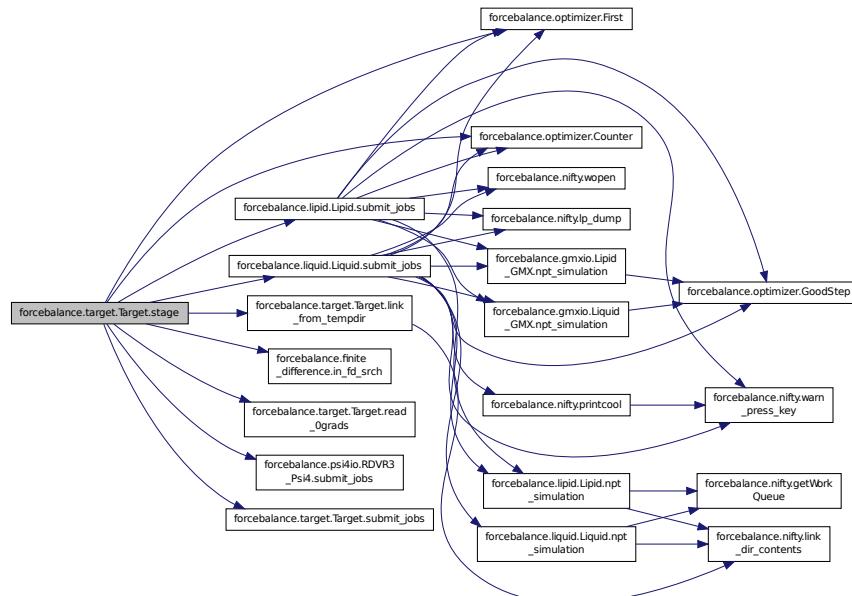
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

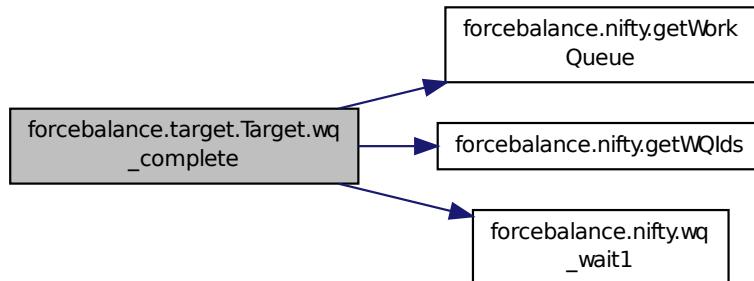


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_0grads( self, Ans ) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.16.4 Member Data Documentation

forcebalance.counterpoise.Counterpoise.cpqm [Counterpoise](#) correction data.

Definition at line 54 of file counterpoise.py.

forcebalance.target.Target.FF [\[inherited\]](#) Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [\[inherited\]](#) Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [\[inherited\]](#) Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.counterpoise.Counterpoise.na Number of atoms.

Definition at line 77 of file counterpoise.py.

forcebalance.counterpoise.Counterpoise.ns Definition at line 90 of file counterpoise.py.

forcebalance.target.Target.pgrad [\[inherited\]](#) Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [\[inherited\]](#) Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [\[inherited\]](#) Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [\[inherited\]](#) Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [\[inherited\]](#) Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [\[inherited\]](#) self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [**inherited**] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [**inherited**] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [**inherited**] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

forcebalance.counterpoise.Counterpoise.xyzs Number of snapshots.

XYZ elements and coordinates

Definition at line 52 of file counterpoise.py.

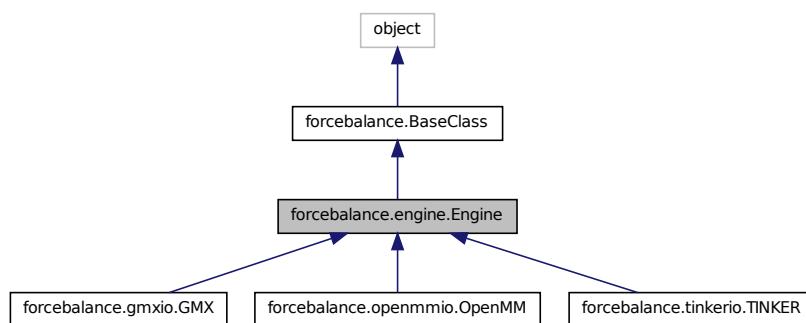
The documentation for this class was generated from the following file:

- [counterpoise.py](#)

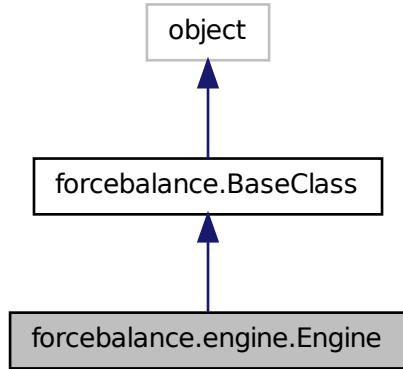
8.17 forcebalance.engine.Engine Class Reference

Base class for all engines.

Inheritance diagram for forcebalance.engine.Engine:



Collaboration diagram for forcebalance.engine.Engine:



Public Member Functions

- def `_init_`
- def `setopts`
- def `readsrc`
- def `prepare`
- def `__setattr__`
- def `set_option`

Public Attributes

- `name`
 - `verbose`
 - `target`
- Engines can get properties from the Target that creates them.*
- `root`
 - `srcdir`
 - `tempdir`
 - `FF`
 - `verbose_options`
 - `PrintOptionDict`

8.17.1 Detailed Description

Base class for all engines.

1. Introduction

In ForceBalance an `Engine` represents a molecular dynamics code and the calculations that may be carried out with that code.

1. Purpose

Previously system calls to MD software have been made by the Target. Duplication of code was occurring, because different Targets were carrying out the same type of calculation.

1. Also

Target objects should contain [Engine](#) objects, because OpenMM [Engine](#) objects need to be initialized at the start of a calculation.

Definition at line 41 of file engine.py.

8.17.2 Constructor & Destructor Documentation

def forcebalance.engine.Engine.__init__ (self, name = "engine", kwargs) Definition at line 44 of file engine.py.

8.17.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited] Definition at line 28 of file __init__.py.

def forcebalance.engine.Engine.prepare (self, kwargs) Definition at line 95 of file engine.py.

def forcebalance.engine.Engine.readsrc (self, kwargs) Definition at line 92 of file engine.py.

def forcebalance.BaseClass.set_option (self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.engine.Engine.setopts (self, kwargs) Definition at line 89 of file engine.py.

8.17.4 Member Data Documentation

forcebalance.engine.Engine.FF Definition at line 65 of file engine.py.

forcebalance.engine.Engine.name Definition at line 48 of file engine.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.engine.Engine.root Definition at line 56 of file engine.py.

forcebalance.engine.Engine.srcdir Definition at line 57 of file engine.py.

forcebalance.engine.Engine.target Engines can get properties from the Target that creates them.
Definition at line 55 of file engine.py.

forcebalance.engine.Engine.tempdir Definition at line 58 of file engine.py.

forcebalance.engine.Engine.verbose Definition at line 50 of file engine.py.

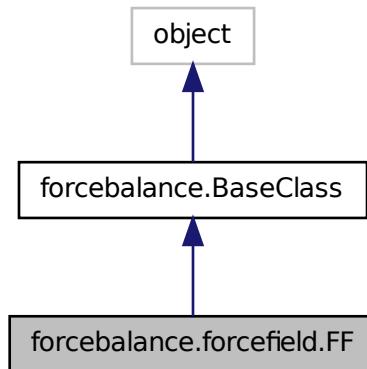
forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.
The documentation for this class was generated from the following file:

- [engine.py](#)

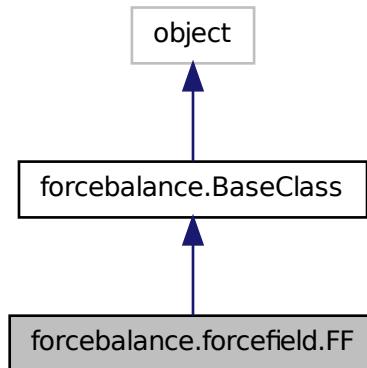
8.18 forcebalance.forcefield.FF Class Reference

Force field class.

Inheritance diagram for forcebalance.forcefield.FF:



Collaboration diagram for forcebalance.forcefield.FF:



Public Member Functions

- def `__init__`
Instantiation of force field class.
- def `addff`
Parse a force field file and add it to the class.
- def `addff_txt`

- def `addff_xml`
Parse a text force field and create several important instance variables.
- def `make`
Create a new force field using provided parameter values.
- def `make_redirect`
- def `find_spacings`
- def `create_pvals`
Converts mathematical to physical parameters.
- def `create_mvals`
Converts physical to mathematical parameters.
- def `rsmake`
Create the rescaling factors for the coordinate transformation in parameter space.
- def `mktransmat`
Create the transformation matrix to rescale and rotate the mathematical parameters.
- def `list_map`
Create the plist, which is like a reversed version of the parameter map.
- def `print_map`
Prints out the (physical or mathematical) parameter indices, IDs and values in a visually appealing way.
- def `sprint_map`
Prints out the (physical or mathematical) parameter indices, IDs and values to a string.
- def `assign_p0`
Assign physical parameter values to the 'pvals0' array.
- def `assign_field`
Record the locations of a parameter in a txt file; [[file name, line number, field number, and multiplier]].
- def `__eq__`
- def `__setattr__`
- def `set_option`

Public Attributes

- `ffdata`
As these options proliferate, the force field class becomes less standalone.
- `ffdata_isxml`
- `map`
The mapping of interaction type -> parameter number.
- `plist`
The listing of parameter number -> interaction types.
- `patoms`
A listing of parameter number -> atoms involved.
- `pfields`
A list where pfields[pnum] = [file',line,field,mult,cmd], basically a new way to modify force field files; when we modify the force field file, we go to the specific line/field in a given file and change the number.
- `rs`
List of rescaling factors.
- `tm`
The transformation matrix for mathematical -> physical parameters.
- `tml`

The transpose of the transformation matrix.

- [excision](#)

Indices to exclude from optimization / Hessian inversion.

- [np](#)

The total number of parameters.

- [pvals0](#)

Initial value of physical parameters.

- [Readers](#)

A dictionary of force field reader classes.

- [atomnames](#)

A list of atom names (this is new, for ESP fitting)

- [FFAtomTypes](#)

WORK IN PROGRESS ## This is a dictionary of { 'AtomType':{ 'Mass' : float, 'Charge' : float, 'ParticleType' : string ('A', 'S', or 'D'), 'AtomicNumber' : int } }.

- [FFMolecules](#)

- [redirect](#)

Creates plist from map.

- [linedestroy_save](#)

Destruction dictionary (experimental).

- [prmdestroy_save](#)

- [linedestroy_this](#)

- [prmdestroy_this](#)

- [tinkerprm](#)

- [openmmxml](#)

- [qmap](#)

- [qid](#)

- [qid2](#)

- [verbose_options](#)

- [PrintOptionDict](#)

8.18.1 Detailed Description

Force field class.

This class contains all methods for force field manipulation. To create an instance of this class, an input file is required containing the list of force field file names. Everything else inside this class pertaining to force field generation is self-contained.

For details on force field parsing, see the detailed documentation for addff.

Definition at line 197 of file forcefield.py.

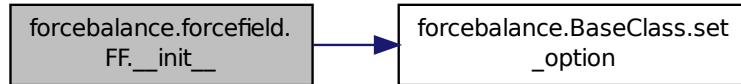
8.18.2 Constructor & Destructor Documentation

def forcebalance.forcefield.FF.__init__(self, options, verbose = True) Instantiation of force field class.

Many variables here are initialized to zero, but they are filled out by methods like addff, rsmake, and mktransmat.

Definition at line 205 of file forcefield.py.

Here is the call graph for this function:



8.18.3 Member Function Documentation

def forcebalance.forcefield.FF.eq_(self, other) Definition at line 1185 of file forcefield.py.

def forcebalance.BaseClass.__setattr__(self, key, value) [inherited] Definition at line 28 of file __init__.py.

def forcebalance.forcefield.FF.addff(self, fname) Parse a force field file and add it to the class.

First, figure out the type of force field file. This is done either by explicitly specifying the type using for example, `ffname force_field.xml:openmm` or we figure it out by looking at the file extension.

Next, parse the file. Currently we support two classes of files - text and XML. The two types are treated very differently; for XML we use the parsers in libxml (via the python lxml module), and for text files we have our own in-house parsing class. Within text files, there is also a specialized GROMACS and TINKER parser as well as a generic text parser.

The job of the parser is to determine the following things: 1) Read the user-specified selection of parameters being fitted 2) Build a mapping (dictionary) of parameter identifier \rightarrow index in parameter vector 3) Build a list of physical parameter values 4) Figure out where to replace the parameter values in the force field file when the values are changed 5) Figure out which parameters need to be repeated or sign-flipped

Generally speaking, each parameter value in the force field file has a unique parameter identifier . The identifier consists of three parts - the interaction type, the parameter subtype (within that interaction type), and the atoms involved.

--- If XML: ---

The force field file is read in using the lxml Python module. Specify which parameter you want to fit using by adding a 'parameterize' element to the end of the force field XML file, like so.

```
1 <AmoebaVdwForce type="BUFFERED-14-7">
2   <Vdw class="74" sigma="0.2655" epsilon="0.056484" reduction="0.910" parameterize="sigma, epsilon,
      reduction" />
```

In this example, the parameter identifier would look like Vdw/74/epsilon .
--- If GROMACS (.itp) or TINKER (.prm) : ---

Follow the rules in the ITP.Reader or Tinker.Reader derived class. Read the documentation in the class documentation or the 'feed' method to learn more. In all cases the parameter is tagged using # PRM 3 (where # denotes a comment, the word PRM stays the same, and 3 is the field number starting from zero.)

--- If normal text : ---

The parameter identifier is simply built using the file name, line number, and field. Thus, the identifier is unique but completely noninformative (which is not ideal for our purposes, but it works.)

--- Endif ---

Warning

My program currently assumes that we are only using one MM program per job. If we use CHARMM and GROMACS to perform simulations as part of the same TARGET, we will get messed up. Maybe this needs to be fixed in the future, with program prefixes to parameters like C_ , G_ .. or simply unit conversions, you get the idea.

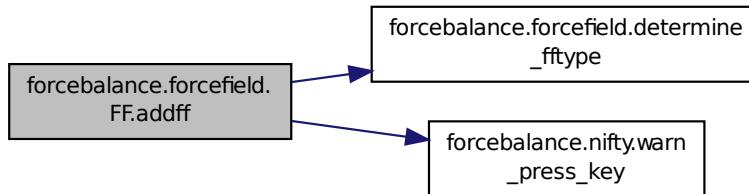
I don't think the multiplier actually works for analytic derivatives unless the interaction calculator knows the multiplier as well. I'm sure I can make this work in the future if necessary.

Parameters

in	ffname	Name of the force field file
----	--------	------------------------------

Definition at line 398 of file forcefield.py.

Here is the call graph for this function:



def forcebalance.forcefield.FF.addff_txt (self, ffname, ffitype) Parse a text force field and create several important instance variables.

Each line is processed using the 'feed' method as implemented in the reader class. This essentially allows us to create the correct parameter identifier (pid), because the pid comes from more than the current line, it also depends on the section that we're in.

When 'PRM' or 'RPT' is encountered, we do several things:

- Build the parameter identifier and insert it into the map
- Point to the file name, line number, and field where the parameter may be modified

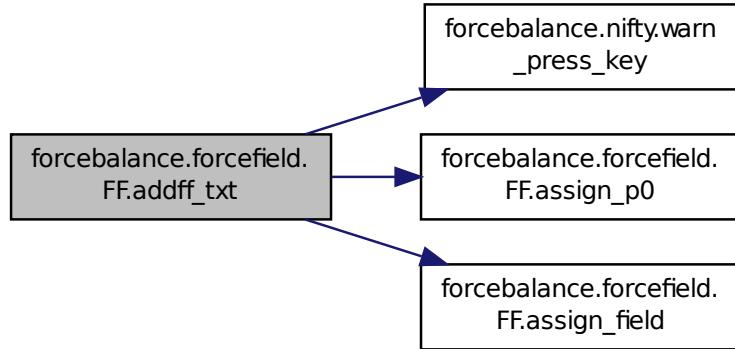
Additionally, when 'PRM' is encountered:

- Store the physical parameter value (this is permanent; it's the original value)
- Increment the total number of parameters

When 'RPT' is encountered we don't expand the parameter vector because this parameter is a copy of an existing one. If the parameter identifier is preceded by MINUS_, we chop off the prefix but remember that the sign needs to be flipped.

Definition at line 468 of file forcefield.py.

Here is the call graph for this function:



```
def forcebalance.forcefield.FF.addff_xml ( self, fname ) Parse an XML force field file and create important instance variables.
```

This was modeled after addff.txt, but XML and text files are fundamentally different, necessitating two different methods.

We begin with an `_ElementTree` object. We search through the tree for the 'parameterize' and 'parameter_repeat' keywords. Each time the keyword is encountered, we do the same four actions that I describe in addff.txt.

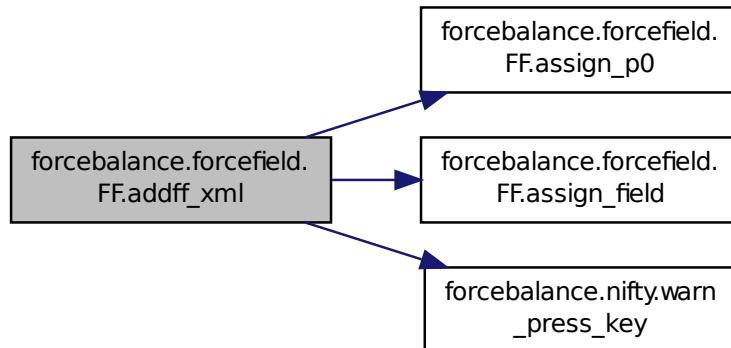
It's hard to specify precisely the location in an XML file to change a force field parameter. I can create a list of tree elements (essentially pointers to elements within a tree), but this method breaks down when I copy the tree because I have no way to refer to the copied tree elements. Fortunately, lxml gives me a way to represent a tree using a flat list, and my XML file 'locations' are represented using the positions in the list.

Warning

The sign-flip hasn't been implemented yet. This shouldn't matter unless your calculation contains repeated parameters with opposite sign.

Definition at line 588 of file forcefield.py.

Here is the call graph for this function:



def forcebalance.forcefield.FF.assign_field (self, idx, fnm, ln, pfld, mult, cmd = None) Record the locations of a parameter in a txt file: [[file name, line number, field number, and multiplier]].

Note that parameters can have multiple locations because of the repetition functionality.

Parameters

in	idx	The index of the parameter.
in	fnm	The file name of the parameter field.
in	ln	The line number within the file (or the node index in the flattened xml)
in	pfld	The field within the line (or the name of the attribute in the xml)
in	mult	The multiplier (this is usually 1.0)

Definition at line 1179 of file forcefield.py.

def forcebalance.forcefield.FF.assign_p0 (self, idx, val) Assign physical parameter values to the 'pvals0' array.

Parameters

in	idx	The index to which we assign the parameter value.
in	val	The parameter value to be inserted.

Definition at line 1161 of file forcefield.py.

def forcebalance.forcefield.FF.create_mvals (self, pvals) Converts physical to mathematical parameters.

We create the inverse transformation matrix using SVD.

Parameters

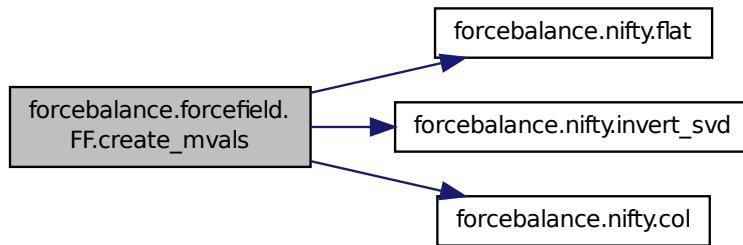
in	<i>pvals</i>	The physical parameters
----	--------------	-------------------------

Returns

mvals The mathematical parameters

Definition at line 870 of file forcefield.py.

Here is the call graph for this function:



def forcebalance.forcefield.FF.create_pvals (*self*, *mvals*) Converts mathematical to physical parameters.

First, mathematical parameters are rescaled and rotated by multiplying by the transformation matrix, followed by adding the original physical parameters.

Parameters

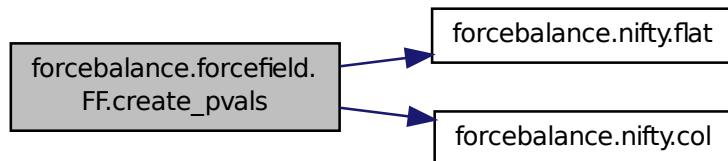
in	<i>mvals</i>	The mathematical parameters
----	--------------	-----------------------------

Returns

pvals The physical parameters

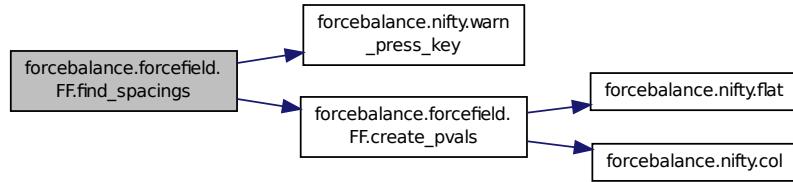
Definition at line 837 of file forcefield.py.

Here is the call graph for this function:



def forcebalance.forcefield.FF.find_spacings (self) Definition at line 792 of file forcefield.py.

Here is the call graph for this function:

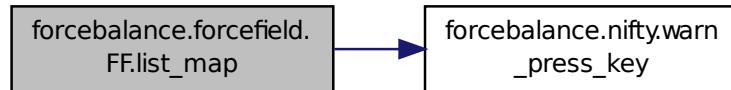


def forcebalance.forcefield.FF.list_map (self) Create the plist, which is like a reversed version of the parameter map.

More convenient for printing.

Definition at line 1129 of file forcefield.py.

Here is the call graph for this function:



def forcebalance.forcefield.FF.make (self, vals = None, use_pvals = False, printdir = None, precision = 12) Create a new force field using provided parameter values.

This big kahuna does a number of things: 1) Creates the physical parameters from the mathematical parameters 2) Creates force fields with physical parameters substituted in 3) Prints the force fields to the specified file.

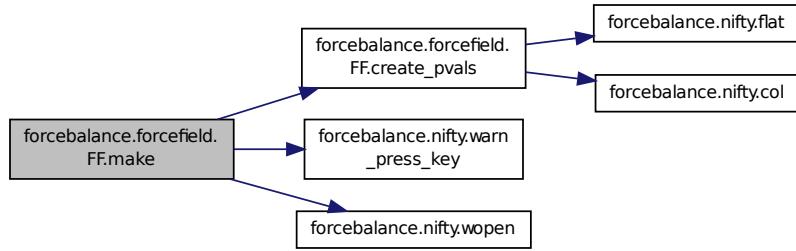
It does NOT store the mathematical parameters in the class state (since we can only hold one set of parameters).

Parameters

in	<i>printdir</i>	The directory that the force fields are printed to; as usual this is relative to the project root directory.
in	<i>vals</i>	Input parameters. I previously had an option where it uses stored values in the class state, but I don't think that's a good idea anymore.
in	<i>use_pvals</i>	Switch for whether to bypass the coordinate transformation and use physical parameters directly.

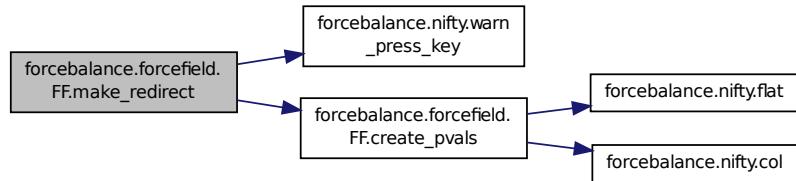
Definition at line 635 of file forcefield.py.

Here is the call graph for this function:



def forcebalance.forcefield.FF.make_redirect (self, mvals) Definition at line 751 of file forcefield.py.

Here is the call graph for this function:



def forcebalance.forcefield.FF.mktransmat (self) Create the transformation matrix to rescale and rotate the mathematical parameters.

For point charge parameters, project out perturbations that change the total charge.

First build these:

'qmap' : Just a list of parameter indices that point to charges.

'qid' : For each parameter in the qmap, a list of the affected atoms :) A potential target for the molecule-specific thang.

Then make this:

'qtrans2' : A transformation matrix that rotates the charge parameters. The first row is all zeros (because it corresponds to increasing the charge on all atoms) The other rows correspond to changing one of the parameters and decreasing all of the others equally such that the overall charge is preserved.

'qmat2' : An identity matrix with 'qtrans2' pasted into the right place

'transmat' : 'qmat2' with rows and columns scaled using self.rs

'excision' : Parameter indices that need to be 'cut out' because they are irrelevant and mess with the matrix diagonalization

Todo Only project out changes in total charge of a molecule, and perhaps generalize to fragments of molecules or other types of parameters.

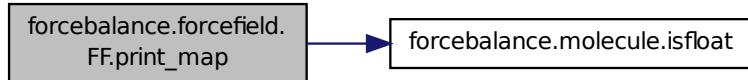
The AMOEBA selection of charge depends not only on the atom type, but what that atom is bonded to.

Definition at line 963 of file forcefield.py.

```
def forcebalance.forcefield.FF.print_map ( self, vals = None, precision = 4 ) Prints out the (physical or mathematical) parameter indices, IDs and values in a visually appealing way.
```

Definition at line 1141 of file forcefield.py.

Here is the call graph for this function:



```
def forcebalance.forcefield.FF.rsmake ( self, printfacs = True ) Create the rescaling factors for the coordinate transformation in parameter space.
```

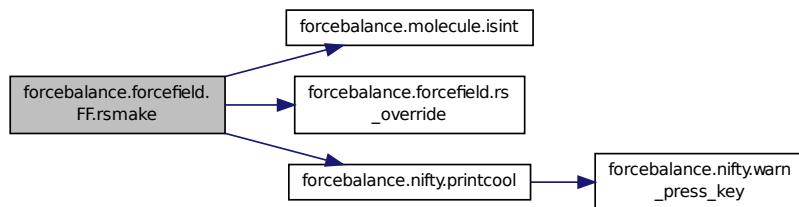
The proper choice of rescaling factors (read: prior widths in maximum likelihood analysis) is still a black art. This is a topic of current research.

Todo Pass in rsfactors through the input file

```
@param[in] printfacs List for printing out the resecaling factors
```

Definition at line 887 of file forcefield.py.

Here is the call graph for this function:

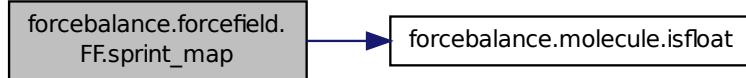


```
def forcebalance.BaseClass.set_option ( self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

```
def forcebalance.forcefield.FF.sprint_map ( self, vals = None, precision = 4 ) Prints out the (physical or mathematical) parameter indices, IDs and values to a string.
```

Definition at line 1149 of file forcefield.py.

Here is the call graph for this function:



8.18.4 Member Data Documentation

forcebalance.forcefield.FF.atomnames A list of atom names (this is new, for ESP fitting)
Definition at line 268 of file forcefield.py.

forcebalance.forcefield.FF.excision Indices to exclude from optimization / Hessian inversion.
Some customized constraints here.
Quadrupoles must be traceless
Definition at line 260 of file forcefield.py.

forcebalance.forcefield.FF.FFAtomTypes WORK IN PROGRESS ## This is a dictionary of {'AtomType': {'Mass' : float, 'Charge' : float, 'ParticleType' : string ('A', 'S', or 'D'), 'AtomicNumber' : int}}.
Definition at line 278 of file forcefield.py.

forcebalance.forcefield.FF.ffdata As these options proliferate, the force field class becomes less standalone.
I need to think of a good solution here... The root directory of the project File names of force fields Directory containing force fields, relative to project directory Priors given by the user :) Whether to constrain the charges. Whether to constrain the charges. Switch for AMOEBA direct or mutual. AMOEBA mutual dipole convergence tolerance. Switch for rigid water molecules Bypass the transformation and use physical parameters directly The content of all force field files are stored in memory
Definition at line 240 of file forcefield.py.

forcebalance.forcefield.FF.ffdata_isxml Definition at line 241 of file forcefield.py.

forcebalance.forcefield.FF.FFMolecules Definition at line 291 of file forcefield.py.

forcebalance.forcefield.FF.linedestroy_save Destruction dictionary (experimental).
Definition at line 319 of file forcefield.py.

forcebalance.forcefield.FF.linedestroy_this Definition at line 321 of file forcefield.py.

forcebalance.forcefield.FF.map The mapping of interaction type -> parameter number.
Definition at line 243 of file forcefield.py.

forcebalance.forcefield.FF.np The total number of parameters.
Definition at line 262 of file forcefield.py.

forcebalance.forcefield.FF.openmmxml Definition at line 414 of file forcefield.py.

forcebalance.forcefield.FF.patoms A listing of parameter number -> atoms involved.

Definition at line 247 of file forcefield.py.

forcebalance.forcefield.FF.pfields A list where pfields[pnum] = [file',line,field,mult,cmd], basically a new way to modify force field files; when we modify the force field file, we go to the specific line/field in a given file and change the number.

Definition at line 252 of file forcefield.py.

forcebalance.forcefield.FF.plist The listing of parameter number -> interaction types.

Definition at line 245 of file forcefield.py.

forcebalance.BaseClass.PrintOptionDict [**inherited**] Definition at line 44 of file __init__.py.

forcebalance.forcefield.FF.prmdestroy_save Definition at line 320 of file forcefield.py.

forcebalance.forcefield.FF.prmdestroy_this Definition at line 322 of file forcefield.py.

forcebalance.forcefield.FF.pvals0 Initial value of physical parameters.

Definition at line 264 of file forcefield.py.

forcebalance.forcefield.FF.qid Definition at line 965 of file forcefield.py.

forcebalance.forcefield.FF.qid2 Definition at line 966 of file forcefield.py.

forcebalance.forcefield.FF.qmap Definition at line 964 of file forcefield.py.

forcebalance.forcefield.FF.Readers A dictionary of force field reader classes.

Definition at line 266 of file forcefield.py.

forcebalance.forcefield.FF.redirect Creates plist from map.

Prints the plist to screen. Make the rescaling factors. Make the transformation matrix. Redirection dictionary (experimental).

Definition at line 317 of file forcefield.py.

forcebalance.forcefield.FF.rs List of rescaling factors.

Takes the dictionary 'BONDS':{3:'B', 4:'K'}, 'VDW':{4:'S', 5:'T'}, and turns it into a list of term types ['BONDSB','B-ONDSK','VDWS','VDWT'].

The array of rescaling factors

Definition at line 254 of file forcefield.py.

forcebalance.forcefield.FF.tinkerprm Definition at line 407 of file forcefield.py.

forcebalance.forcefield.FF.tm The transformation matrix for mathematical -> physical parameters.

Definition at line 256 of file forcefield.py.

forcebalance.forcefield.FF.tml The transpose of the transformation matrix.

Definition at line 258 of file forcefield.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

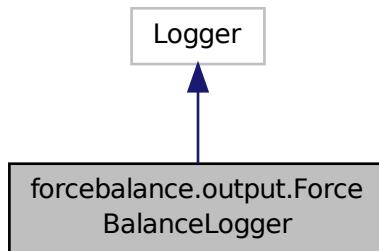
The documentation for this class was generated from the following file:

- [forcefield.py](#)

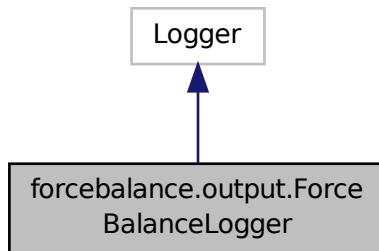
8.19 forcebalance.output.ForceBalanceLogger Class Reference

This logger starts out with a default handler that writes to stdout addHandler removes this default the first time another handler is added.

Inheritance diagram for forcebalance.output.ForceBalanceLogger:



Collaboration diagram for forcebalance.output.ForceBalanceLogger:



Public Member Functions

- def [__init__](#)
- def [addHandler](#)
- def [removeHandler](#)

Public Attributes

- [defaultHandler](#)

8.19.1 Detailed Description

This logger starts out with a default handler that writes to stdout addHandler removes this default the first time another handler is added.

This is used for forcebalance package level logging, where a logger should always be present unless otherwise specified. To silence, add a NullHandler We also by default set the log level to INFO (logging.Logger starts at WARNING)

Definition at line 10 of file output.py.

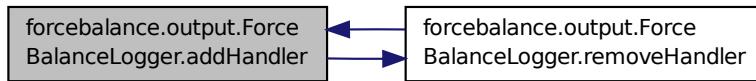
8.19.2 Constructor & Destructor Documentation

```
def forcebalance.output.ForceBalanceLogger.__init__ ( self, name ) Definition at line 11 of file output.py.
```

8.19.3 Member Function Documentation

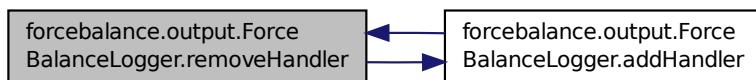
```
def forcebalance.output.ForceBalanceLogger.addHandler ( self, hdlr ) Definition at line 17 of file output.py.
```

Here is the call graph for this function:



```
def forcebalance.output.ForceBalanceLogger.removeHandler ( self, hdlr ) Definition at line 23 of file output.py.
```

Here is the call graph for this function:



8.19.4 Member Data Documentation

```
forcebalance.output.ForceBalanceLogger.defaultHandler Definition at line 13 of file output.py.
```

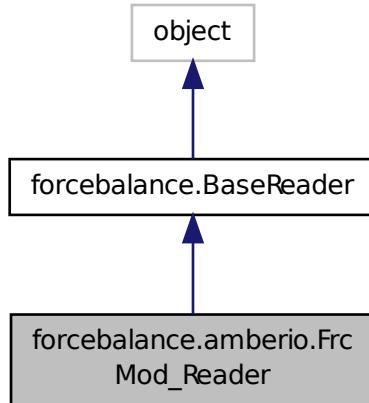
The documentation for this class was generated from the following file:

- [output.py](#)

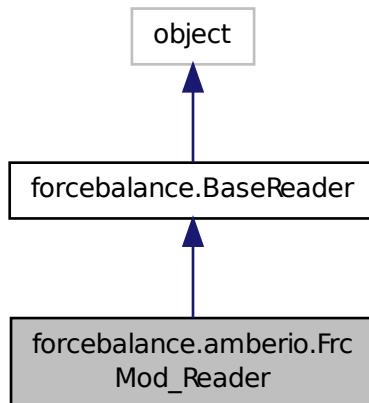
8.20 forcebalance.amberio.FrcMod.Reader Class Reference

Finite state machine for parsing FrcMod force field file.

Inheritance diagram for forcebalance.amberio.FrcMod.Reader:



Collaboration diagram for forcebalance.amberio.FrcMod.Reader:



Public Member Functions

- def `_init_`
- def `Split`
- def `Whites`
- def `feed`
- def `build.pid`

Returns the parameter type (e.g.

Public Attributes

- [pdict](#)
The parameter dictionary (defined in this file)
- [atom](#)
The atom numbers in the interaction (stored in the parser)
- [dihe](#)
Whether we're inside the dihedral section.
- [adict](#)
The frcmod file never has any atoms in it.
- [itype](#)
- [suffix](#)
- [In](#)
- [molatom](#)
The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.
- [Molecules](#)
- [AtomTypes](#)

8.20.1 Detailed Description

Finite state machine for parsing FrcMod force field file.

Definition at line 99 of file amberio.py.

8.20.2 Constructor & Destructor Documentation

def forcebalance.amberio.FrcMod_Reader.__init__ (self, fnm) Definition at line 101 of file amberio.py.

8.20.3 Member Function Documentation

def forcebalance.BaseReader.build_pid (self, pfd) [inherited] Returns the parameter type (e.g. K in BOND\$K) based on the current interaction type.

Both the 'pdict' dictionary (see [gmlio.pdict](#)) and the interaction type 'state' (here, BONDS) are needed to get the parameter type.

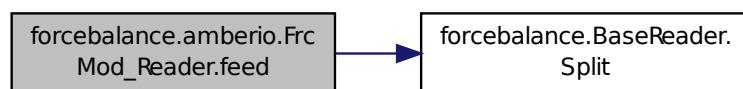
If, however, 'pdict' does not contain the ptype value, a suitable substitute is simply the field number.

Note that if the interaction type state is not set, then it defaults to the file name, so a generic parameter ID is 'filename.line_num.field_num'

Definition at line 124 of file __init__.py.

def forcebalance.amberio.FrcMod_Reader.feed (self, line) Definition at line 119 of file amberio.py.

Here is the call graph for this function:



def forcebalance.amberio.FrcMod.Reader.Split (*self*, *line*) Definition at line 113 of file amberio.py.

def forcebalance.amberio.FrcMod.Reader.Whites (*self*, *line*) Definition at line 116 of file amberio.py.

8.20.4 Member Data Documentation

forcebalance.amberio.FrcMod.Reader.adict The frcmod file never has any atoms in it.
Definition at line 111 of file amberio.py.

forcebalance.amberio.FrcMod.Reader.atom The atom numbers in the interaction (stored in the parser)
Definition at line 107 of file amberio.py.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file __init__.py.

forcebalance.amberio.FrcMod.Reader.dihe Whether we're inside the dihedral section.
Definition at line 109 of file amberio.py.

forcebalance.amberio.FrcMod.Reader.itype Definition at line 130 of file amberio.py.

forcebalance.BaseReader.In [inherited] Definition at line 84 of file __init__.py.

forcebalance.BaseReader.molatom [inherited] The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

self.moleculedict = OrderedDict() The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.

Definition at line 94 of file __init__.py.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file __init__.py.

forcebalance.amberio.FrcMod.Reader.pdict The parameter dictionary (defined in this file)
Definition at line 105 of file amberio.py.

forcebalance.amberio.FrcMod.Reader.suffix Definition at line 165 of file amberio.py.

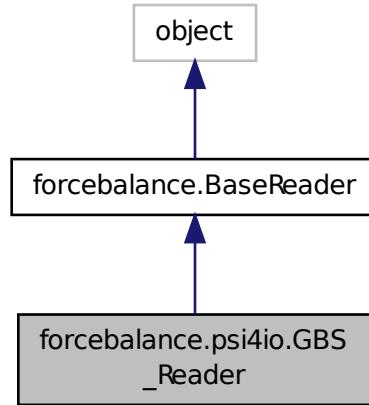
The documentation for this class was generated from the following file:

- [amberio.py](#)

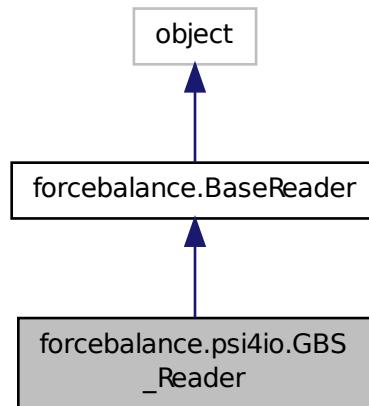
8.21 forcebalance.psi4io.GBS_Reader Class Reference

Interaction type -> Parameter Dictionary.

Inheritance diagram for forcebalance.psi4io.GBS_Reader:



Collaboration diagram for forcebalance.psi4io.GBS_Reader:



Public Member Functions

- def `_init_`
- def `build_pid`
- def `feed`
Feed in a line.
- def `Split`

- def `Whites`
- def `feed`

Public Attributes

- `element`
- `amom`
- `last_amom`
- `basis_number`
- `contraction_number`
- `adict`
- `isdata`
- `destroy`
- `In`
- `itype`
- `suffix`
- `pdict`
- `molatom`

The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

- `Molecules`
- `AtomTypes`

8.21.1 Detailed Description

Interaction type -> Parameter Dictionary.

`pdict = {'Exponent':{0:'A', 1:'C'}, 'BASSP' :{0:'A', 1:'B', 2:'C'} }` Finite state machine for parsing basis set files.
Definition at line 35 of file psi4io.py.

8.21.2 Constructor & Destructor Documentation

`def forcebalance.psi4io.GBS_Reader.__init__ (self, fnm = None)` Definition at line 37 of file psi4io.py.

8.21.3 Member Function Documentation

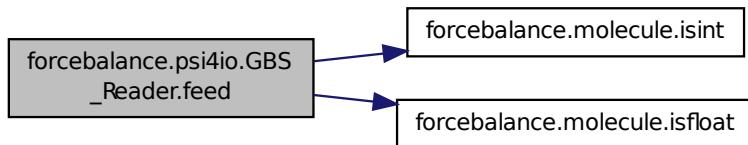
`def forcebalance.psi4io.GBS_Reader.build_pid (self, pfld)` Definition at line 48 of file psi4io.py.

`def forcebalance.psi4io.GBS_Reader.feed (self, line, linindep = False)` Feed in a line.
Parameters

in	line	The line of data
----	------	------------------

Definition at line 61 of file psi4io.py.

Here is the call graph for this function:



```
def forcebalance.BaseReader.feed( self, line ) [inherited] Definition at line 105 of file __init__.py.

def forcebalance.BaseReader.Split( self, line ) [inherited] Definition at line 99 of file __init__.py.

def forcebalance.BaseReader.Whites( self, line ) [inherited] Definition at line 102 of file __init__.py.
```

8.21.4 Member Data Documentation

```
forcebalance.psi4io.GBS_Reader.adict Definition at line 44 of file psi4io.py.

forcebalance.psi4io.GBS_Reader.amom Definition at line 40 of file psi4io.py.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file __init__.py.

forcebalance.psi4io.GBS_Reader.basis_number Definition at line 42 of file psi4io.py.

forcebalance.psi4io.GBS_Reader.contraction_number Definition at line 43 of file psi4io.py.

forcebalance.psi4io.GBS_Reader.destroy Definition at line 46 of file psi4io.py.

forcebalance.psi4io.GBS_Reader.element Definition at line 39 of file psi4io.py.

forcebalance.psi4io.GBS_Reader.isdata Definition at line 45 of file psi4io.py.

forcebalance.BaseReader.itype [inherited] Definition at line 85 of file __init__.py.

forcebalance.psi4io.GBS_Reader.last_amom Definition at line 41 of file psi4io.py.

forcebalance.BaseReader.In [inherited] Definition at line 84 of file __init__.py.

forcebalance.BaseReader.molatom [inherited] The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.  
self.molecdict = OrderedDict() The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.  
Definition at line 94 of file __init__.py.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file __init__.py.

forcebalance.BaseReader.pdict [inherited] Definition at line 87 of file __init__.py.

forcebalance.BaseReader.suffix [inherited] Definition at line 86 of file __init__.py.  
The documentation for this class was generated from the following file:

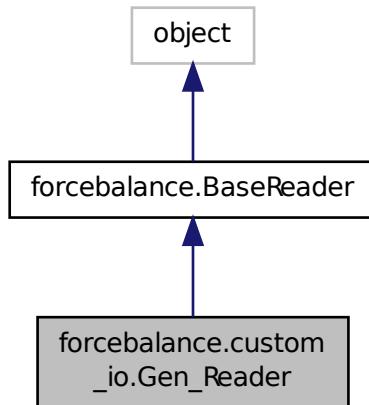
- psi4io.py

```

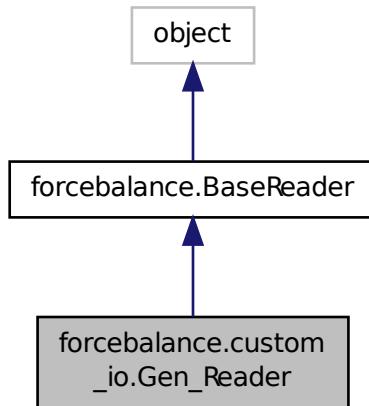
8.22 forcebalance.custom.io.Gen_Reader Class Reference

Finite state machine for parsing custom GROMACS force field files.

Inheritance diagram for forcebalance.custom.io.Gen_Reader:



Collaboration diagram for forcebalance.custom.io.Gen_Reader:



Public Member Functions

- def `__init__`
- def `feed`

Feed in a line.

- def [Split](#)
- def [Whites](#)
- def [build.pid](#)

Returns the parameter type (e.g.

Public Attributes

- [sec](#)
The current section that we're in.
- [pdict](#)
The parameter dictionary (defined in this file)
- [itype](#)
- [suffix](#)
- [In](#)
- [adict](#)
The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.
- [molatom](#)
The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.
- [Molecules](#)
- [AtomTypes](#)

8.22.1 Detailed Description

Finite state machine for parsing custom GROMACS force field files.

This class is instantiated when we begin to read in a file. The feed(line) method updates the state of the machine, giving it information like the residue we're currently on, the nonbonded interaction type, and the section that we're in. Using this information we can look up the interaction type and parameter type for building the parameter ID.

Definition at line 41 of file `custom.io.py`.

8.22.2 Constructor & Destructor Documentation

def forcebalance.custom.io.Gen_Reader.__init__ (self, fnm) Definition at line 43 of file `custom.io.py`.

8.22.3 Member Function Documentation

def forcebalance.BaseReader.build.pid (self, pfd) [inherited] Returns the parameter type (e.g. K in BONDSK) based on the current interaction type.

Both the 'pdict' dictionary (see [gmlio.pdict](#)) and the interaction type 'state' (here, BONDS) are needed to get the parameter type.

If, however, 'pdict' does not contain the ptype value, a suitable substitute is simply the field number.

Note that if the interaction type state is not set, then it defaults to the file name, so a generic parameter ID is 'filename.line_num.field_num'

Definition at line 124 of file `__init__.py`.

def forcebalance.custom.io.Gen_Reader.feed (self, line) Feed in a line.

Parameters

in	line	The line of data
----	------	------------------

Definition at line 57 of file custom_io.py.

def forcebalance.BaseReader.Split(self, line) [inherited] Definition at line 99 of file __init__.py.

def forcebalance.BaseReader.Whites(self, line) [inherited] Definition at line 102 of file __init__.py.

8.22.4 Member Data Documentation

forcebalance.BaseReader.adict [inherited] The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

Definition at line 89 of file __init__.py.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file __init__.py.

forcebalance.custom_io.Gen_Reader.itype Definition at line 60 of file custom_io.py.

forcebalance.BaseReader.In [inherited] Definition at line 84 of file __init__.py.

forcebalance.BaseReader.molatom [inherited] The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

self.molecdict = OrderedDict() The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.

Definition at line 94 of file __init__.py.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file __init__.py.

forcebalance.custom_io.Gen_Reader.pdict The parameter dictionary (defined in this file)

Definition at line 49 of file custom_io.py.

forcebalance.custom_io.Gen_Reader.sec The current section that we're in.

Definition at line 47 of file custom_io.py.

forcebalance.custom_io.Gen_Reader.suffix Definition at line 79 of file custom_io.py.

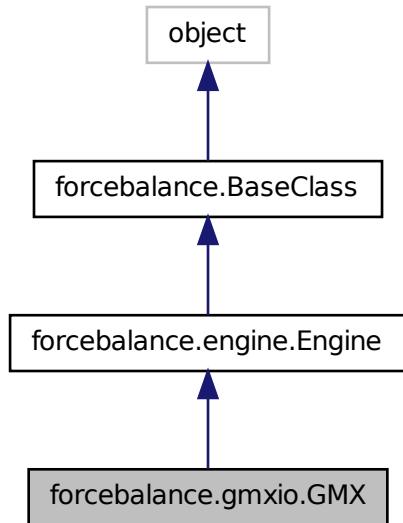
The documentation for this class was generated from the following file:

- [custom.io.py](#)

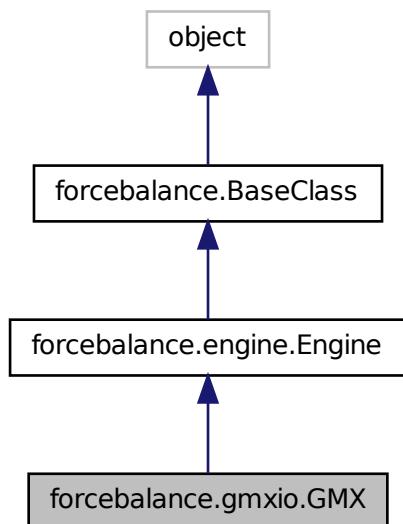
8.23 forcebalance.gmxio.GMX Class Reference

Derived from Engine object for carrying out general purpose GROMACS calculations.

Inheritance diagram for forcebalance.gmxio.GMX:



Collaboration diagram for forcebalance.gmxio.GMX:



Public Member Functions

- def `_init_`
`Called by init ; Set GROMACS-specific options.`
- def `readsrc`
`Called by init ; read files from the source directory.`
- def `prepare`
`Called by init ; prepare the temp directory and figure out the topology.`
- def `links`
- def `callgmx`
`Call GROMACS; prepend the gmxpath to the call to the GROMACS program.`
- def `warngmx`
`Call gromacs and allow for certain expected warnings.`
- def `energy_termnames`
`Get a list of energy term names from the .edr file by parsing a system call to g_energy.`
- def `optimize`
`Optimize the geometry and align the optimized geometry to the starting geometry.`
- def `evaluate_`
`Utility function for computing energy, and (optionally) forces and dipoles using GROMACS.`
- def `evaluate_snapshot`
`Evaluate variables (energies, force and/or dipole) using GROMACS for a single snapshot.`
- def `evaluate_trajectory`
`Evaluate variables (energies, force and/or dipole) using GROMACS over a trajectory.`
- def `energy_one`
`Compute the energy using GROMACS for a snapshot.`
- def `energy_force_one`
`Compute the energy and force using GROMACS for a single snapshot; interfaces with AbInitio target.`
- def `energy`
`Compute the energy using GROMACS over a trajectory.`
- def `energy_force`
`Compute the energy and force using GROMACS over a trajectory.`
- def `energy_dipole`
- def `energy_rmsd`
`Calculate energy of the selected structure (optionally minimize and return the minimized energy and RMSD).`
- def `interaction_energy`
`Computes the interaction energy between two fragments over a trajectory.`
- def `multipole_moments`
`Return the multipole moments of the 1st snapshot in Debye and Buckingham units.`
- def `normal_modes`
- def `generate_vsite_positions`
- def `n_snaps`
- def `scd_persnap`
- def `calc_scd`
- def `molecular_dynamics`
`Method for running a molecular dynamics simulation.`
- def `md`
`Method for running a molecular dynamics simulation.`
- def `prepare`
- def `__setattr__`
- def `set_option`

Public Attributes

- **valkw**
Valid GROMACS-specific keywords.
- **gmxsuffix**
Disable some optimizations.
- **gmxpath**
The directory containing GROMACS executables (e.g.
- **top**
Attempt to determine file names of .gro, .top, and .mdp files.
- **mdp**
- **mol**
- **gmx_defs**
- **pbc**
- **double**
Write out the trajectory coordinates to a .gro file.
- **AtomMask**
- **AtomLists**
- **mdtraj**
- **mdene**
- **name**
- **verbose**
- **target**
Engines can get properties from the Target that creates them.
- **root**
- **srcdir**
- **tempdir**
- **FF**
- **verbose_options**
- **PrintOptionDict**

8.23.1 Detailed Description

Derived from Engine object for carrying out general purpose GROMACS calculations.

Definition at line 490 of file gmxio.py.

8.23.2 Constructor & Destructor Documentation

def forcebalance.gmxio.GMX.__init__ (self, name = "gmx", kwargs) Definition at line 493 of file gmxio.py.

8.23.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited] Definition at line 28 of file __init__.py.

def forcebalance.gmxio.GMX.calc_scd (self, n_snap, timestep) Definition at line 1069 of file gmxio.py.

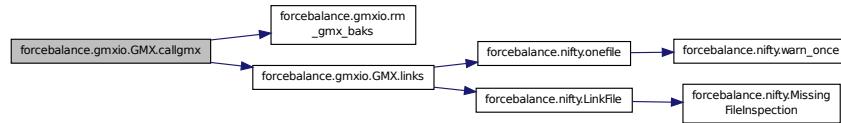
Here is the call graph for this function:



```
def forcebalance.gmxio.GMX.callgmx ( self, command, stdin = None, print_to_screen = False, print_command = False, kwargs ) Call GROMACS; prepend the gmxpath to the call to the GROMACS program.
```

Definition at line 691 of file gmxio.py.

Here is the call graph for this function:



```
def forcebalance.gmxio.GMX.energy ( self, traj = None ) Compute the energy using GROMACS over a trajectory.
```

Definition at line 890 of file gmxio.py.

Here is the call graph for this function:



```
def forcebalance.gmxio.GMX.energy_dipole ( self, traj = None ) Definition at line 903 of file gmxio.py.
```

Here is the call graph for this function:



```
def forcebalance.gmxio.GMX.energy_force ( self, force = True, traj = None ) Compute the energy and force using GROMACS over a trajectory.
```

Definition at line 897 of file gmxio.py.

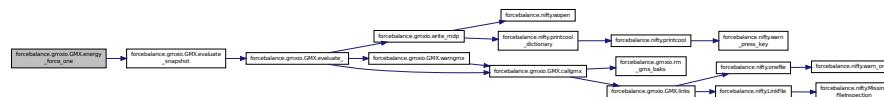
Here is the call graph for this function:



def forcebalance.gmxio.GMX.energy_force_one (self, shot) Compute the energy and force using GROMACS for a single snapshot; interfaces with Ablinitio target.

Definition at line 882 of file gmxio.py.

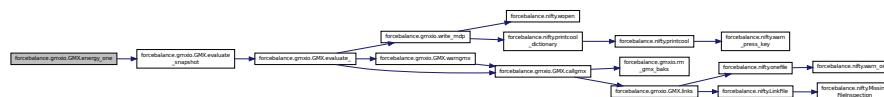
Here is the call graph for this function:



def forcebalance.gmxio.GMX.energy_one (self, shot) Compute the energy using GROMACS for a snapshot.

Definition at line 875 of file gmxio.py.

Here is the call graph for this function:

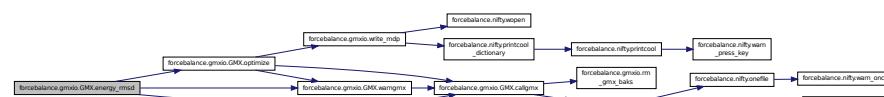


def forcebalance.gmxio.GMX.energy_rmsd (self, shot, optimize = True) Calculate energy of the selected structure (optionally minimize and return the minimized energy and RMSD).

In kcal/mol.

Definition at line 909 of file gmxio.py.

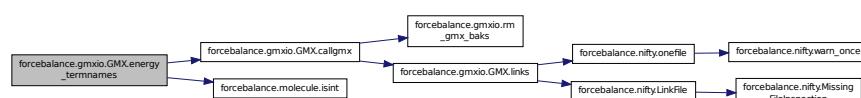
Here is the call graph for this function:



def forcebalance.gmxio.GMX.energy_termnames (self, edrfile = None) Get a list of energy term names from the .edr file by parsing a system call to g_energy.

Definition at line 748 of file gmxio.py.

Here is the call graph for this function:



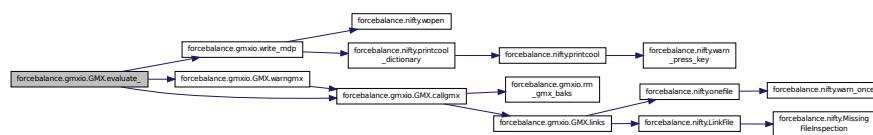
def forcebalance.gmxio.GMX.evaluate_(self, force = False, dipole = False, traj = None) Utility function for computing energy, and (optionally) forces and dipoles using GROMACS.

Inputs: force: Switch for calculating the force. dipole: Switch for calculating the dipole. traj: Trajectory file name. If present, will loop over these snapshots. Otherwise will do a single point evaluation at the current geometry.

Outputs: Result: Dictionary containing energies, forces and/or dipoles.

Definition at line 820 of file gmxio.py.

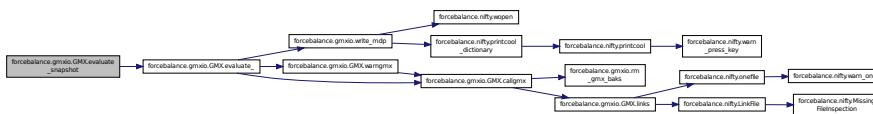
Here is the call graph for this function:



def forcebalance.gmxio.GMX.evaluate_snapshot(self, shot, force = False, dipole = False) Evaluate variables (energies, force and/or dipole) using GROMACS for a single snapshot.

Definition at line 853 of file gmxio.py.

Here is the call graph for this function:

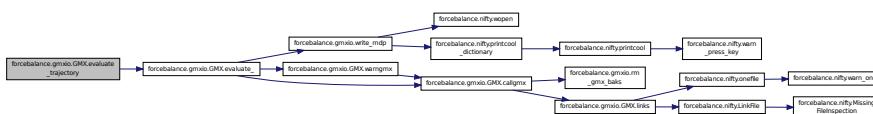


def forcebalance.gmxio.GMX.evaluate_trajectory(self, force = False, dipole = False, traj = None)

Evaluate variables (energies, force and/or dipole) using GROMACS over a trajectory.

Definition at line 862 of file gmxio.py.

Here is the call graph for this function:



def forcebalance.gmxio.GMX.generate_vsites_positions(self) Definition at line 1047 of file gmxio.py.

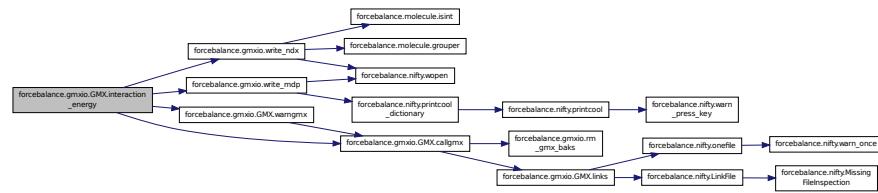
Here is the call graph for this function:



def forcebalance.gmxio.GMX.interaction_energy (self, fraga, fragb) Computes the interaction energy between two fragments over a trajectory.

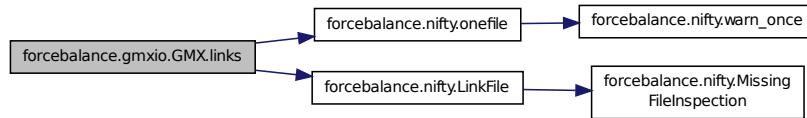
Definition at line 924 of file gmxio.py.

Here is the call graph for this function:



def forcebalance.gmxio.GMX.links (self) Definition at line 675 of file gmxio.py.

Here is the call graph for this function:



def forcebalance.gmxio.GMX.md (self, nsteps = 0, nequil = 0, verbose = False, deffnm = None, kwargs)

) Method for running a molecular dynamics simulation.

A little different than molecular_dynamics (for [thermo.py](#))

Required arguments:

nsteps = (int) Number of total time steps

nequil = (int) Number of additional time steps at the beginning
for equilibration

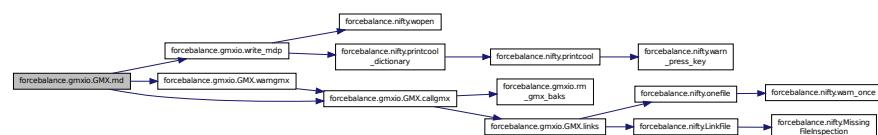
verbose = (bool) Be loud and noisy

deffnm = (string) default names for simulation output files

The simulation data is written to the working directory.

Definition at line 1260 of file gmxio.py.

Here is the call graph for this function:



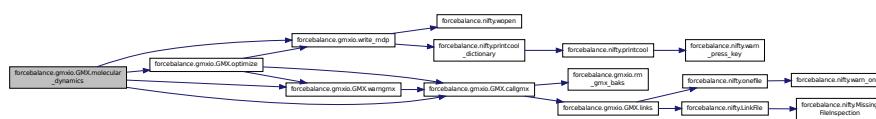
```
def forcebalance.gmxio.GMX.molecular_dynamics ( self, nsteps, timestep, temperature = None, pressure = None, nequil = 0, nsave = 0, minimize = True, threads = None, verbose = False, bilayer = False, kwargs ) Method for running a molecular dynamics simulation.
```

Required arguments: nsteps = (int) Number of total time steps timestep = (float) Time step in FEMTOSECOND-S temperature = (float) Temperature control (Kelvin) pressure = (float) Pressure control (atmospheres) nequil = (int) Number of additional time steps at the beginning for equilibration nsave = (int) Step interval for saving data minimize = (bool) Perform an energy minimization prior to dynamics threads = (int) Number of MPI-threads

Returns simulation data: Rhos = (array) Density in kilogram m⁻³ Potentials = (array) Potential energies Kinetics = (array) Kinetic energies Volumes = (array) Box volumes Dips = (3xN array) Dipole moments EComps = (dict) Energy components Als = (array) Average area per lipid in nm² Scds = (Nx28 array) Deuterium order parameter

Definition at line 1110 of file gmxio.py.

Here is the call graph for this function:

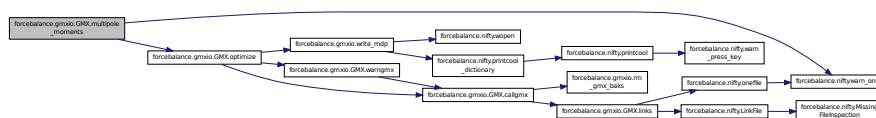


```
def forcebalance.gmxio.GMX.multipole_moments ( self, shot = 0, optimize = True, polarizability = False )
```

) Return the multipole moments of the 1st snapshot in Debye and Buckingham units.

Definition at line 960 of file gmxio.py.

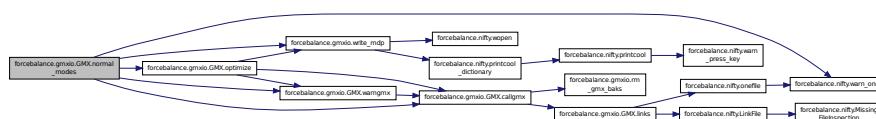
Here is the call graph for this function:



```
def forcebalance.gmxio.GMX.n_snaps ( self, nsteps, step_interval, timestep ) Definition at line 1055 of file gmxio.py.
```

```
def forcebalance.gmxio.GMX.normal_modes ( self, shot = 0, optimize = True ) Definition at line 1011 of file gmxio.py.
```

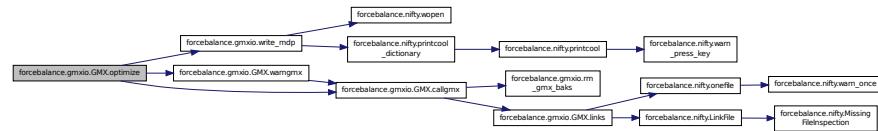
Here is the call graph for this function:



```
def forcebalance.gmxio.GMX.optimize ( self, shot = 0, crit = 1e-4, kwargs ) Optimize the geometry and align the optimized geometry to the starting geometry.
```

Definition at line 779 of file gmxio.py.

Here is the call graph for this function:



def forcebalance.engine.Engine.prepare(self, kwargs) [inherited] Definition at line 95 of file engine.py.

def forcebalance.gmxio.GMX.prepare(self, pbc = False, kwargs) Called by **init** ; prepare the temp directory and figure out the topology.

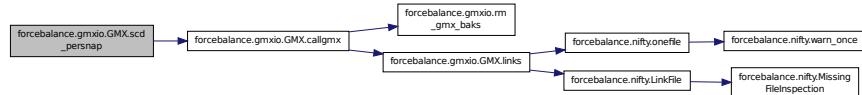
Definition at line 552 of file gmxio.py.

def forcebalance.gmxio.GMX.readsrc(self, kwargs) Called by **init** ; read files from the source directory.

Definition at line 536 of file gmxio.py.

def forcebalance.gmxio.GMX.scd_persnap(self, ndx, timestep, final_frame) Definition at line 1058 of file gmxio.py.

Here is the call graph for this function:



def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

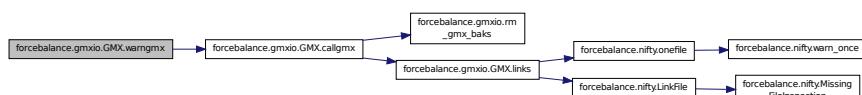
def forcebalance.gmxio.GMX.setopts(self, kwargs) Called by **init** ; Set GROMACS-specific options.

Definition at line 500 of file gmxio.py.

def forcebalance.gmxio.GMX.warngmx(self, command, warnings = [], maxwarn = 1, kwargs) Call gromacs and allow for certain expected warnings.

Definition at line 707 of file gmxio.py.

Here is the call graph for this function:



8.23.4 Member Data Documentation

forcebalance.gmxio.GMX.AtomLists Definition at line 643 of file gmxio.py.

forcebalance.gmxio.GMX.AtomMask Definition at line 642 of file gmxio.py.

forcebalance.gmxio.GMX.double Write out the trajectory coordinates to a .gro file.

At this point, we could have gotten a .mdp file from the target folder or as part of the force field. If it still missing, then we may write a default. Call grompp followed by gmxdump to read the trajectory

Definition at line 637 of file gmxio.py.

forcebalance.engine.Engine.FF [inherited] Definition at line 65 of file engine.py.

forcebalance.gmxio.GMX.gmx_defs Definition at line 555 of file gmxio.py.

forcebalance.gmxio.GMX.gmxpath The directory containing GROMACS executables (e.g.

mdrun)

Definition at line 518 of file gmxio.py.

forcebalance.gmxio.GMX.gmxsuffix Disable some optimizations.

The suffix to GROMACS executables, e.g. '_d' for double precision.

Definition at line 510 of file gmxio.py.

forcebalance.gmxio.GMX.mdene Definition at line 1313 of file gmxio.py.

forcebalance.gmxio.GMX.mdp Definition at line 541 of file gmxio.py.

forcebalance.gmxio.GMX.mdtraj Definition at line 1183 of file gmxio.py.

forcebalance.gmxio.GMX.mol Definition at line 543 of file gmxio.py.

forcebalance.engine.Engine.name [inherited] Definition at line 48 of file engine.py.

forcebalance.gmxio.GMX.pbc Definition at line 560 of file gmxio.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.engine.Engine.root [inherited] Definition at line 56 of file engine.py.

forcebalance.engine.Engine.srkdir [inherited] Definition at line 57 of file engine.py.

forcebalance.engine.Engine.target [inherited] Engines can get properties from the Target that creates them.

Definition at line 55 of file engine.py.

forcebalance.engine.Engine.tempdir [inherited] Definition at line 58 of file engine.py.

forcebalance.gmxio.GMX.top Attempt to determine file names of .gro, .top, and .mdp files.

Link files into the temp directory.

Write the appropriate coordinate files.

Definition at line 540 of file gmxio.py.

forcebalance.gmxio.GMX.valkwd Valid GROMACS-specific keywords.

Definition at line 495 of file gmxio.py.

forcebalance.engine.Engine.verbose [inherited] Definition at line 50 of file engine.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

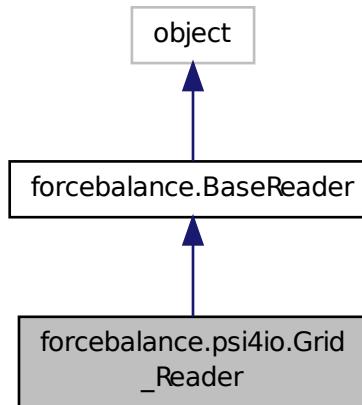
The documentation for this class was generated from the following file:

- [gmxio.py](#)

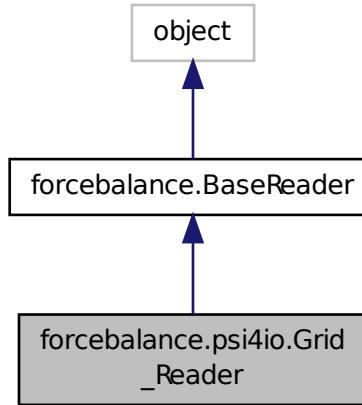
8.24 forcebalance.psi4io.Grid_Reader Class Reference

Finite state machine for parsing DVR grid files.

Inheritance diagram for forcebalance.psi4io.Grid_Reader:



Collaboration diagram for forcebalance.psi4io.Grid_Reader:



Public Member Functions

- def `_init_`
- def `build_pid`
- def `feed`
Feed in a line.
- def `Split`
- def `Whites`
- def `feed`

Public Attributes

- `element`
- `point`
- `radii`
- `isdata`
- `In`
- `itype`
- `suffix`
- `pdict`
- `adict`

The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

- `molatom`

The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

- `Molecules`
- `AtomTypes`

8.24.1 Detailed Description

Finite state machine for parsing DVR grid files.
Definition at line 250 of file psi4io.py.

8.24.2 Constructor & Destructor Documentation

def forcebalance.psi4io.Grid_Reader.__init__ (self, fnm = None) Definition at line 252 of file psi4io.py.

8.24.3 Member Function Documentation

def forcebalance.psi4io.Grid_Reader.build_pid (self, pfd) Definition at line 258 of file psi4io.py.

def forcebalance.BaseReader.feed (self, line) [inherited] Definition at line 105 of file __init__.py.

def forcebalance.psi4io.Grid_Reader.feed (self, line, linindep = False) Feed in a line.
Parameters

in	line	The line of data
----	------	------------------

Definition at line 273 of file psi4io.py.

def forcebalance.BaseReader.Split (self, line) [inherited] Definition at line 99 of file __init__.py.

def forcebalance.BaseReader.Whites (self, line) [inherited] Definition at line 102 of file __init__.py.

8.24.4 Member Data Documentation

forcebalance.BaseReader.adict [inherited] The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

Definition at line 89 of file __init__.py.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file __init__.py.

forcebalance.psi4io.Grid_Reader.element Definition at line 254 of file psi4io.py.

forcebalance.psi4io.Grid_Reader.isdata Definition at line 284 of file psi4io.py.

forcebalance.BaseReader.itype [inherited] Definition at line 85 of file __init__.py.

forcebalance.BaseReader.In [inherited] Definition at line 84 of file __init__.py.

forcebalance.BaseReader.molatom [inherited] The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

self.molecdict = OrderedDict() The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.

Definition at line 94 of file __init__.py.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file __init__.py.

forcebalance.BaseReader.pdict [inherited] Definition at line 87 of file __init__.py.

forcebalance.psi4io.Grid_Reader.point Definition at line 255 of file psi4io.py.

forcebalance.psi4io.Grid_Reader.radius Definition at line 256 of file psi4io.py.

forcebalance.BaseReader.suffix [inherited] Definition at line 86 of file __init__.py.

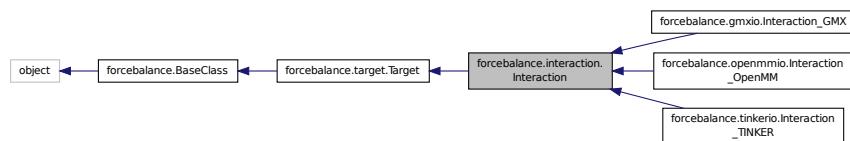
The documentation for this class was generated from the following file:

- [psi4io.py](#)

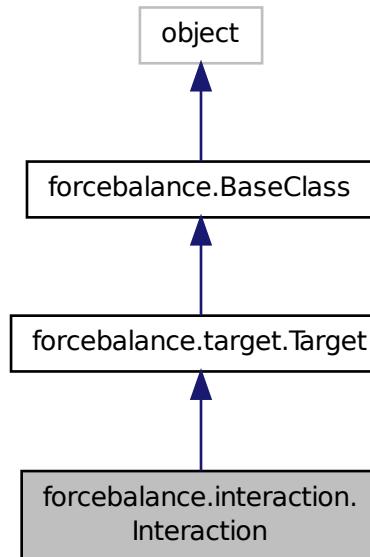
8.25 forcebalance.interaction.Interaction Class Reference

Subclass of Target for fitting force fields to interaction energies.

Inheritance diagram for forcebalance.interaction.Interaction:



Collaboration diagram for forcebalance.interaction.Interaction:



Public Member Functions

- def [__init__](#)
- def [read_reference_data](#)

Read the reference ab initio data from a file such as qdata.txt.

- def `indicate`
- def `get`
Evaluate objective function.
- def `get_X`
Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
Computes the objective function contribution and its gradient.
- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `select1`
Number of snapshots.
- `select2`
Set fragment 2.
- `eqm`
Set upper cutoff energy.
- `label`
Snapshot label, useful for graphing.

- **qfnm**
The qdata.txt file that contains the QM energies and forces.
- **e_err**
- **e_err_pct**
- **ns**
Read in the trajectory file.
- **mol**
- **engine**
Build keyword dictionaries to pass to engine.
- **divisor**
Read in the reference data.
- **prefactor**
- **weight**
- **emm**
- **objective**
- **rd**
Root directory of the whole project.
- **pgrad**
Iteration where we turn on zero-gradient skipping.
- **tempbase**
Relative directory of target.
- **tempdir**
- **rundir**
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**
Whether to write indicate.log at every iteration (true for all but remote.)
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

8.25.1 Detailed Description

Subclass of Target for fitting force fields to interaction energies.

Currently TINKER is supported.

We introduce the following concepts:

- The number of snapshots
- The reference interaction energies and the file they belong in (qdata.txt)

This subclass contains the 'get' method for building the objective function from any simulation software (a driver to run the program and read output is still required).

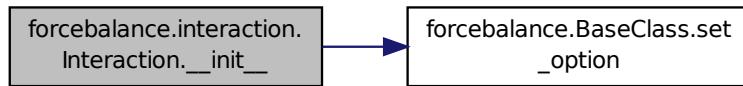
Definition at line 35 of file interaction.py.

8.25.2 Constructor & Destructor Documentation

```
def forcebalance.interaction.Interaction.__init__( self, options, tgt_opts, forcefield )
```

 Definition at line 38 of file interaction.py.

Here is the call graph for this function:



8.25.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited]
```

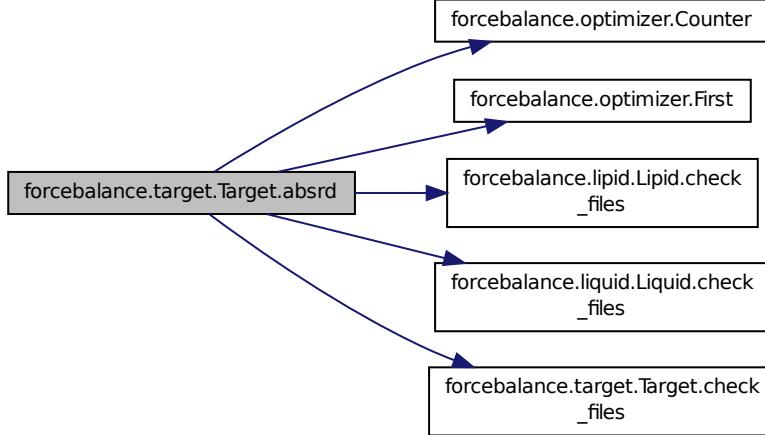
 Definition at line 28 of file __init__.py.

```
def forcebalance.target.Target.absrd( self, inum = None ) [inherited]
```

 Supply the correct directory specified by user's "read" option.

Definition at line 393 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.check_files(self, there) [inherited] Check this directory for the presence of readable files when the 'read' option is set.

Definition at line 364 of file target.py.

def forcebalance.interaction.Interaction.get(self, mvals, AGrad = False, AHess = False) Evaluate objective function.

Definition at line 157 of file interaction.py.

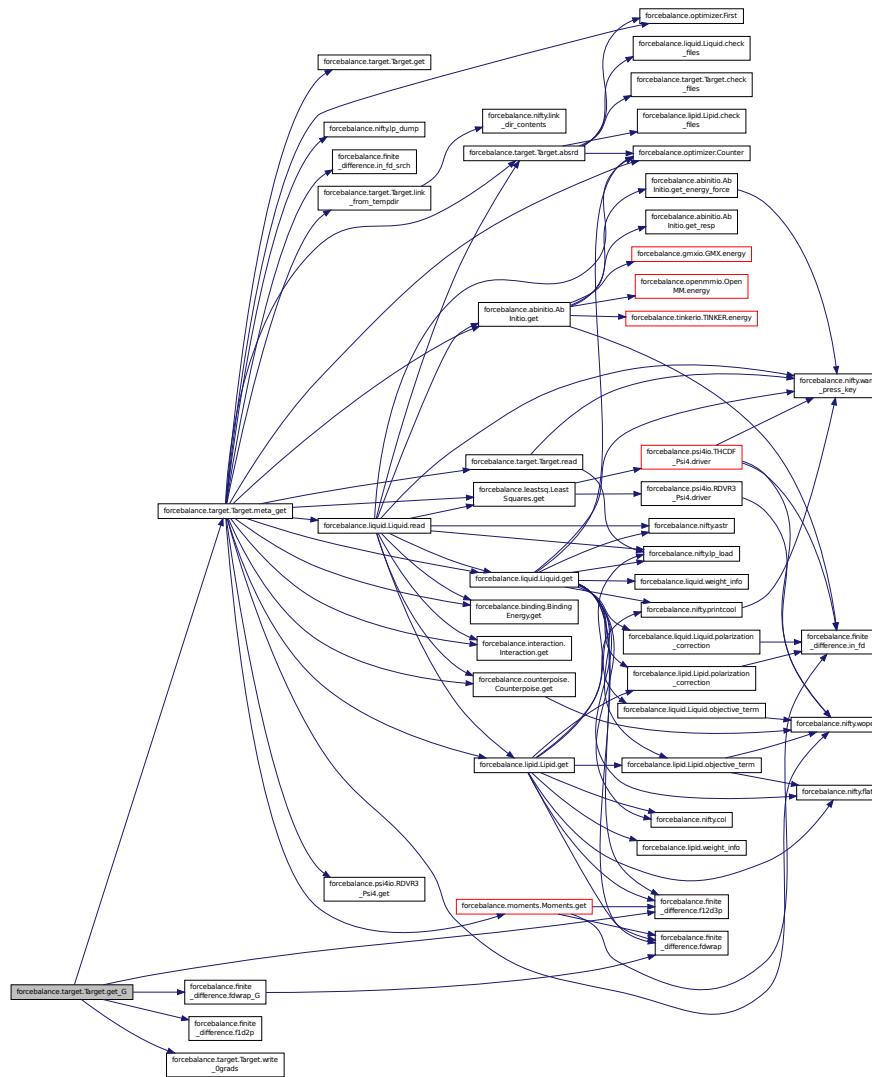
def forcebalance.target.Target.get_G(self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the `fd1.pids` and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



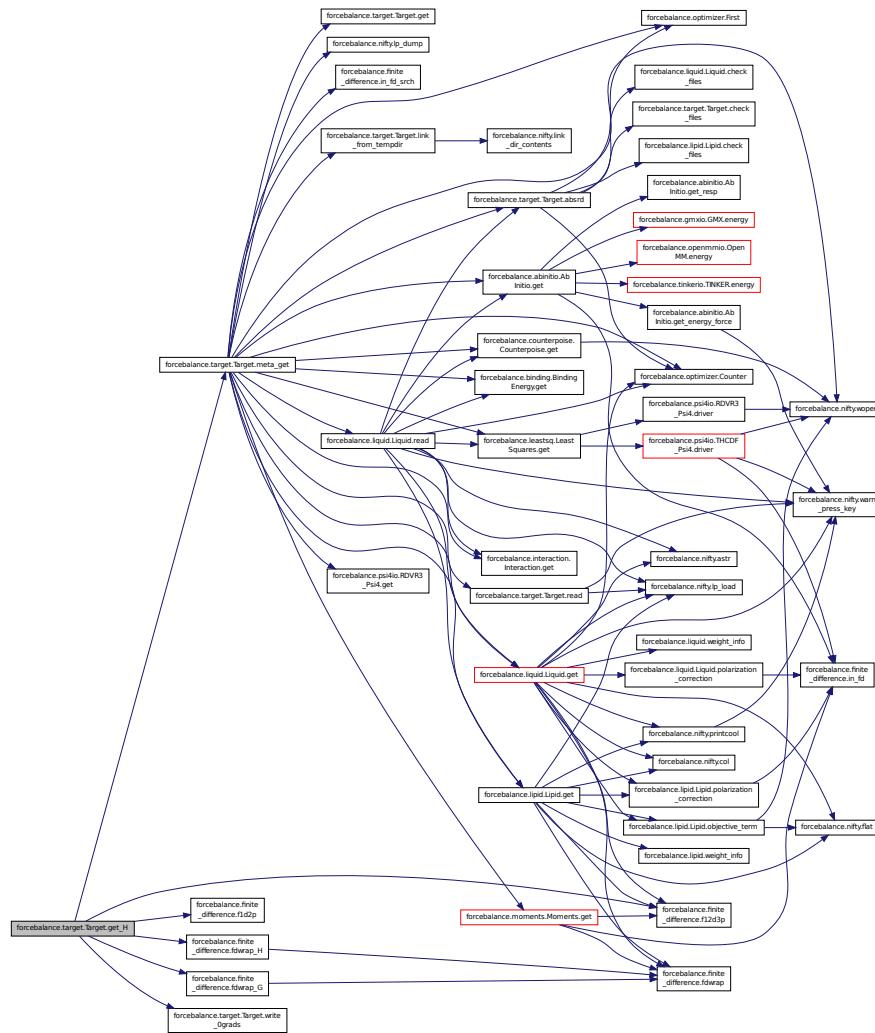
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

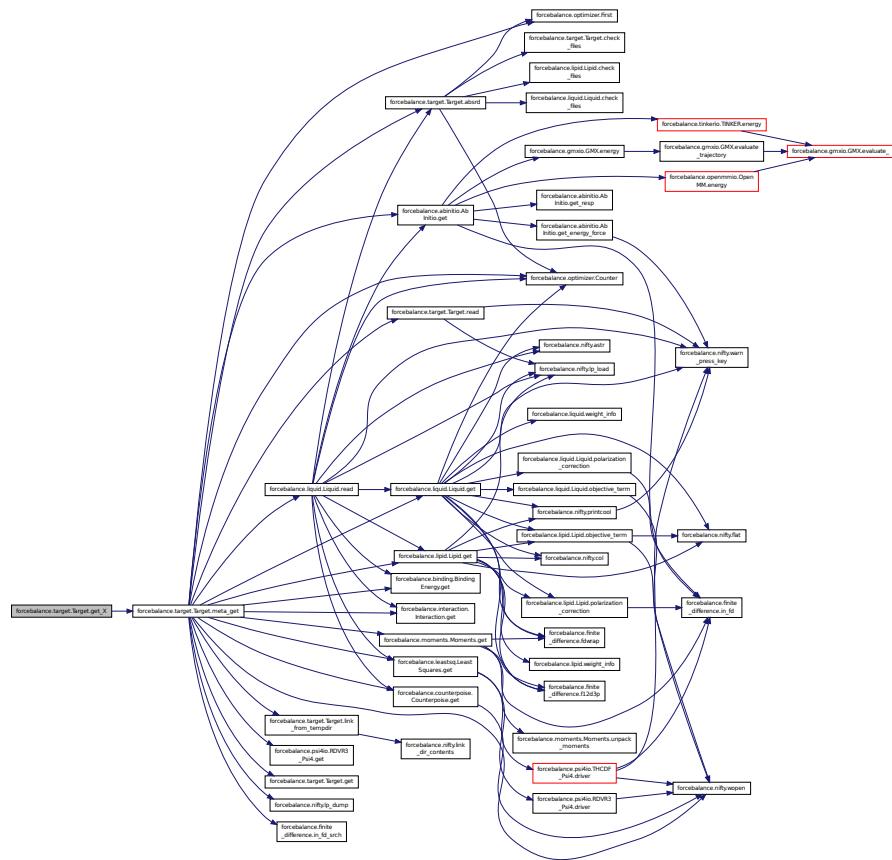
Here is the call graph for this function:



def forcebalance.target.Target.get.X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

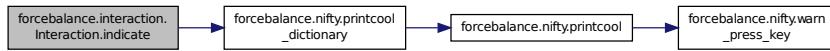
Definition at line 184 of file target.py.

Here is the call graph for this function:



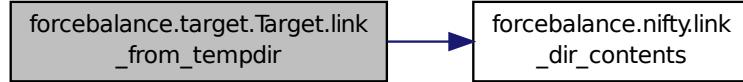
def forcebalance.interaction.Interaction.indicate (self) Definition at line 141 of file interaction.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

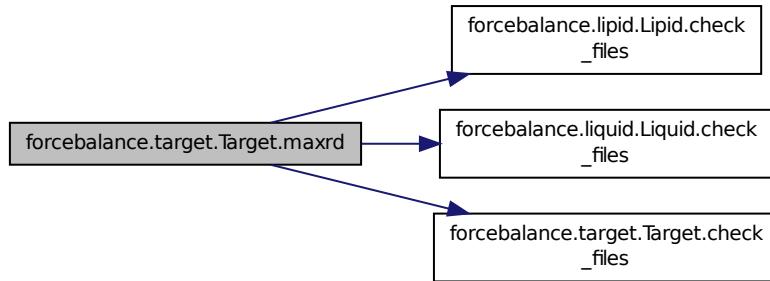
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

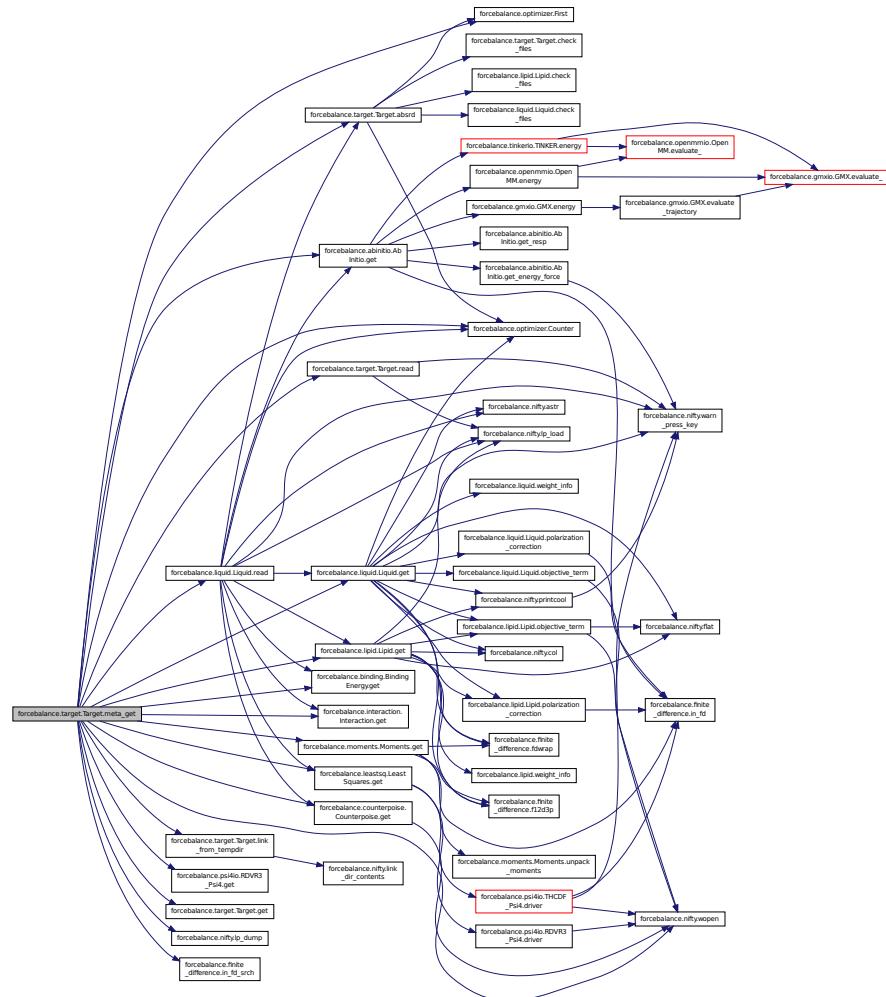


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

Here is the call graph for this function:

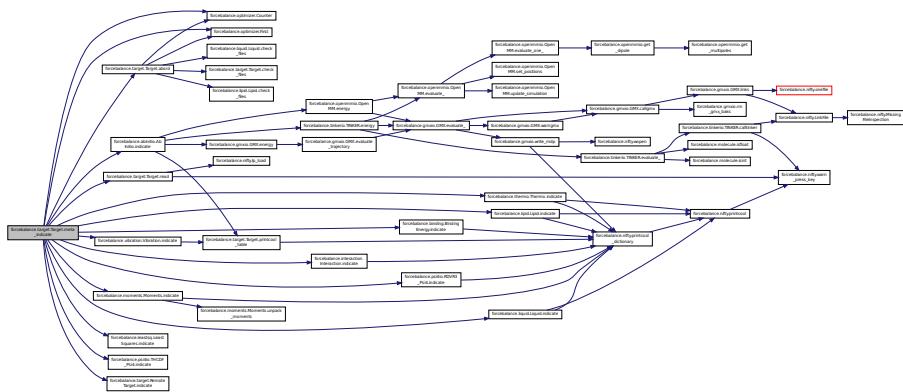


def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.

Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

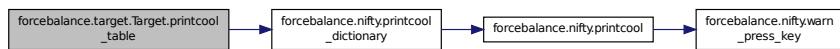
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

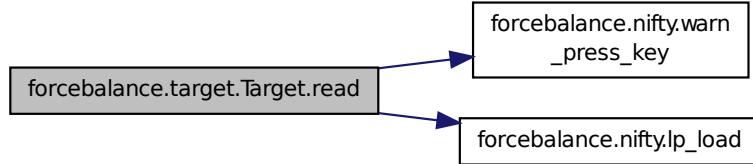
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.interaction.Interaction.read_reference_data (self) Read the reference ab initio data from a file such as qdata.txt.

After reading in the information from qdata.txt, it is converted into kcal/mol.

Definition at line 124 of file interaction.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

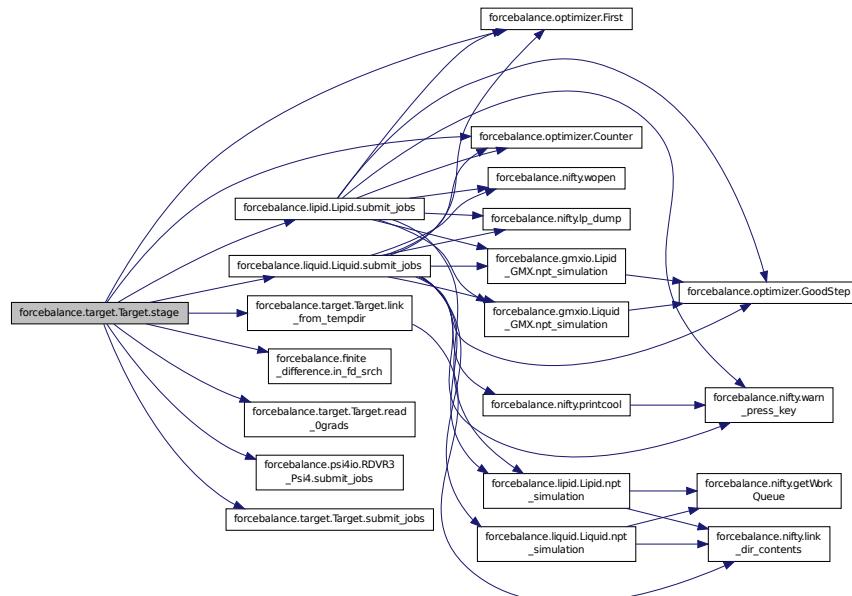
def forcebalance.BaseClass.set_option (self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

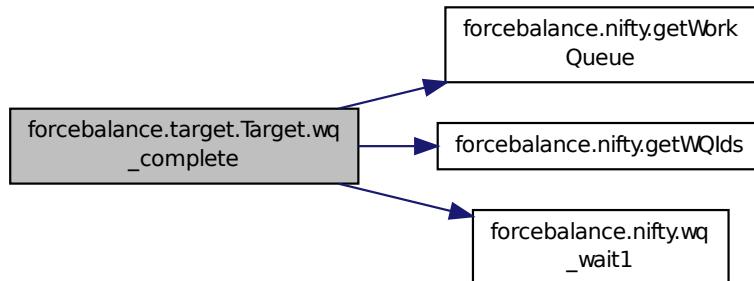


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_0grads( self, Ans ) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.25.4 Member Data Documentation

forcebalance.interaction.Interaction.divisor Read in the reference data.

Definition at line 95 of file interaction.py.

forcebalance.interaction.Interaction.e_err Definition at line 77 of file interaction.py.

forcebalance.interaction.Interaction.e_err_pct Definition at line 78 of file interaction.py.

forcebalance.interaction.Interaction.emm Definition at line 194 of file interaction.py.

forcebalance.interaction.Interaction.engine Build keyword dictionaries to pass to engine.

Definition at line 88 of file interaction.py.

forcebalance.interaction.Interaction.eqm Set upper cutoff energy.

Reference (QM) interaction energies

Definition at line 72 of file interaction.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.interaction.Interaction.label Snapshot label, useful for graphing.

Definition at line 74 of file interaction.py.

forcebalance.interaction.Interaction.mol Definition at line 81 of file interaction.py.

forcebalance.interaction.Interaction.ns Read in the trajectory file.

Definition at line 80 of file interaction.py.

forcebalance.interaction.Interaction.objective Definition at line 195 of file interaction.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.interaction.Interaction.prefactor Definition at line 113 of file interaction.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.interaction.Interaction.qfnm The qdata.txt file that contains the QM energies and forces.

Definition at line 76 of file interaction.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.interaction.Interaction.select1 Number of snapshots.

Do we call Q-Chem for dielectric energies? (Currently needs to be fixed) Do we put the reference energy into the denominator? Do we put the reference energy into the denominator? What is the energy denominator? Set fragment 1

Definition at line 60 of file interaction.py.

forcebalance.interaction.Interaction.select2 Set fragment 2.

Definition at line 65 of file interaction.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.interaction.Interaction.weight Definition at line 161 of file interaction.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

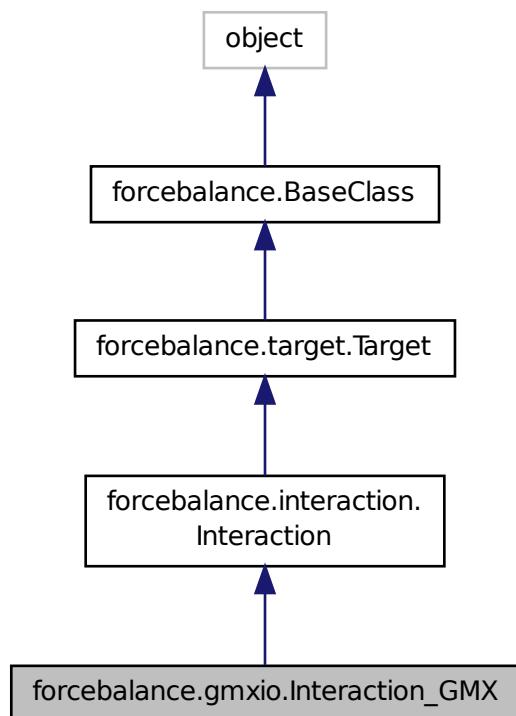
Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.
Definition at line 162 of file target.py.
The documentation for this class was generated from the following file:
• [interaction.py](#)

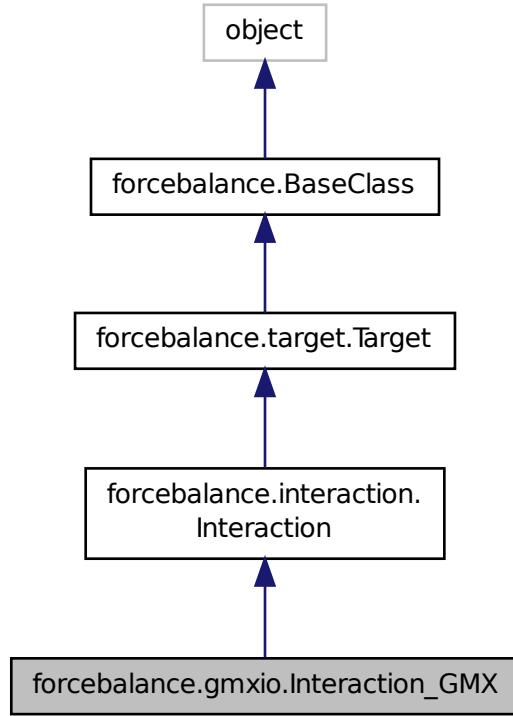
8.26 forcebalance.gmxio.Interaction_GMX Class Reference

Interaction energy matching using GROMACS.

Inheritance diagram for forcebalance.gmxio.Interaction_GMX:



Collaboration diagram for forcebalance.gmxio.Interaction_GMX:



Public Member Functions

- def `__init__`
- def `read_reference_data`

Read the reference ab initio data from a file such as qdata.txt.
- def `indicate`
- def `get`

Evaluate objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`

- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
Default file names for coordinates, top and mdp files.
- `select1`
Number of snapshots.
- `select2`
Set fragment 2.
- `eqm`
Set upper cutoff energy.
- `label`
Snapshot label, useful for graphing.
- `qfnm`
The qdata.txt file that contains the QM energies and forces.
- `e_err`
- `e_err_pct`
- `ns`
Read in the trajectory file.
- `mol`
- `engine`
Build keyword dictionaries to pass to engine.
- `divisor`
Read in the reference data.
- `prefactor`

- `weight`
- `emm`
- `objective`
- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`
Relative directory of target.
- `tempdir`
- `rundir`
`self.tempdir = os.path.join('temp',self.name)` *The directory in which the simulation is running - this can be updated.*
- `FF`
Need the forcefield (here for now)
- `xct`
Counts how often the objective function was computed.
- `gct`
Counts how often the gradient was computed.
- `hct`
Counts how often the Hessian was computed.
- `read_indicate`
Whether to read indicate.log from file when restarting an aborted run.
- `write_indicate`
Whether to write indicate.log at every iteration (true for all but remote.)
- `read_objective`
Whether to read objective.p from file when restarting an aborted run.
- `write_objective`
Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.26.1 Detailed Description

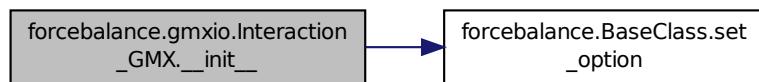
Interaction energy matching using GROMACS.

Definition at line 1469 of file gmxio.py.

8.26.2 Constructor & Destructor Documentation

`def forcebalance.gmxio.Interaction_GMX.__init__(self, options, tgt_opts, forcefield)` Definition at line 1470 of file gmxio.py.

Here is the call graph for this function:



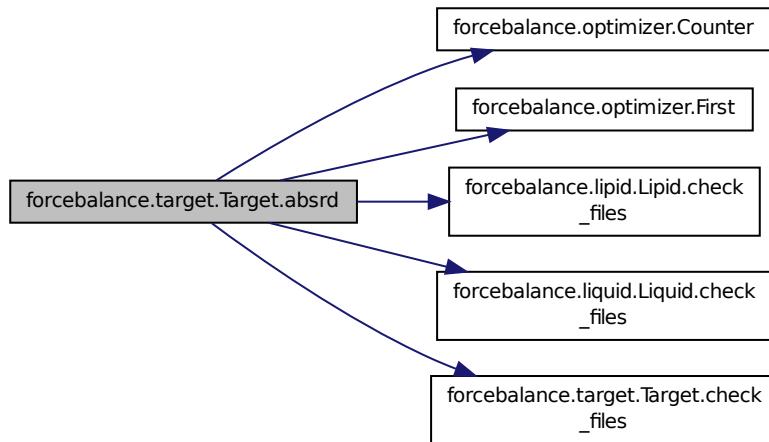
8.26.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.interaction.Interaction.get( self, mvals, AGrad = False, AHess = False ) [inherited] Evaluate objective function.
```

Definition at line 157 of file interaction.py.

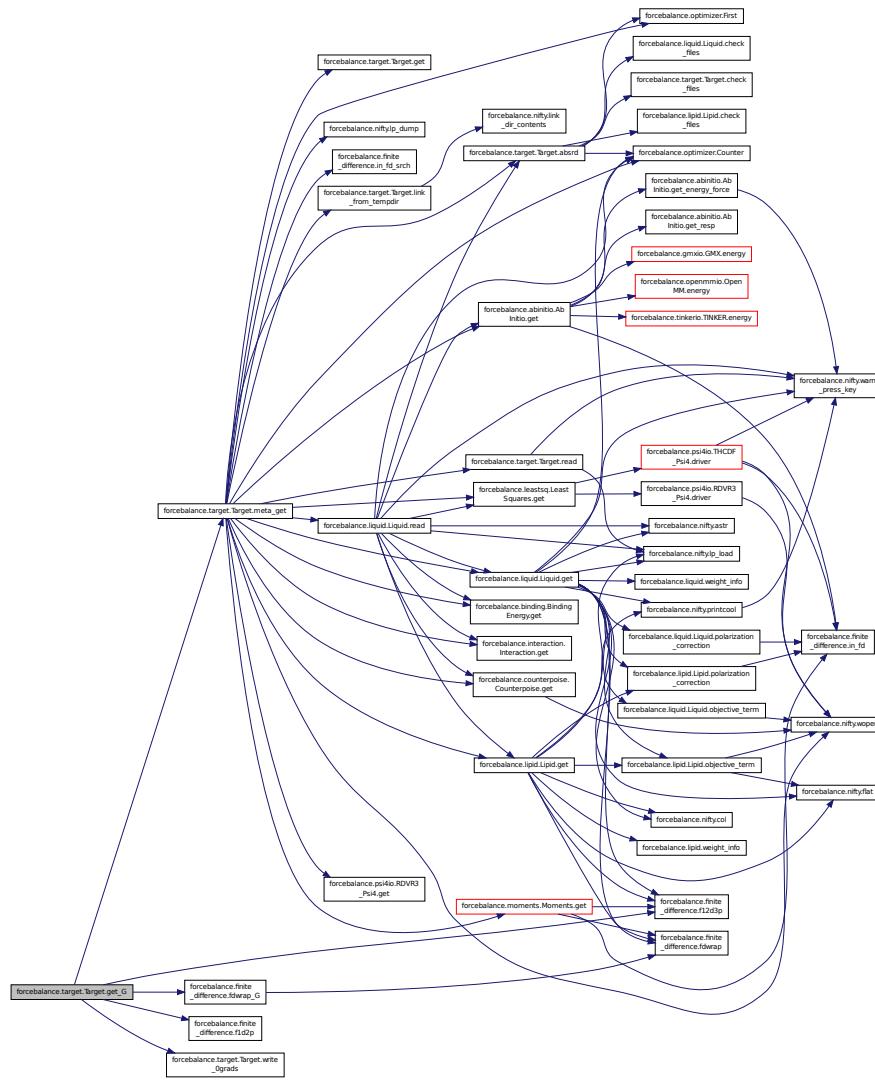
```
def forcebalance.target.Target.get_G( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



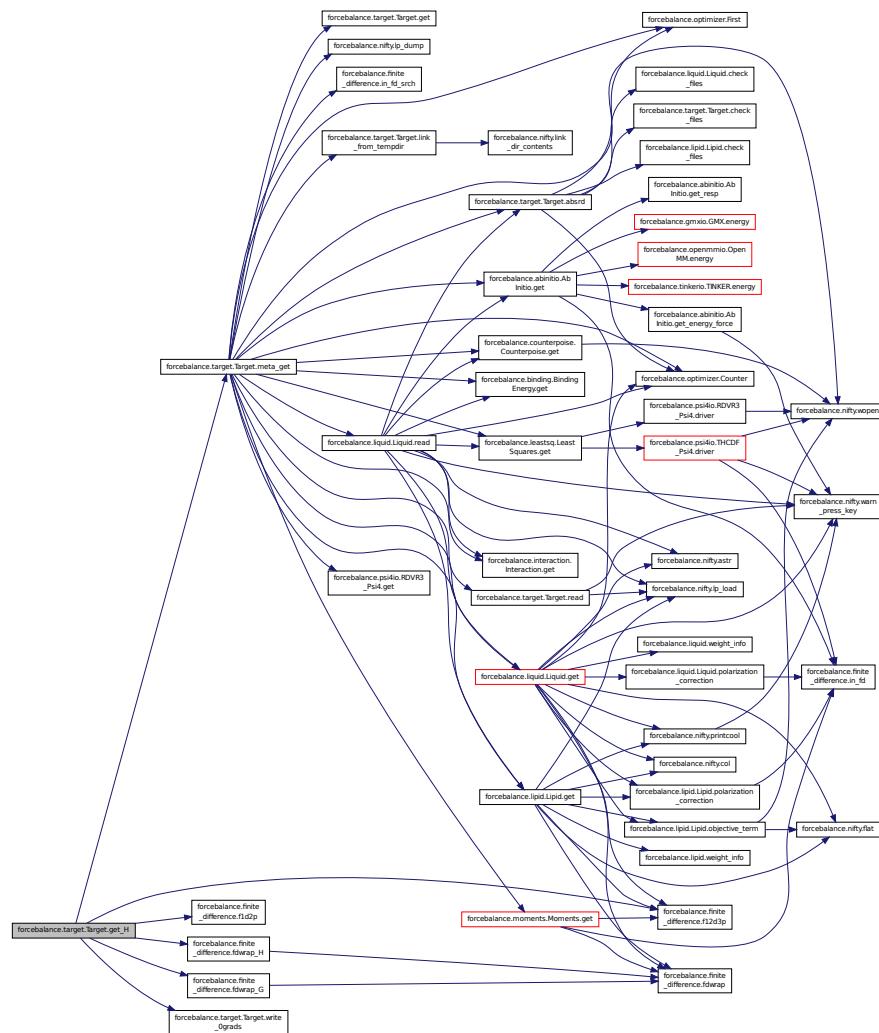
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

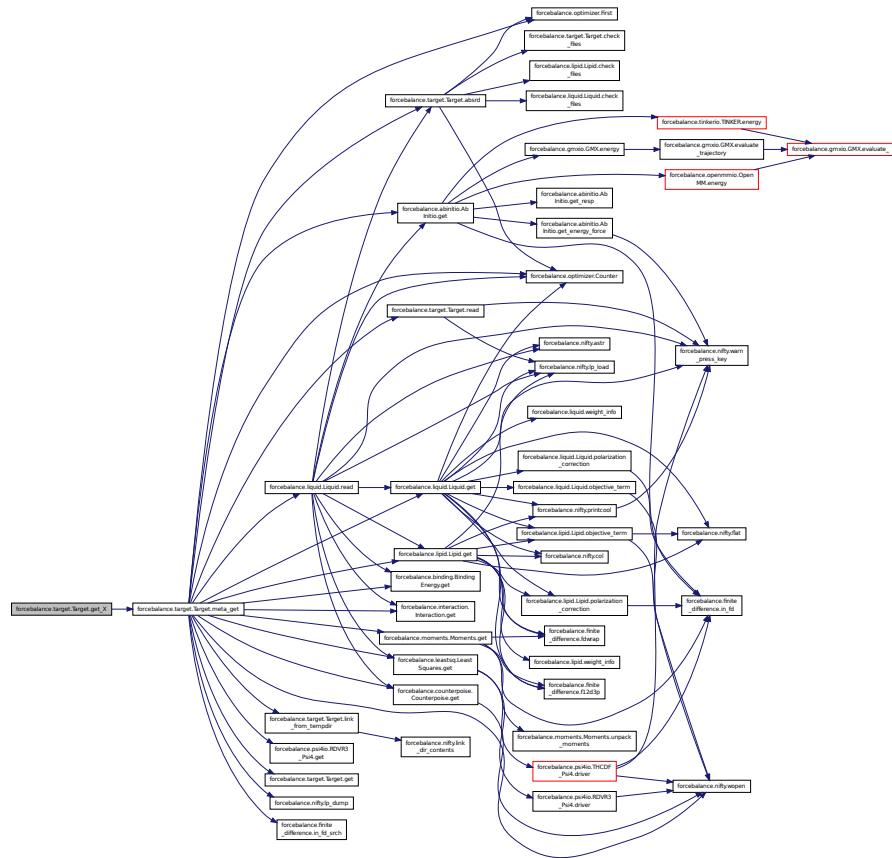
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

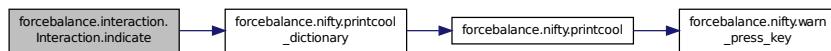
Definition at line 184 of file target.py.

Here is the call graph for this function:



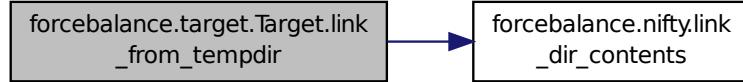
def forcebalance.interaction.Interaction.indicate (self) [inherited] Definition at line 141 of file interaction.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

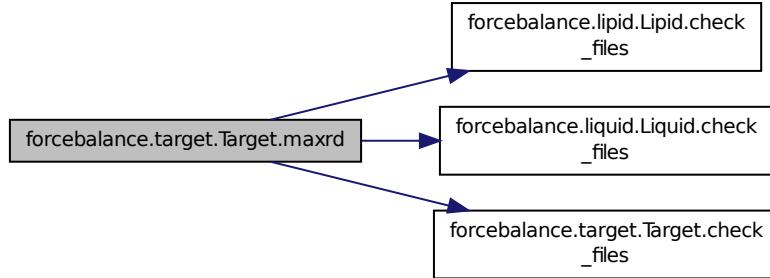
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

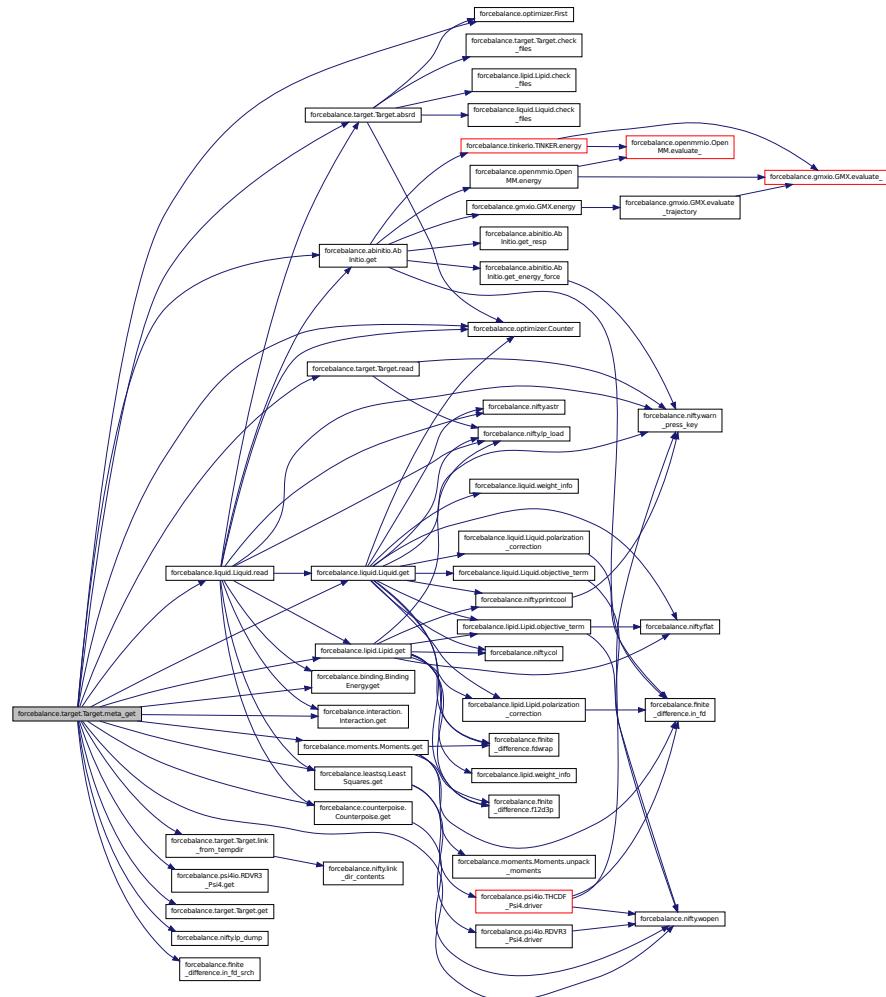


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

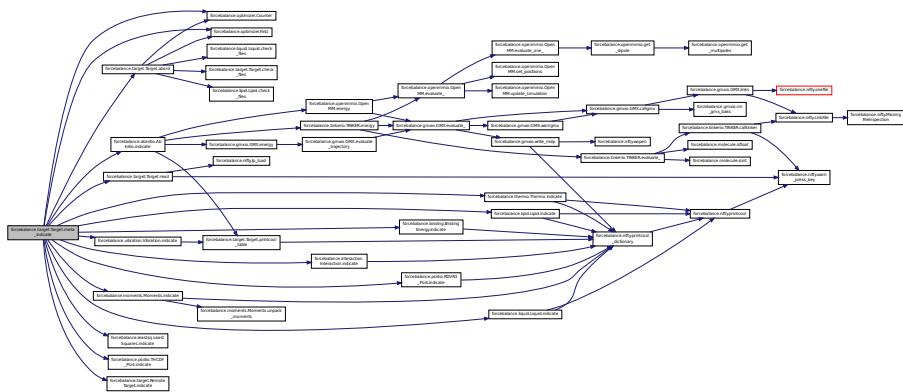
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

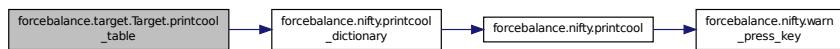
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

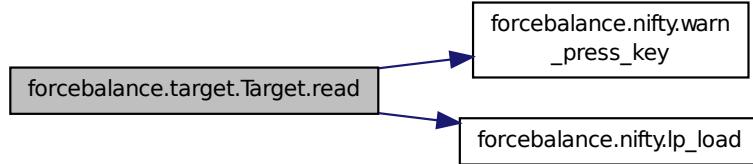
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.interaction.Interaction.read_reference_data (self) [inherited] Read the reference ab initio data from a file such as qdata.txt.

After reading in the information from qdata.txt, it is converted into kcal/mol.

Definition at line 124 of file interaction.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

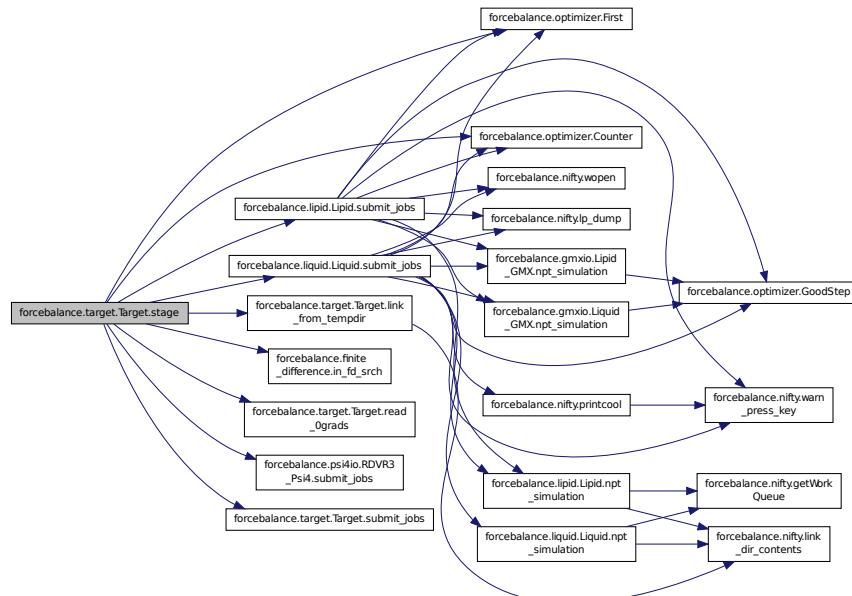
def forcebalance.BaseClass.set_option (self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

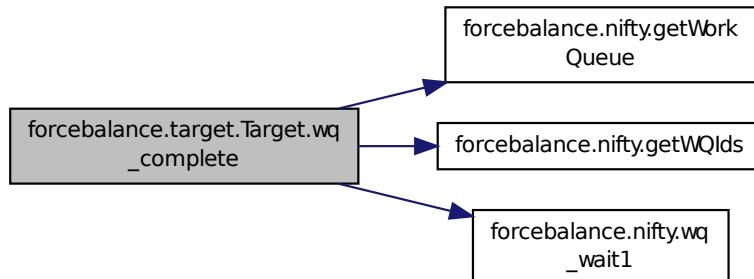


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_0grads( self, Ans ) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.26.4 Member Data Documentation

forcebalance.interaction.Interaction.divisor [inherited] Read in the reference data.

Definition at line 95 of file interaction.py.

forcebalance.interaction.Interaction.e_err [inherited] Definition at line 77 of file interaction.py.

forcebalance.interaction.Interaction.e_err_pct [inherited] Definition at line 78 of file interaction.py.

forcebalance.interaction.Interaction.emm [inherited] Definition at line 194 of file interaction.py.

forcebalance.interaction.Interaction.engine [inherited] Build keyword dictionaries to pass to engine.

Definition at line 88 of file interaction.py.

forcebalance.gmxio.Interaction_GMX.engine Default file names for coordinates, top and mdp files.

Definition at line 1475 of file gmxio.py.

forcebalance.interaction.Interaction.eqm [inherited] Set upper cutoff energy.

Reference (QM) interaction energies

Definition at line 72 of file interaction.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.interaction.Interaction.label [inherited] Snapshot label, useful for graphing.

Definition at line 74 of file interaction.py.

forcebalance.interaction.Interaction.mol [inherited] Definition at line 81 of file interaction.py.

forcebalance.interaction.Interaction.ns [inherited] Read in the trajectory file.

Definition at line 80 of file interaction.py.

forcebalance.interaction.Interaction.objective [inherited] Definition at line 195 of file interaction.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.interaction.Interaction.prefactor [inherited] Definition at line 113 of file interaction.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.interaction.Interaction.qfnm [inherited] The qdata.txt file that contains the QM energies and forces.

Definition at line 76 of file interaction.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.interaction.Interaction.select1 [inherited] Number of snapshots.

Do we call Q-Chem for dielectric energies? (Currently needs to be fixed) Do we put the reference energy into the denominator? Do we put the reference energy into the denominator? What is the energy denominator? Set fragment 1

Definition at line 60 of file interaction.py.

forcebalance.interaction.Interaction.select2 [inherited] Set fragment 2.

Definition at line 65 of file interaction.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.interaction.Interaction.weight [inherited] Definition at line 161 of file interaction.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

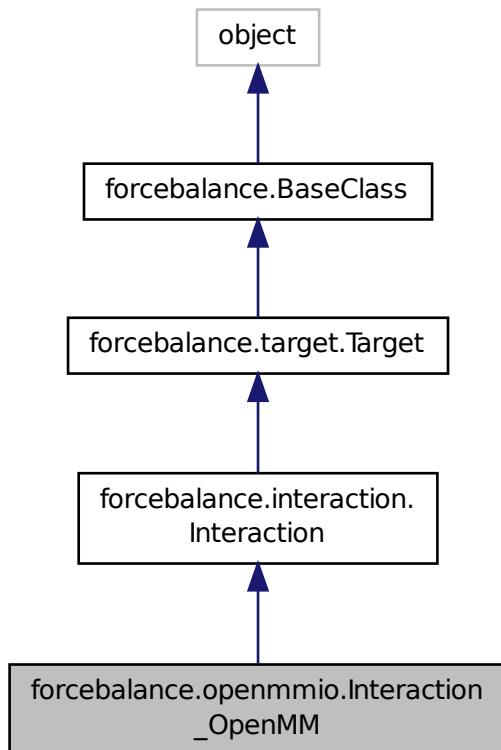
The documentation for this class was generated from the following file:

- [gmxio.py](#)

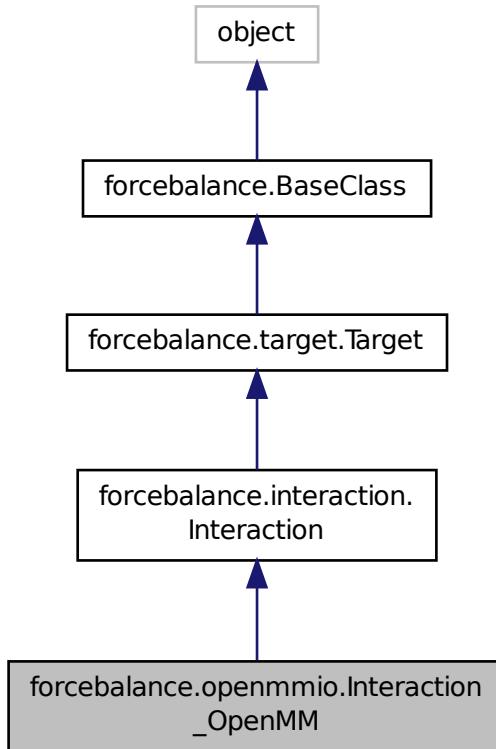
8.27 forcebalance.openmmio.Interaction_OpenMM Class Reference

Interaction matching using [OpenMM](#).

Inheritance diagram for forcebalance.openmmio.Interaction_OpenMM:



Collaboration diagram for forcebalance.openmmio.Interaction_OpenMM:



Public Member Functions

- def `_init_`
- def `read_reference_data`

Read the reference ab initio data from a file such as qdata.txt.
- def `indicate`
- def `get`

Evaluate objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.

- def `link_from_tempdir`
 Back up the temporary directory if desired, delete it and then create a new one.
- def `refresh_temp_directory`
 Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
 Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
 Supply the correct directory specified by user's "read" option.
- def `maxrd`
 Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
 Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
 Wrapper around the get function.
- def `submit_jobs`
- def `stage`
 Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
 This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
 Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
 Default file names for coordinates and key file.
- `select1`
 Number of snapshots.
- `select2`
 Set fragment 2.
- `eqm`
 Set upper cutoff energy.
- `label`
 Snapshot label, useful for graphing.
- `qfnm`
 The qdata.txt file that contains the QM energies and forces.
- `e_err`
- `e_err_pct`
- `ns`
 Read in the trajectory file.
- `mol`
- `engine`
 Build keyword dictionaries to pass to engine.
- `divisor`
 Read in the reference data.

- **prefactor**
- **weight**
- **emm**
- **objective**
- **rd**
Root directory of the whole project.
- **pgrad**
Iteration where we turn on zero-gradient skipping.
- **tempbase**
Relative directory of target.
- **tempdir**
- **rundir**
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**
Whether to write indicate.log at every iteration (true for all but remote.)
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

8.27.1 Detailed Description

Interaction matching using [OpenMM](#).

Definition at line 1190 of file openmmio.py.

8.27.2 Constructor & Destructor Documentation

def forcebalance.openmmio.Interaction_OpenMM.__init__(self, options, tgt_opts, forcefield) Definition at line 1191 of file openmmio.py.

Here is the call graph for this function:



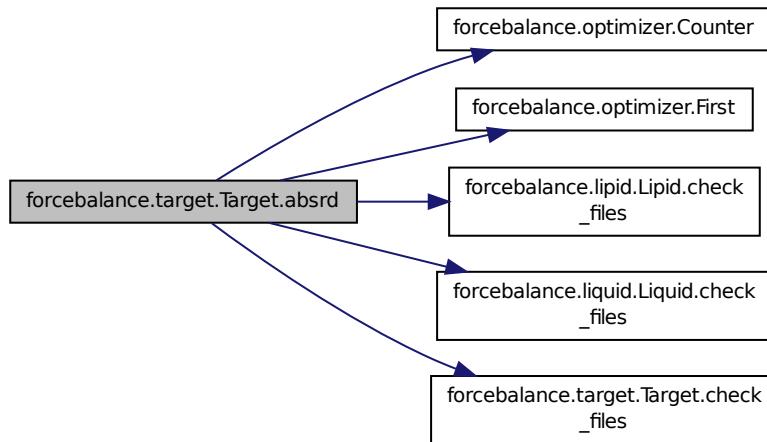
8.27.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.interaction.Interaction.get( self, mvals, AGrad = False, AHess = False ) [inherited] Evaluate objective function.
```

Definition at line 157 of file interaction.py.

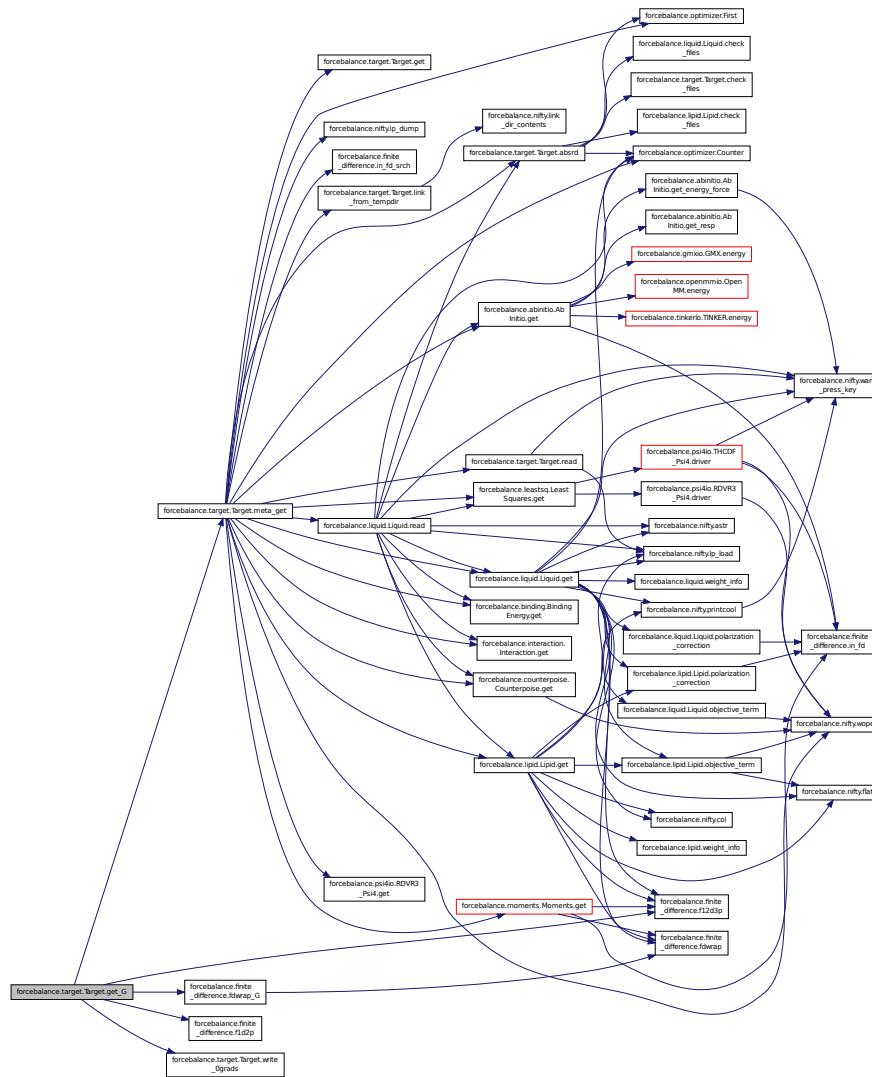
```
def forcebalance.target.Target.get_G( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



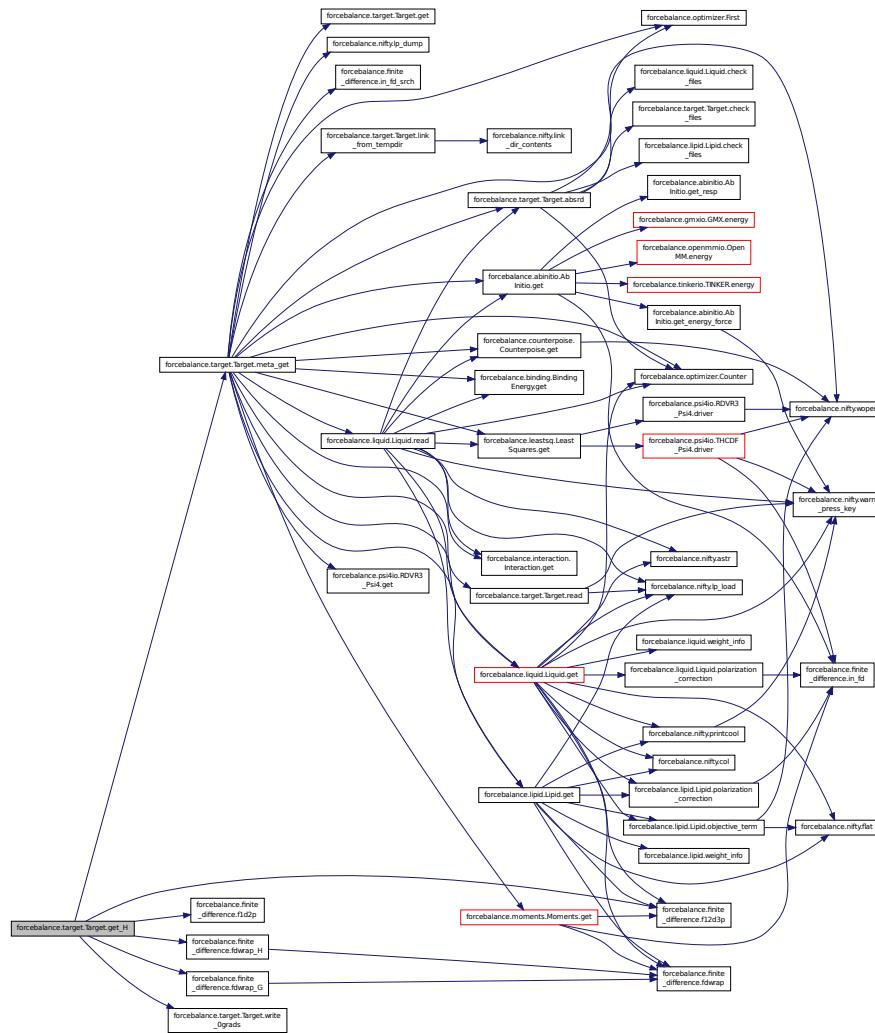
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

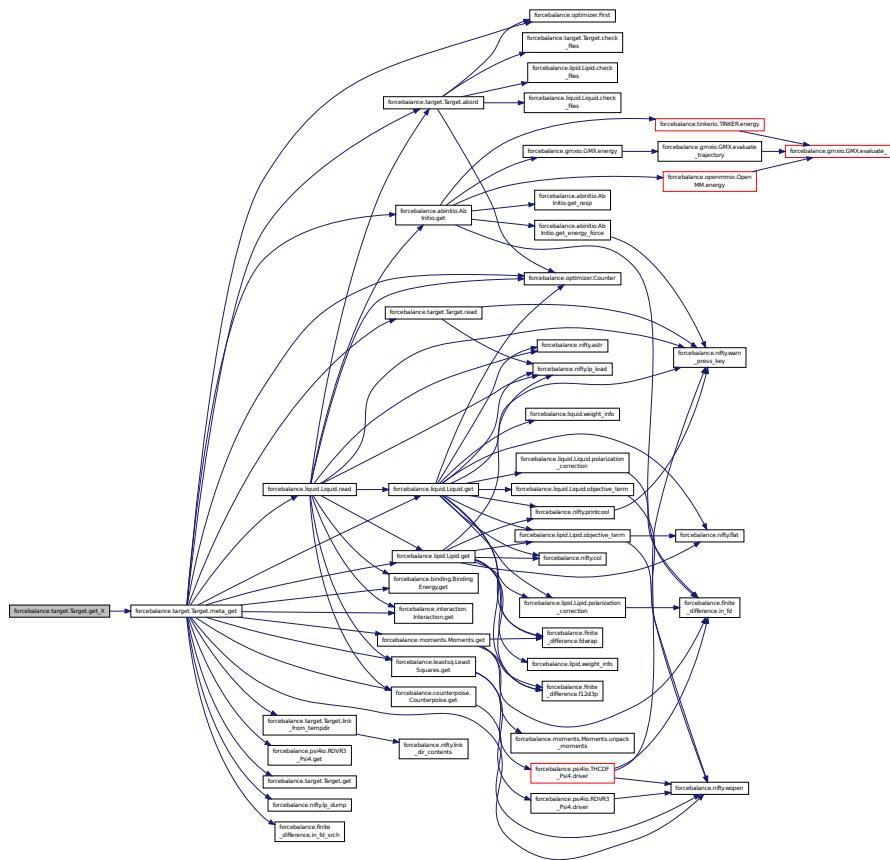
Here is the call graph for this function:



def forcebalance.target.Target.get.X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

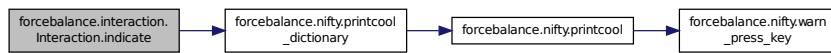
Definition at line 184 of file target.py.

Here is the call graph for this function:



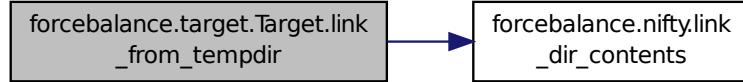
```
def forcebalance.interaction.Interaction.indicate ( self ) [inherited] Definition at line 141 of file interaction.py.
```

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

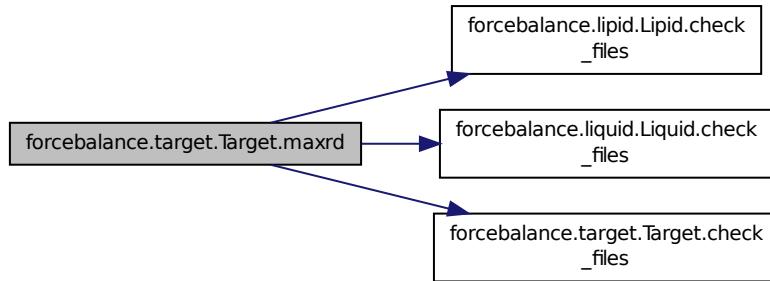
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

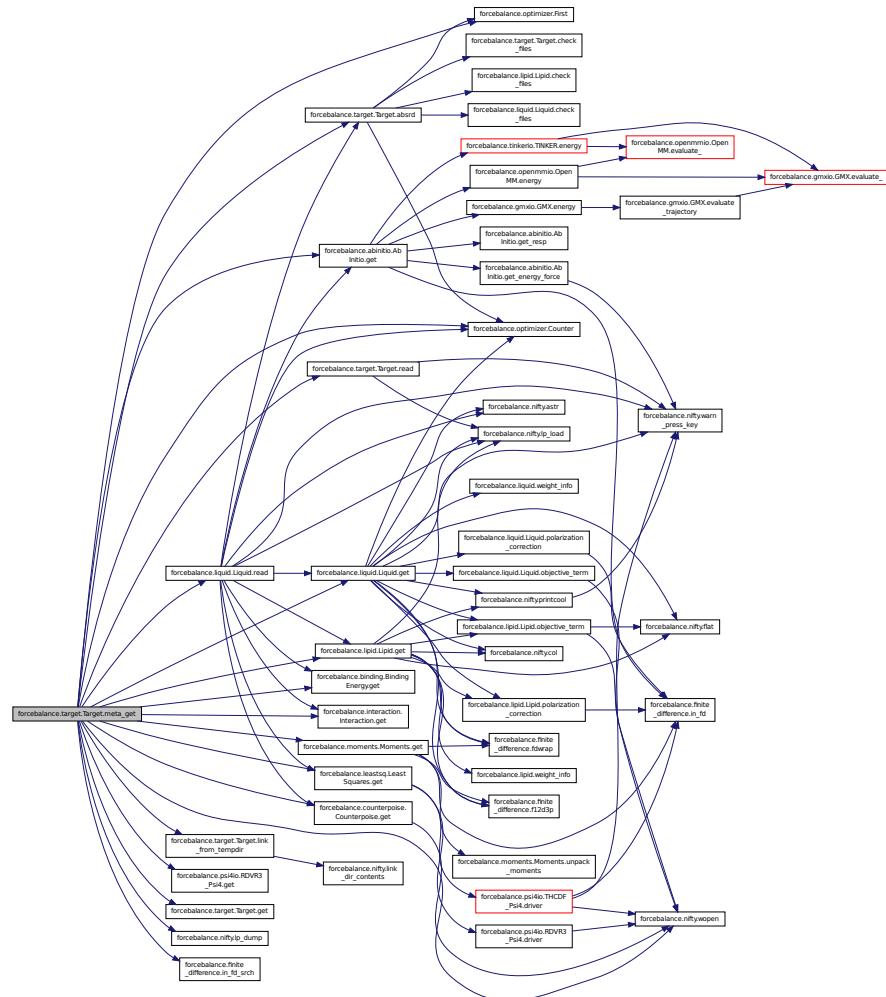


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

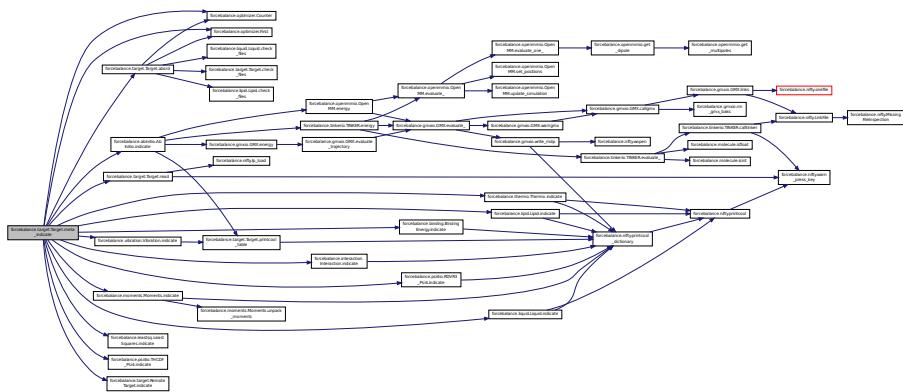
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict ([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

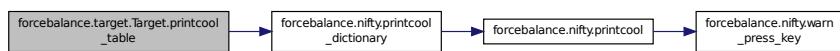
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

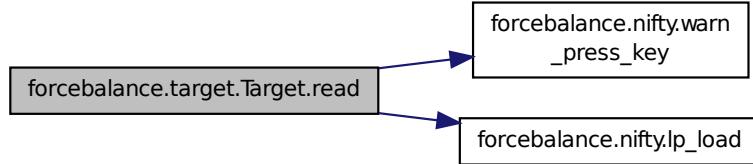
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.interaction.Interaction.read_reference_data (self) [inherited] Read the reference ab initio data from a file such as qdata.txt.

After reading in the information from qdata.txt, it is converted into kcal/mol.

Definition at line 124 of file interaction.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

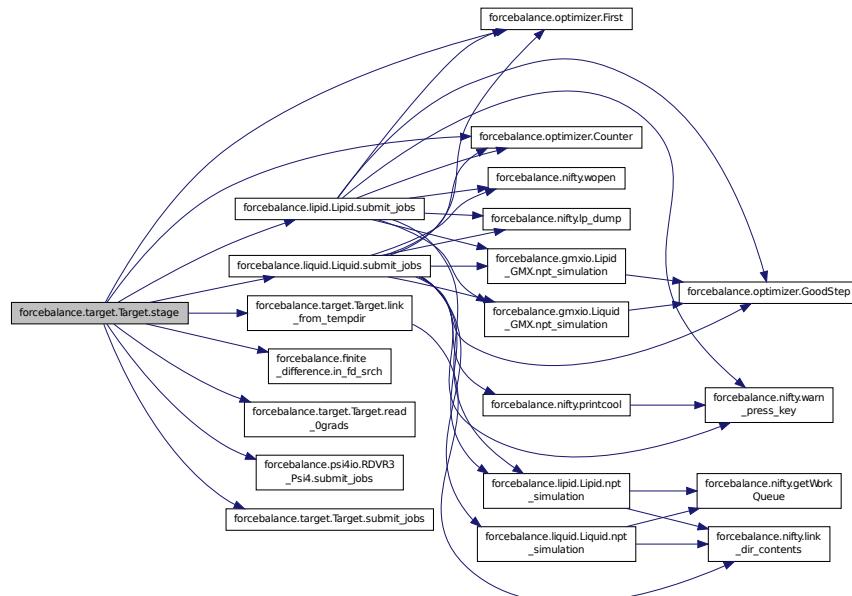
def forcebalance.BaseClass.set_option (self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

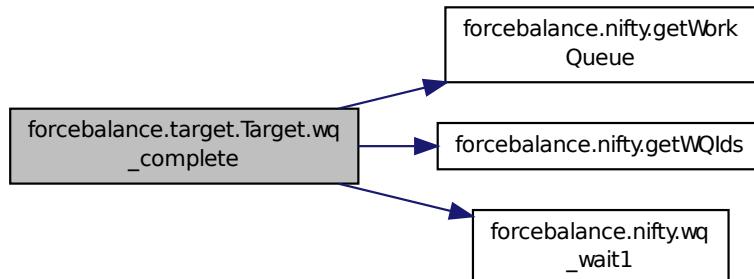


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_0grads( self, Ans ) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.27.4 Member Data Documentation

forcebalance.interaction.Interaction.divisor [inherited] Read in the reference data.

Definition at line 95 of file interaction.py.

forcebalance.interaction.Interaction.e_err [inherited] Definition at line 77 of file interaction.py.

forcebalance.interaction.Interaction.e_err_pct [inherited] Definition at line 78 of file interaction.py.

forcebalance.interaction.Interaction.emm [inherited] Definition at line 194 of file interaction.py.

forcebalance.interaction.Interaction.engine [inherited] Build keyword dictionaries to pass to engine.

Definition at line 88 of file interaction.py.

forcebalance.openmmio.Interaction_OpenMM.engine Default file names for coordinates and key file.

Definition at line 1196 of file openmmio.py.

forcebalance.interaction.Interaction.eqm [inherited] Set upper cutoff energy.

Reference (QM) interaction energies

Definition at line 72 of file interaction.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.interaction.Interaction.label [inherited] Snapshot label, useful for graphing.

Definition at line 74 of file interaction.py.

forcebalance.interaction.Interaction.mol [inherited] Definition at line 81 of file interaction.py.

forcebalance.interaction.Interaction.ns [inherited] Read in the trajectory file.

Definition at line 80 of file interaction.py.

forcebalance.interaction.Interaction.objective [inherited] Definition at line 195 of file interaction.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.interaction.Interaction.prefactor [inherited] Definition at line 113 of file interaction.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.interaction.Interaction.qfnm [inherited] The qdata.txt file that contains the QM energies and forces.

Definition at line 76 of file interaction.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.interaction.Interaction.select1 [inherited] Number of snapshots.

Do we call Q-Chem for dielectric energies? (Currently needs to be fixed) Do we put the reference energy into the denominator? Do we put the reference energy into the denominator? What is the energy denominator? Set fragment 1

Definition at line 60 of file interaction.py.

forcebalance.interaction.Interaction.select2 [inherited] Set fragment 2.

Definition at line 65 of file interaction.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.interaction.Interaction.weight [inherited] Definition at line 161 of file interaction.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

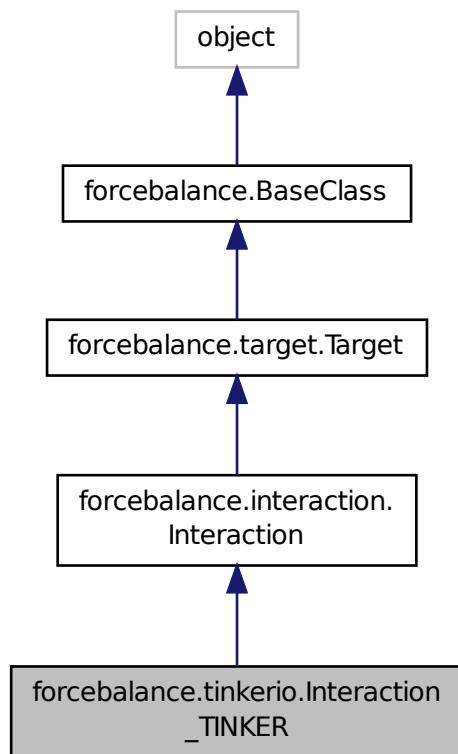
The documentation for this class was generated from the following file:

- [openmmio.py](#)

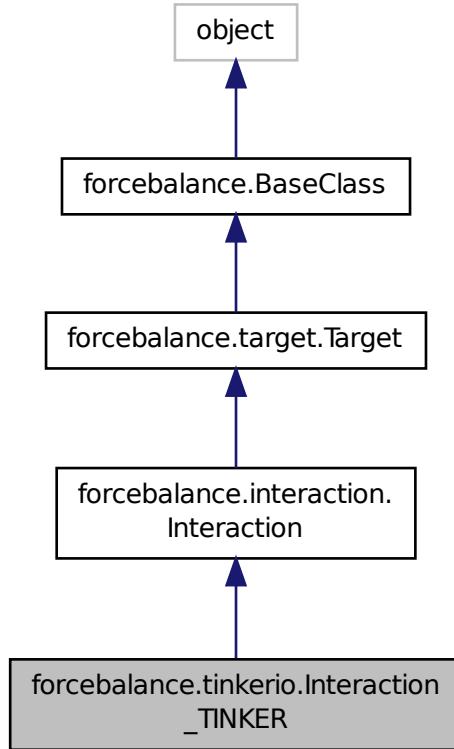
8.28 forcebalance.tinkerio.Interaction_TINKER Class Reference

Subclass of Target for interaction matching using [TINKER](#).

Inheritance diagram for forcebalance.tinkerio.Interaction_TINKER:



Collaboration diagram for forcebalance.tinkerio.Interaction_TINKER:



Public Member Functions

- def `_init_`
- def `read_reference_data`

Read the reference ab initio data from a file such as qdata.txt.
- def `indicate`
- def `get`

Evaluate objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.

- def `link_from_tempdir`
 Back up the temporary directory if desired, delete it and then create a new one.
- def `refresh_temp_directory`
 Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
 Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
 Supply the correct directory specified by user's "read" option.
- def `maxrd`
 Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
 Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
 Wrapper around the get function.
- def `submit_jobs`
- def `stage`
 Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
 This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
 Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
 Default file names for coordinates and key file.
- `select1`
 Number of snapshots.
- `select2`
 Set fragment 2.
- `eqm`
 Set upper cutoff energy.
- `label`
 Snapshot label, useful for graphing.
- `qfnm`
 The qdata.txt file that contains the QM energies and forces.
- `e_err`
- `e_err_pct`
- `ns`
 Read in the trajectory file.
- `mol`
- `engine`
 Build keyword dictionaries to pass to engine.
- `divisor`
 Read in the reference data.

- `prefactor`
- `weight`
- `emm`
- `objective`
- `rd`
`Root directory of the whole project.`
- `pgrad`
`Iteration where we turn on zero-gradient skipping.`
- `tempbase`
`Relative directory of target.`
- `tempdir`
- `rundir`
`self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.`
- `FF`
`Need the forcefield (here for now)`
- `xct`
`Counts how often the objective function was computed.`
- `gct`
`Counts how often the gradient was computed.`
- `hct`
`Counts how often the Hessian was computed.`
- `read_indicate`
`Whether to read indicate.log from file when restarting an aborted run.`
- `write_indicate`
`Whether to write indicate.log at every iteration (true for all but remote.)`
- `read_objective`
`Whether to read objective.p from file when restarting an aborted run.`
- `write_objective`
`Whether to write objective.p at every iteration (true for all but remote.)`
- `verbose_options`
- `PrintOptionDict`

8.28.1 Detailed Description

Subclass of Target for interaction matching using [TINKER](#).

Definition at line 1086 of file tinkerio.py.

8.28.2 Constructor & Destructor Documentation

`def forcebalance.tinkerio.Interaction_TINKER.__init__ (self, options, tgt_opts, forcefield)` Definition at line 1087 of file tinkerio.py.

Here is the call graph for this function:



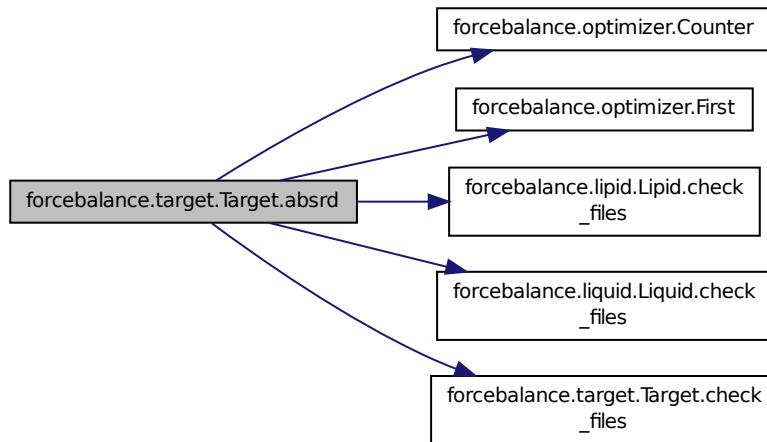
8.28.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.interaction.Interaction.get( self, mvals, AGrad = False, AHess = False ) [inherited] Evaluate objective function.
```

Definition at line 157 of file interaction.py.

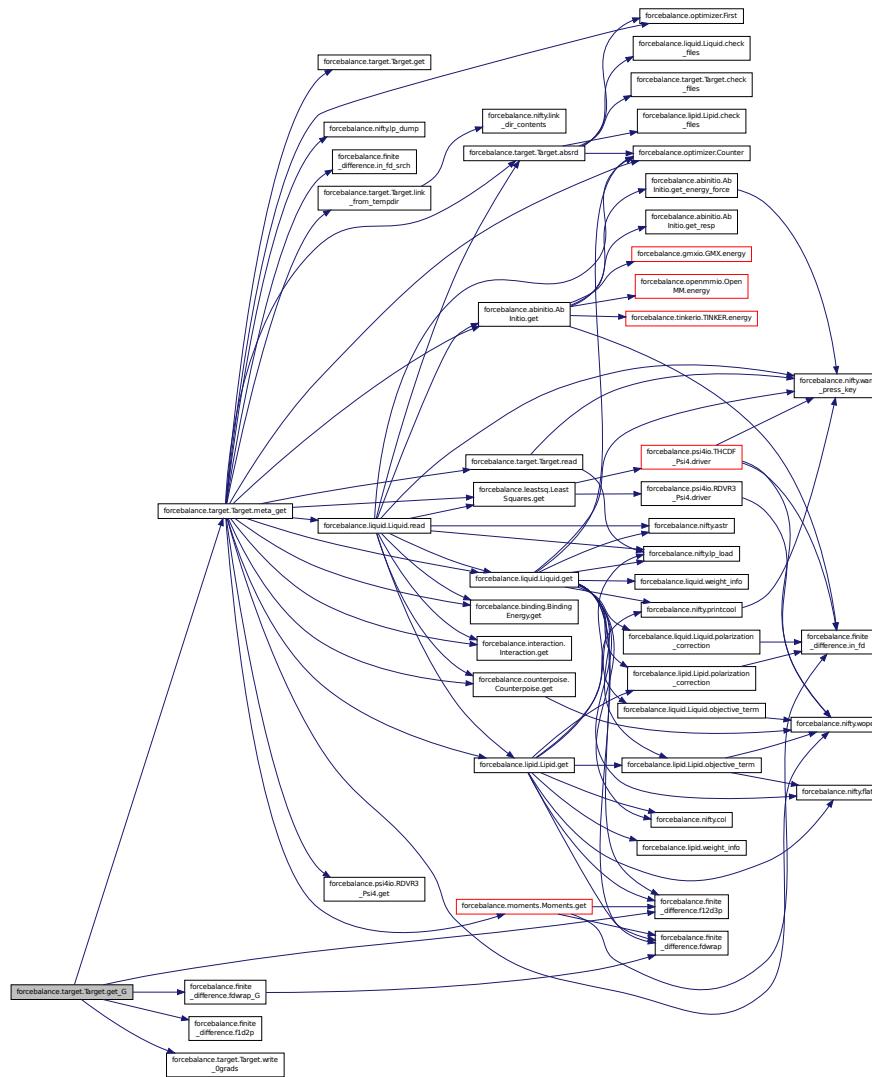
```
def forcebalance.target.Target.get_G( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



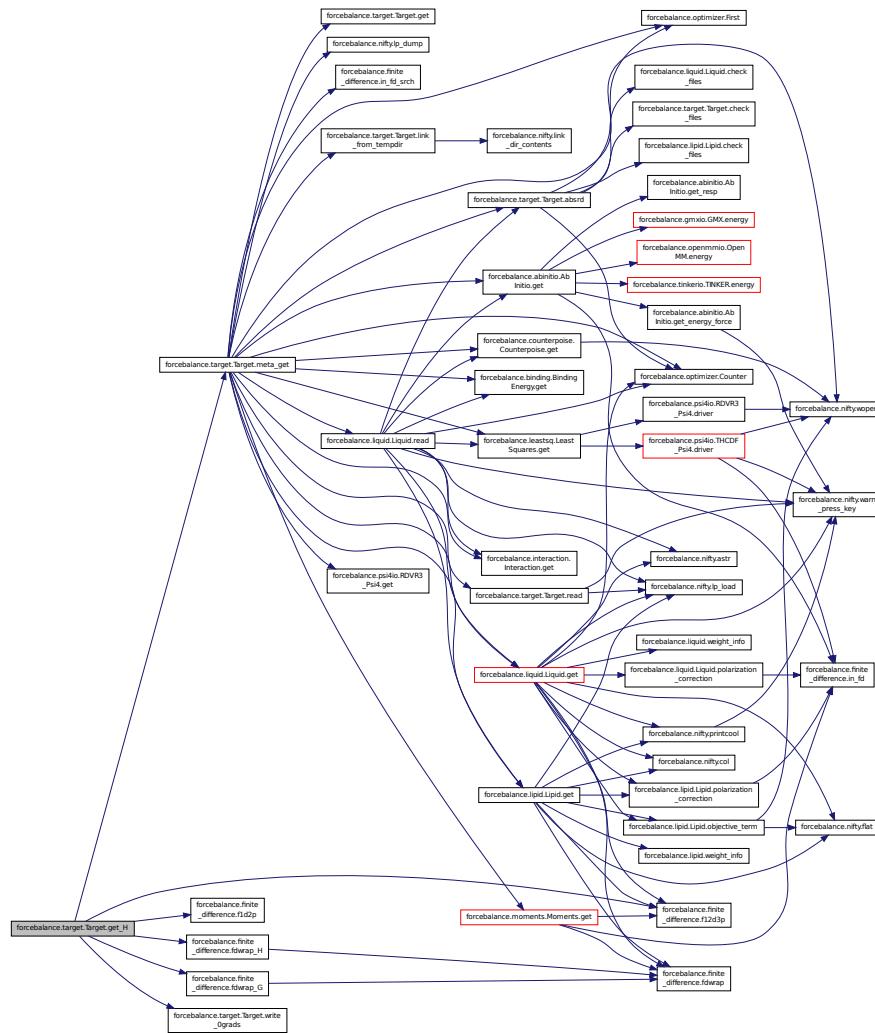
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

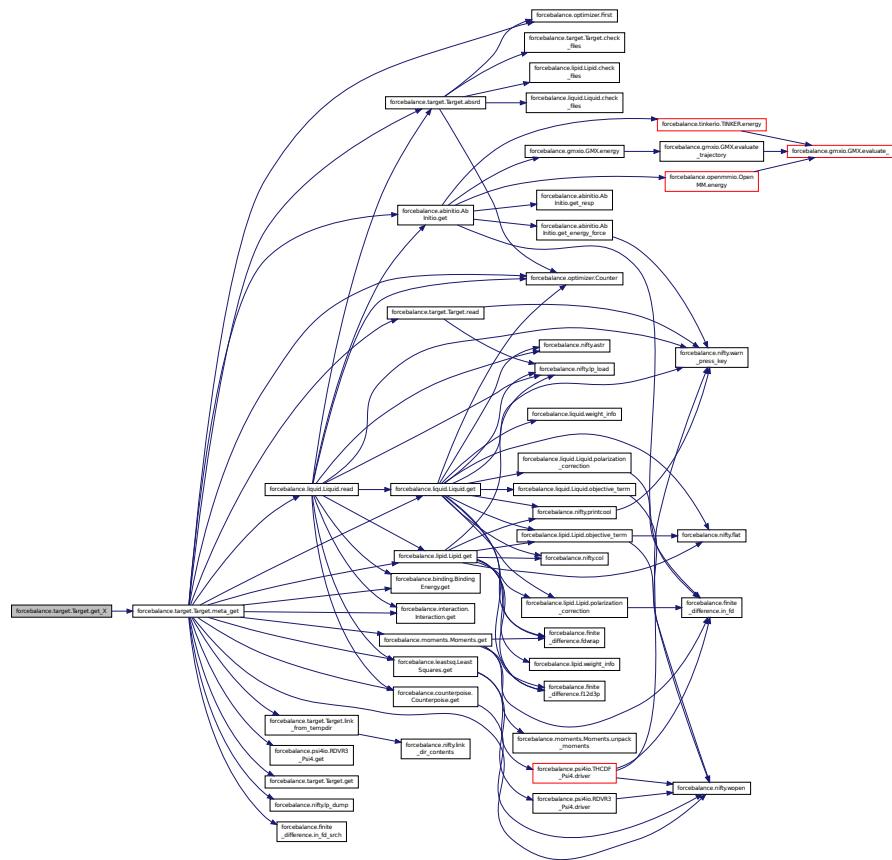
Here is the call graph for this function:



def forcebalance.target.Target.get.X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

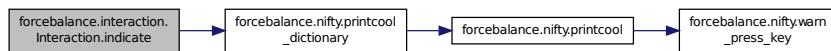
Definition at line 184 of file target.py.

Here is the call graph for this function:



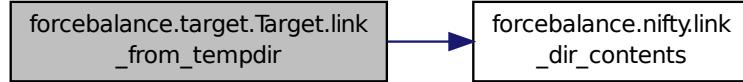
```
def forcebalance.optimizer.optimize ( self ) [inherited] Definition at line 141 of file
optimizer.py.
```

Here is the call graph for this function:



```
def forcebalance.target.Target.link_from_tempdir( self, absdestdir ) [inherited] Definition at line 315 of
file target.py.
```

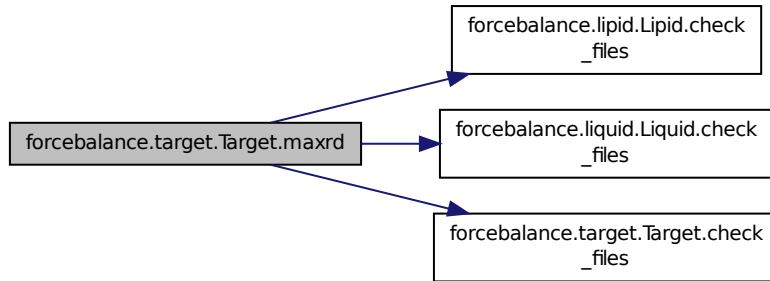
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

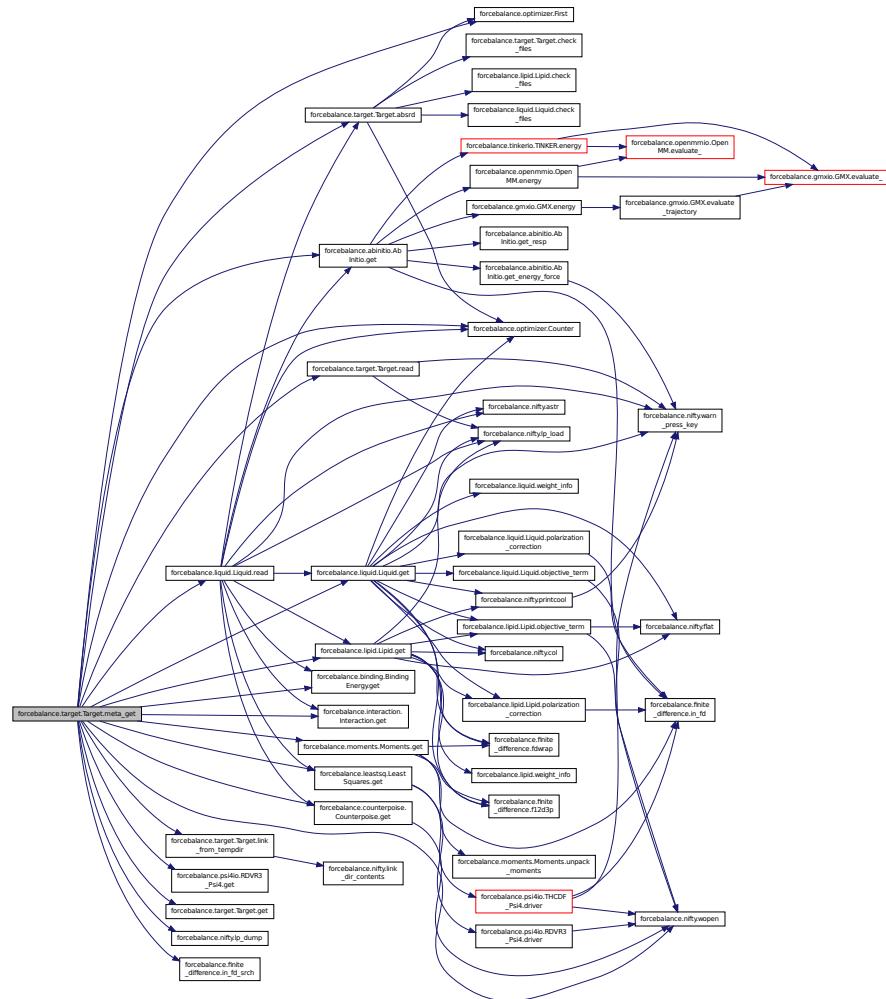


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

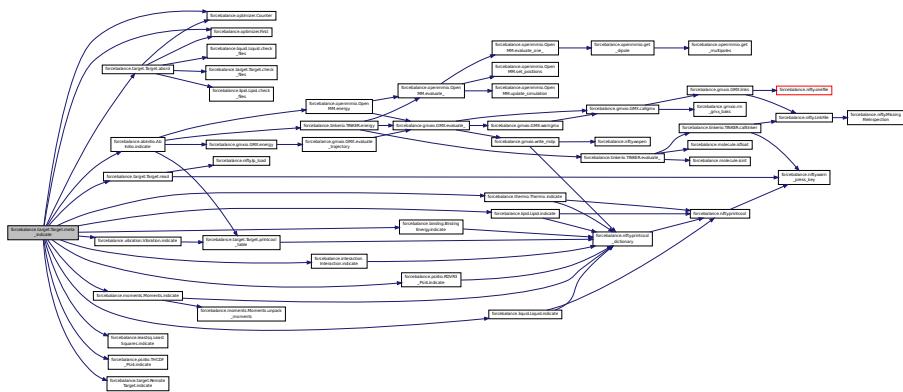
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

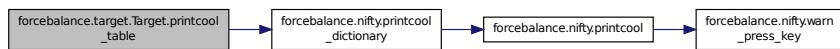
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

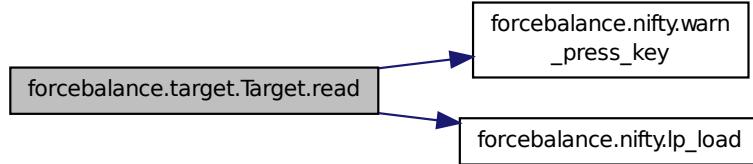
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.interaction.Interaction.read_reference_data (self) [inherited] Read the reference ab initio data from a file such as qdata.txt.

After reading in the information from qdata.txt, it is converted into kcal/mol.

Definition at line 124 of file interaction.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

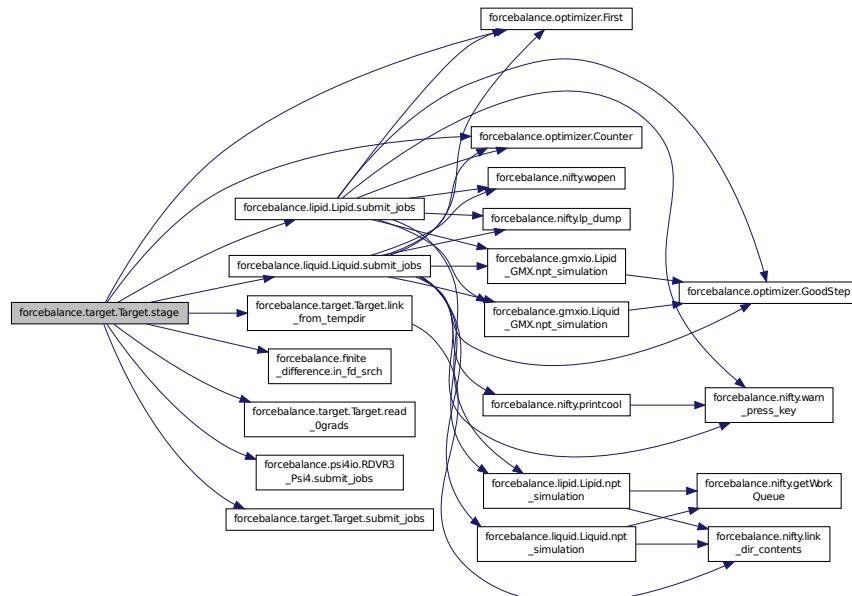
def forcebalance.BaseClass.set_option (self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

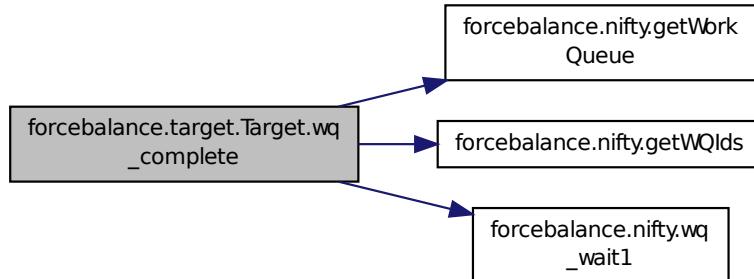


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_0grads( self, Ans ) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.28.4 Member Data Documentation

forcebalance.interaction.Interaction.divisor [inherited] Read in the reference data.

Definition at line 95 of file interaction.py.

forcebalance.interaction.Interaction.e_err [inherited] Definition at line 77 of file interaction.py.

forcebalance.interaction.Interaction.e_err_pct [inherited] Definition at line 78 of file interaction.py.

forcebalance.interaction.Interaction.emm [inherited] Definition at line 194 of file interaction.py.

forcebalance.interaction.Interaction.engine [inherited] Build keyword dictionaries to pass to engine.

Definition at line 88 of file interaction.py.

forcebalance.tinkerio.Interaction_TINKER.engine Default file names for coordinates and key file.

Definition at line 1091 of file tinkerio.py.

forcebalance.interaction.Interaction.eqm [inherited] Set upper cutoff energy.

Reference (QM) interaction energies

Definition at line 72 of file interaction.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.interaction.Interaction.label [inherited] Snapshot label, useful for graphing.

Definition at line 74 of file interaction.py.

forcebalance.interaction.Interaction.mol [inherited] Definition at line 81 of file interaction.py.

forcebalance.interaction.Interaction.ns [inherited] Read in the trajectory file.

Definition at line 80 of file interaction.py.

forcebalance.interaction.Interaction.objective [inherited] Definition at line 195 of file interaction.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.interaction.Interaction.prefactor [inherited] Definition at line 113 of file interaction.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.interaction.Interaction.qfnm [inherited] The qdata.txt file that contains the QM energies and forces.

Definition at line 76 of file interaction.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.interaction.Interaction.select1 [inherited] Number of snapshots.

Do we call Q-Chem for dielectric energies? (Currently needs to be fixed) Do we put the reference energy into the denominator? Do we put the reference energy into the denominator? What is the energy denominator? Set fragment 1

Definition at line 60 of file interaction.py.

forcebalance.interaction.Interaction.select2 [inherited] Set fragment 2.

Definition at line 65 of file interaction.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.interaction.Interaction.weight [inherited] Definition at line 161 of file interaction.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

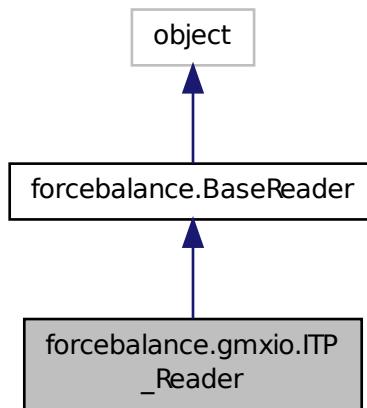
The documentation for this class was generated from the following file:

- [tinkerio.py](#)

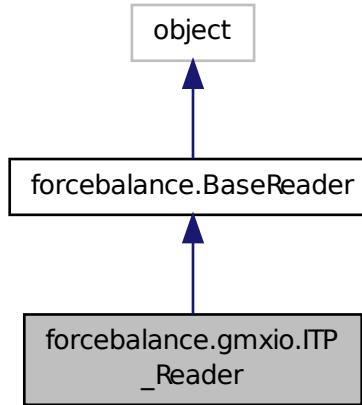
8.29 forcebalance.gmxio.ITP_Reader Class Reference

Finite state machine for parsing GROMACS force field files.

Inheritance diagram for forcebalance.gmxio.ITP_Reader:



Collaboration diagram for forcebalance.gmxio.ITP_Reader:



Public Member Functions

- def `__init__`
- def `feed`

Given a line, determine the interaction type and the atoms involved (the suffix).
- def `Split`
- def `Whites`
- def `build.pid`

Returns the parameter type (e.g.

Public Attributes

- `sec`

The current section that we're in.
- `nbttype`

Nonbonded type.
- `mol`

The current molecule (set by the moleculetype keyword)
- `pdict`

The parameter dictionary (defined in this file)
- `atomnames`

Listing of all atom names in the file, (probably unnecessary)
- `atomtypes`

Listing of all atom types in the file, (probably unnecessary)
- `atomtype_to_mass`

A dictionary of atomic masses.
- `itype`
- `suffix`

- [molatom](#)
- [In](#)
- [adict](#)

The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

- [Molecules](#)
- [AtomTypes](#)

8.29.1 Detailed Description

Finite state machine for parsing GROMACS force field files.

We open the force field file and read all of its lines. As we loop through the force field file, we look for two types of tags: (1) section markers, in [GMX](#) indicated by [section_name], which allows us to determine the section, and (2) parameter tags, indicated by the 'PRM' or 'RPT' keywords.

As we go through the file, we figure out the atoms involved in the interaction described on each line.

When a 'PRM' keyword is indicated, it is followed by a number which is the field in the line to be modified, starting with zero. Based on the field number and the section name, we can figure out the parameter type. With the parameter type and the atoms in hand, we construct a 'parameter identifier' or pid which uniquely identifies that parameter. We also store the physical parameter value in an array called 'pvals0' and the precise location of that parameter (by filename, line number, and field number) in a list called 'pfields'.

An example: Suppose in 'my_ff.itp' I encounter the following on lines 146 and 147:

```
1 [ angletypes ]
2 CA   CB   O   1   109.47  350.00 ; PRM 4 5
```

From reading [angletypes] I know I'm in the 'angletypes' section.

On the next line, I notice two parameters on fields 4 and 5.

From the atom types, section type and field number I know the parameter IDs are 'ANGLESBCACBO' and 'ANGLESKCACBO'.

After building map={'ANGLESBCACBO':1,'ANGLESKCACBO':2}, I store the values in an array: pvals0=array([109.47,350.00]), and I put the parameter locations in pfields: pfields=[['my_ff.itp',147,4,1.0],['my_ff.itp',146,5,1.0]]. The 1.0 is a 'multiplier' and I will explain it below.

Note that in the creation of parameter IDs, we run into the issue that the atoms involved in the interaction may be labeled in reverse order (e.g. OCACB). Thus, we store both the normal and the reversed parameter ID in the map.

Parameter repetition and multiplier:

If 'RPT' is encountered in the line, it is always in the syntax: 'RPT 4 ANGLESBCACAH 5 MINUS_ANGLES-KCACAH /RPT'. In this case, field 4 is replaced by the stored parameter value corresponding to ANGLESBCACAH and field 5 is replaced by -1 times the stored value of ANGLESKCACAH. Now I just picked this as an example, I don't think people actually want a negative angle force constant .. :) the MINUS keyword does come in handy for assigning atomic charges and virtual site positions. In order to achieve this, a multiplier of -1.0 is stored into pfields instead of 1.0.

Todo Note that I can also create the opposite virtual site position by changing the atom labeling, woo!

Definition at line 328 of file gmxio.py.

8.29.2 Constructor & Destructor Documentation

def forcebalance.gmxio.ITP_Reader.__init__ (self, fnm) Definition at line 331 of file gmxio.py.

8.29.3 Member Function Documentation

def forcebalance.BaseReader.build.pid (self, pfd) [inherited] Returns the parameter type (e.g. K in BONDSK) based on the current interaction type.

Both the 'pdic' dictionary (see [gmxio.pdic](#)) and the interaction type 'state' (here, BONDS) are needed to get the parameter type.

If, however, 'pdic' does not contain the ptype value, a suitable substitute is simply the field number.

Note that if the interaction type state is not set, then it defaults to the file name, so a generic parameter ID is 'filename.line_num.field_num'

Definition at line 124 of file __init__.py.

def forcebalance.gmxio.ITP_Reader.feed (self, line) Given a line, determine the interaction type and the atoms involved (the suffix).

For example, we want

```
H O H 5 1.231258497536e+02 4.269161426840e+02 -1.033397697685e-02 1.304674117410e+04  
; PRM 4 5 6 7
```

to give us itype = 'UREY_BRADLEY' and suffix = 'HOH'

If we are in a TypeSection, it returns a list of atom types;

If we are in a TopolSection, it returns a list of atom names.

The section is essentially a case statement that picks out the appropriate interaction type and makes a list of the atoms involved

Note that we can call gmxdump for this as well, but I prefer to read the force field file directly.

ToDo: [atoms] section might need to be more flexible to accommodate optional fields

Definition at line 369 of file gmxio.py.

def forcebalance.BaseReader.Split (self, line) [inherited] Definition at line 99 of file __init__.py.

def forcebalance.BaseReader.Whites (self, line) [inherited] Definition at line 102 of file __init__.py.

8.29.4 Member Data Documentation

forcebalance.BaseReader.adict [inherited] The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

Definition at line 89 of file __init__.py.

forcebalance.gmxio.ITP_Reader.atomnames Listing of all atom names in the file, (probably unnecessary)

Definition at line 343 of file gmxio.py.

forcebalance.gmxio.ITP_Reader.atomtype_to_mass A dictionary of atomic masses.

Definition at line 347 of file gmxio.py.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file __init__.py.

forcebalance.gmxio.ITP_Reader.atomtypes Listing of all atom types in the file, (probably unnecessary)

Definition at line 345 of file gmxio.py.

forcebalance.gmxio.ITP_Reader.itype Definition at line 372 of file gmxio.py.

forcebalance.BaseReader.in [inherited] Definition at line 84 of file __init__.py.

forcebalance.gmxio.ITP_Reader.mol The current molecule (set by the moleculetype keyword)

Definition at line 339 of file gmxio.py.

forcebalance.gmxio.ITP_Reader.molatom Definition at line 479 of file gmxio.py.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file __init__.py.

forcebalance.gmxio.ITP_Reader.nbtype Nonbonded type.

Definition at line 337 of file gmxio.py.

forcebalance.gmxio.ITP_Reader.pdict The parameter dictionary (defined in this file)

Definition at line 341 of file gmxio.py.

forcebalance.gmxio.ITP_Reader.sec The current section that we're in.

Definition at line 335 of file gmxio.py.

forcebalance.gmxio.ITP_Reader.suffix Definition at line 474 of file gmxio.py.

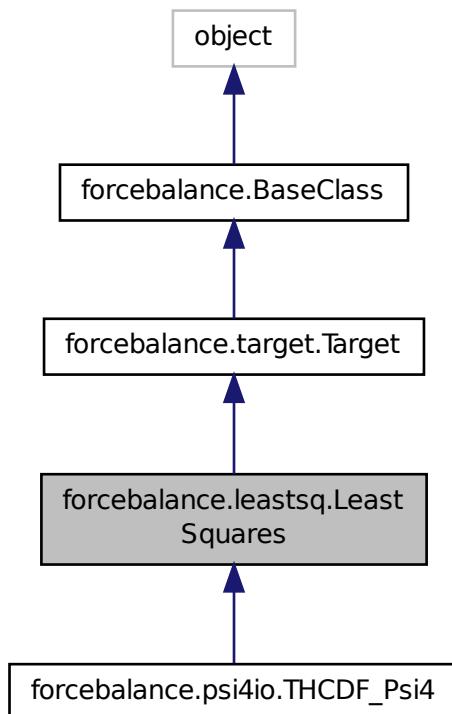
The documentation for this class was generated from the following file:

- [gmxio.py](#)

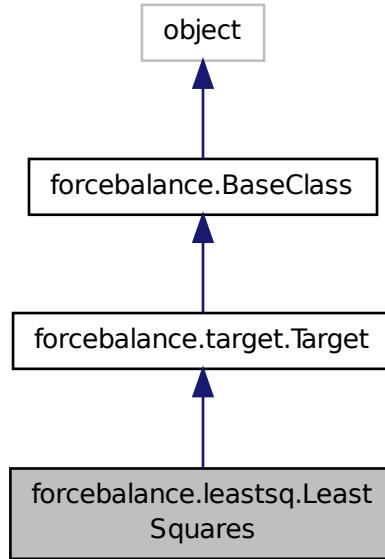
8.30 forcebalance.leastsq.LeastSquares Class Reference

Subclass of Target for general least squares fitting.

Inheritance diagram for forcebalance.leastsq.LeastSquares:



Collaboration diagram for forcebalance.leastsq.LeastSquares:



Public Member Functions

- def `_init_`
- def `indicate`
- def `get`
 LPW 05-30-2012.
- def `get_X`
 Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`
 Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`
 Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
 Computes the objective function contribution and its gradient.
- def `get_H`
 Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
 Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
 Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
 Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

- def **absrd**
Supply the correct directory specified by user's "read" option.
- def **maxrd**
Supply the latest existing temp-directory containing valid data.
- def **meta_indicate**
Wrap around the indicate function, so it can print to screen and also to a file.
- def **meta_get**
Wrapper around the get function.
- def **submit_jobs**
- def **stage**
Stages the directory for the target, and then launches Work Queue processes if any.
- def **wq_complete**
This method determines whether the Work Queue tasks for the current target have completed.
- def **printcool_table**
Print target information in an organized table format.
- def **__setattr__**
- def **set_option**

Public Attributes

- **MAQ**
Dictionary for derivative terms.
- **D**
- **objective**
- **rd**
Root directory of the whole project.
- **pgrad**
Iteration where we turn on zero-gradient skipping.
- **tempbase**
Relative directory of target.
- **tempdir**
- **rundir**
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**
Whether to write indicate.log at every iteration (true for all but remote.)
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

8.30.1 Detailed Description

Subclass of Target for general least squares fitting.
Definition at line 35 of file leastsq.py.

8.30.2 Constructor & Destructor Documentation

```
def forcebalance.leastsq.LeastSquares.__init__ ( self, options, tgt_opts, forcefield )
```

 Definition at line 38 of file leastsq.py.

8.30.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited]
```

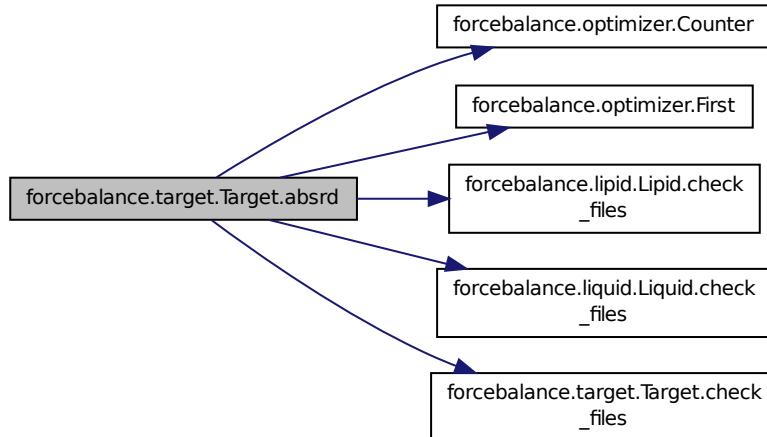
 Definition at line 28 of file __init__.py.

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited]
```

 Supply the correct directory specified by user's "read" option.

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files ( self, there ) [inherited]
```

 Check this directory for the presence of readable files when the 'read' option is set.

Definition at line 364 of file target.py.

```
def forcebalance.leastsq.LeastSquares.get ( self, mvals, AGrad = False, AHess = False )
```

 LPW 05-30-2012.

This subroutine builds the objective function (and optionally its derivatives) from a general software.

This subroutine interfaces with simulation software 'drivers'. The driver is expected to give exact values, fitting values, and weights.

Parameters

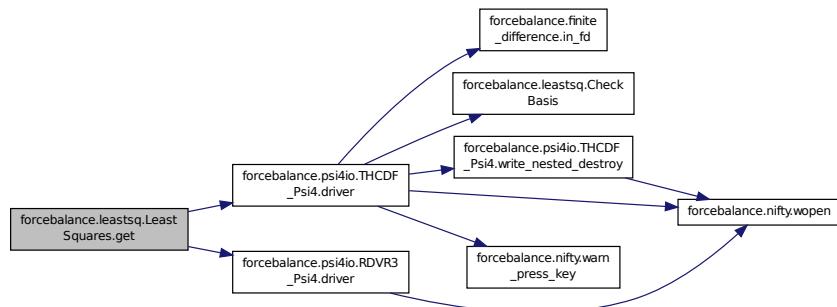
in	<i>mvals</i>	Mathematical parameter values
in	<i>AGrad</i>	Switch to turn on analytic gradient
in	<i>AHess</i>	Switch to turn on analytic Hessian

Returns

Answer Contribution to the objective function

Definition at line 62 of file leastsq.py.

Here is the call graph for this function:



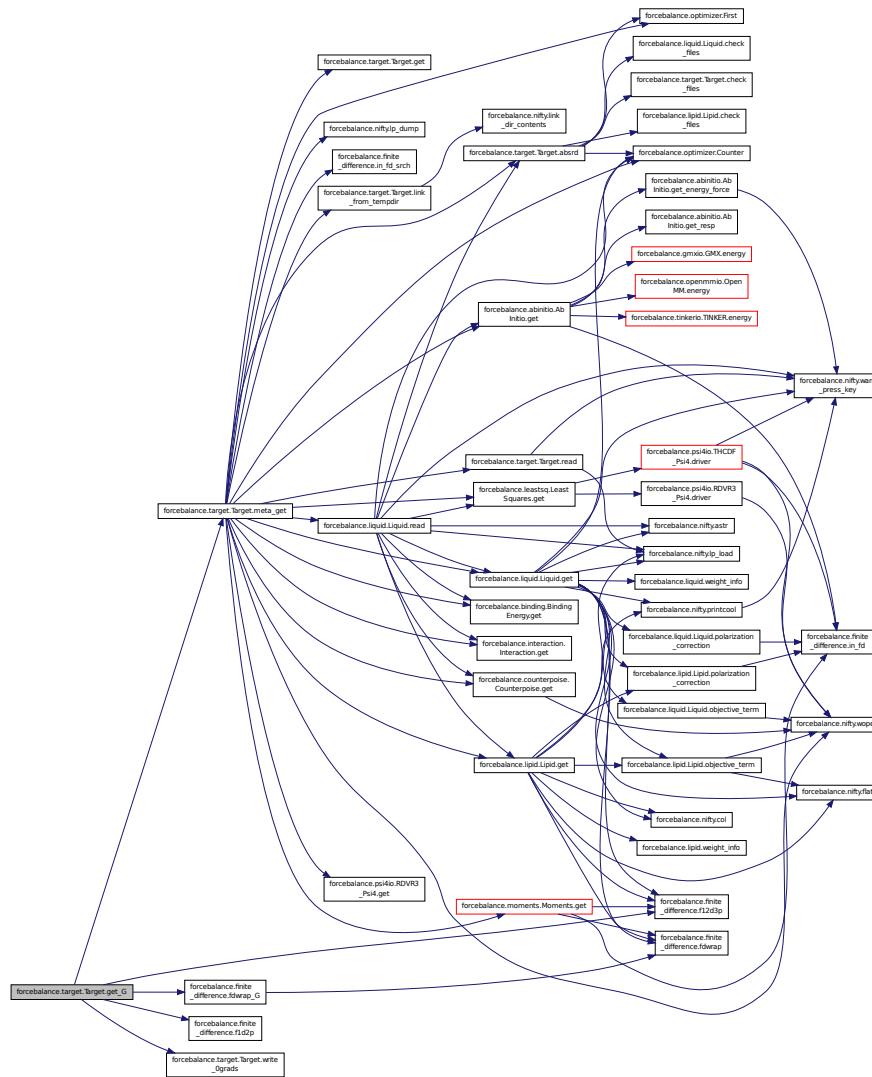
def forcebalance.target.Target.get_G (*self*, *mvals = None*) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1.pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



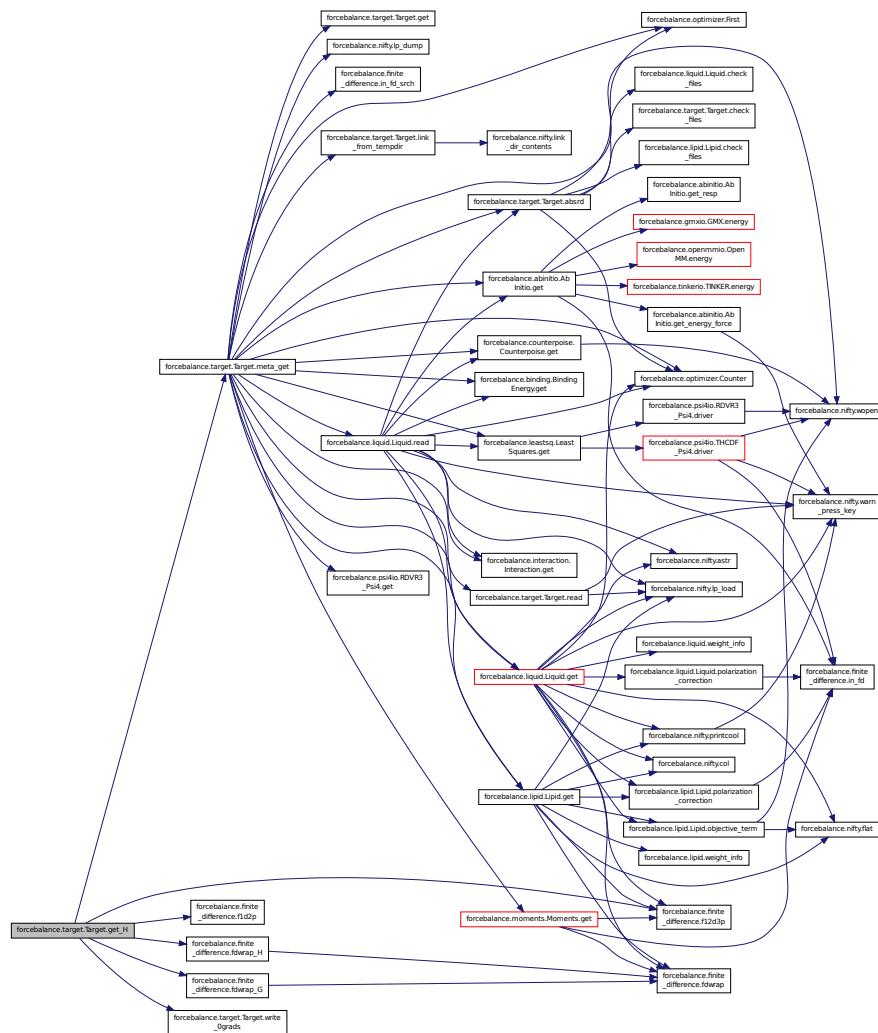
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

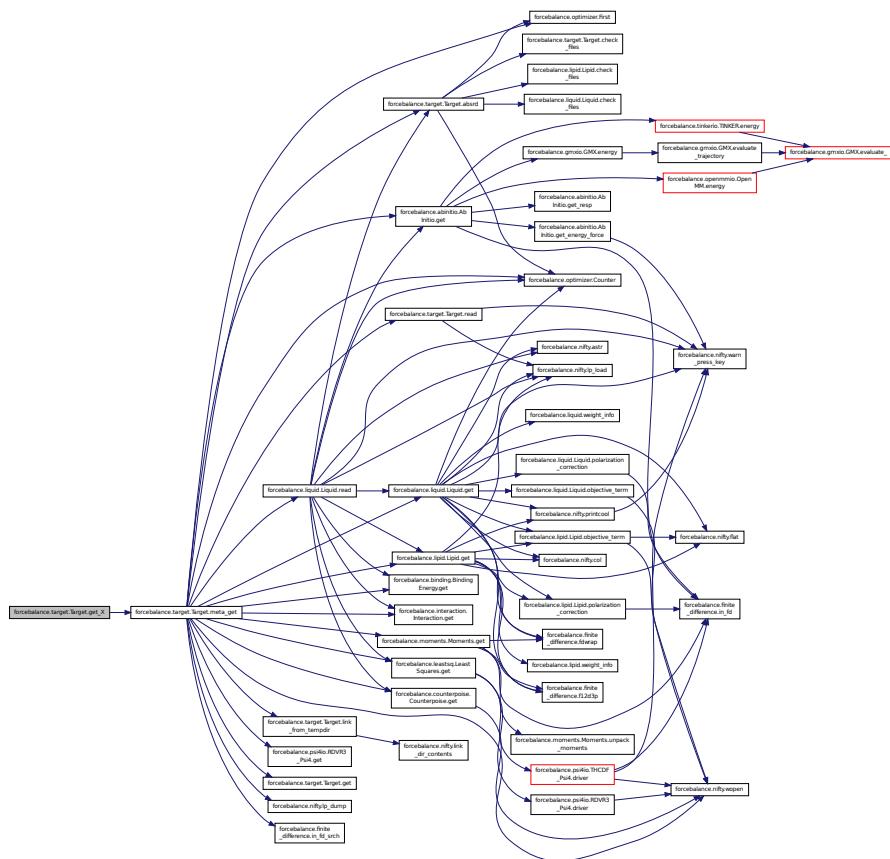
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

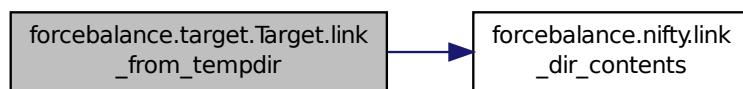
Here is the call graph for this function:



def forcebalance.leastsq.LeastSquares.indicate (self) Definition at line 41 of file leastsq.py.

def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

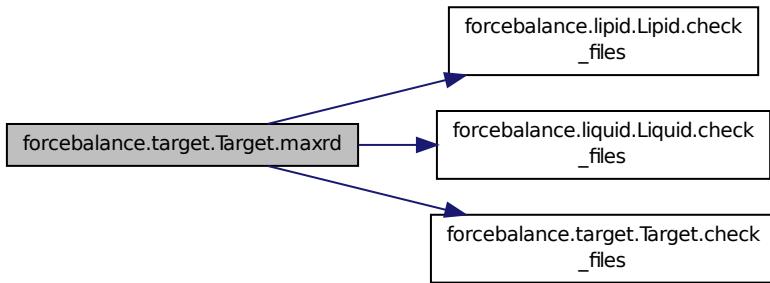
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

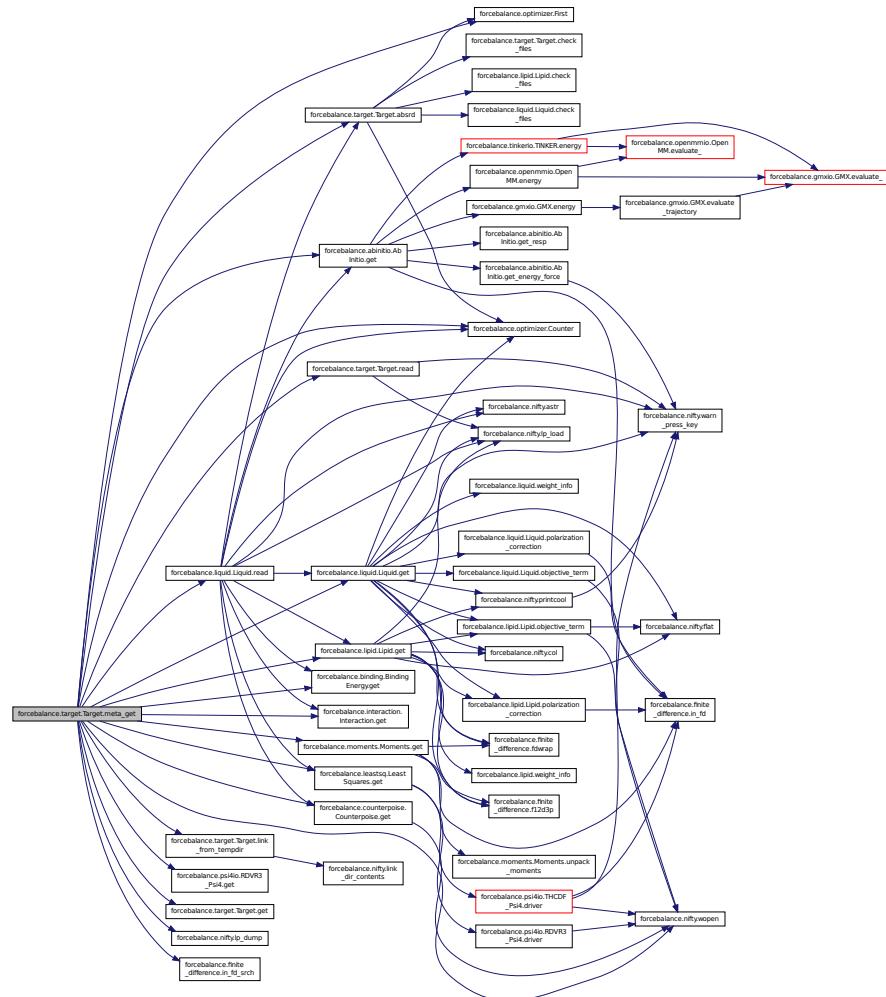
Definition at line 447 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.meta_get( self, mvals, AGrad=False, AHess=False, customdir=None ) [inherited] Wrapper around the get function.  
Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call read\(\) instead. The 'get' method should not worry about the directory that it's running in.  
Definition at line 511 of file target.py.
```

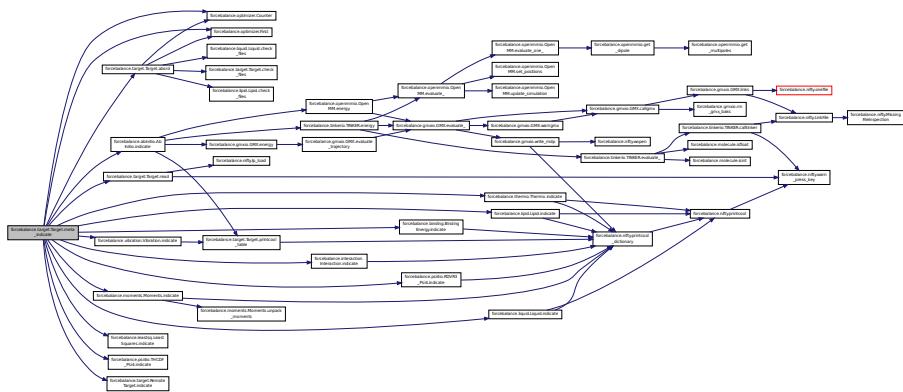
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

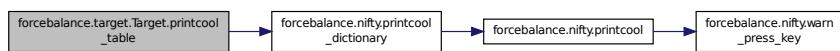
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

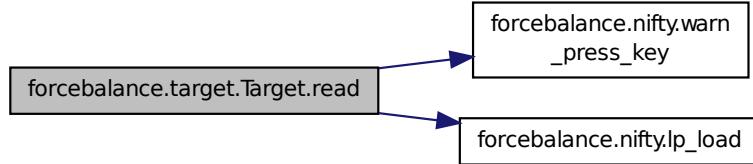
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

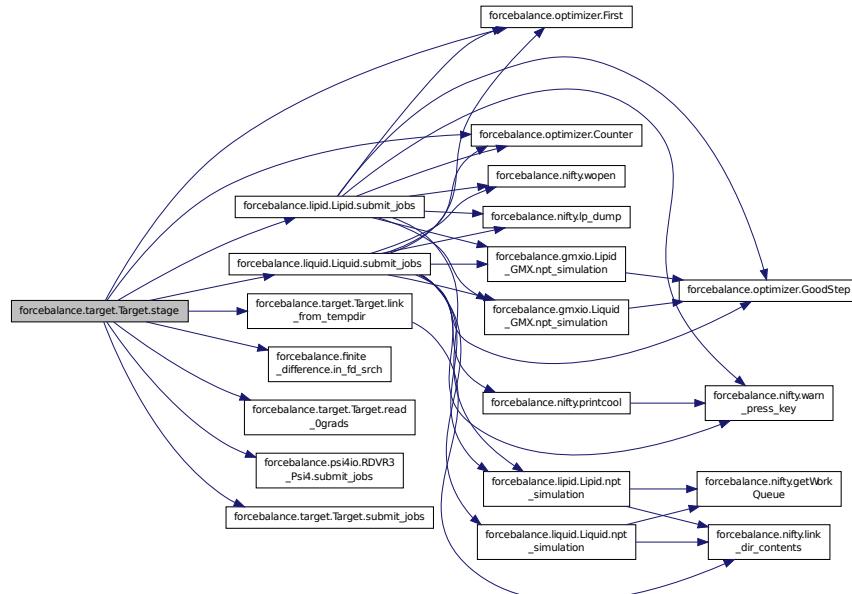
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

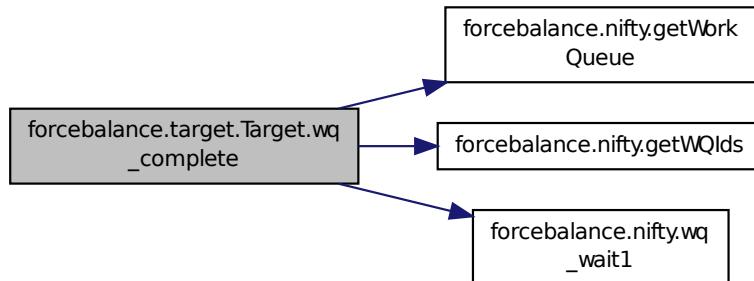


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_0grads( self, Ans ) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.30.4 Member Data Documentation

forcebalance.leastsq.LeastSquares.D Definition at line 126 of file leastsq.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.leastsq.LeastSquares.MAQ Dictionary for derivative terms.
Definition at line 88 of file leastsq.py.

forcebalance.leastsq.LeastSquares.objective Definition at line 127 of file leastsq.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.
Dictionary of whether to call the derivatives.
Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.
Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.
Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.
Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number
The 'customdir' is customizable and can go below anything.
Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.
Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [**inherited**] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [**inherited**] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [**inherited**] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

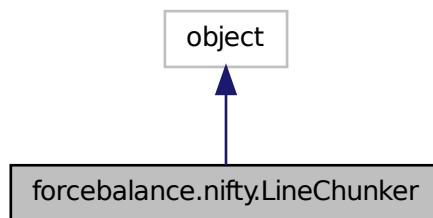
Definition at line 162 of file target.py.

The documentation for this class was generated from the following file:

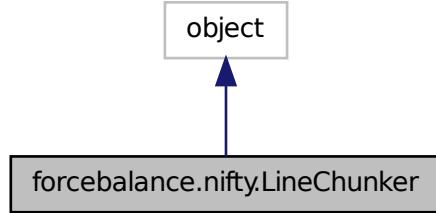
- [leastsq.py](#)

8.31 forcebalance.nifty.LineChunker Class Reference

Inheritance diagram for forcebalance.nifty.LineChunker:



Collaboration diagram for forcebalance.nifty.LineChunker:



Public Member Functions

- def `__init__`
- def `push`
- def `close`
- def `nomnom`
- def `__enter__`
- def `__exit__`

Public Attributes

- `callback`
- `buf`

8.31.1 Detailed Description

Definition at line 943 of file nifty.py.

8.31.2 Constructor & Destructor Documentation

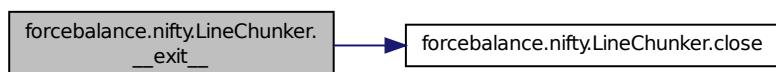
`def forcebalance.nifty.LineChunker.__init__(self, callback)` Definition at line 944 of file nifty.py.

8.31.3 Member Function Documentation

`def forcebalance.nifty.LineChunker.__enter__(self)` Definition at line 963 of file nifty.py.

`def forcebalance.nifty.LineChunker.__exit__(self, args, kwargs)` Definition at line 966 of file nifty.py.

Here is the call graph for this function:



```
def forcebalance.nifty.LineChunker.close ( self ) Definition at line 952 of file nifty.py.  
  
def forcebalance.nifty.LineChunker.nomnom ( self ) Definition at line 956 of file nifty.py.  
  
def forcebalance.nifty.LineChunker.push ( self, data ) Definition at line 948 of file nifty.py.  
Here is the call graph for this function:
```



8.31.4 Member Data Documentation

forcebalance.nifty.LineChunker.buf Definition at line 946 of file nifty.py.

forcebalance.nifty.LineChunker.callback Definition at line 945 of file nifty.py.

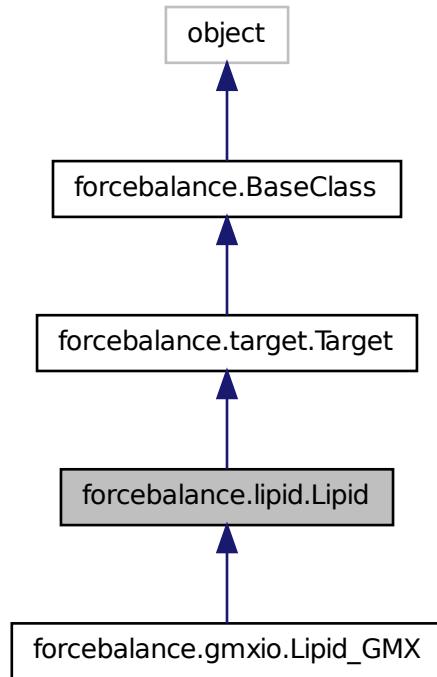
The documentation for this class was generated from the following file:

- [nifty.py](#)

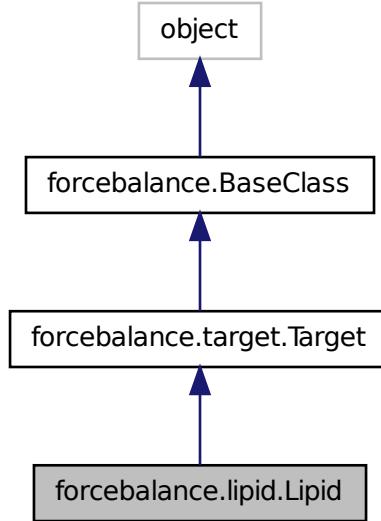
8.32 forcebalance.lipid.Lipid Class Reference

Subclass of Target for lipid property matching.

Inheritance diagram for forcebalance.lipid.Lipid:



Collaboration diagram for forcebalance.lipid.Lipid:



Public Member Functions

- def `_init_`
- def `prepare_temp_directory`

Prepare the temporary directory by copying in important files.
- def `read_data`
- def `check_files`
- def `npt_simulation`

Submit a NPT simulation to the Work Queue.
- def `polarization_correction`
- def `indicate`
- def `objective_term`
- def `submit_jobs`
- def `get`

Fitting of lipid bulk properties.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

- def `link_from_tempdir`
Computes the objective function contribution and its gradient / Hessian.
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `do_self_pol`
- `lipid_mol`
- `last_traj`
- `extra_output`
- `gas_engine`
Read the reference data.
- `read_indicate`
- `write_indicate`
- `read_objective`
- `SavedMVal`
Saved force field mvals for all iterations.
- `SavedTraj`
Saved trajectories for all iterations and all temperatures.
- `MBarEnergy`
Evaluated energies for all trajectories (i.e.
- `RefData`
- `PhasePoints`
- `Labels`
- `engname`
- `w_rho`
Density.
- `w_alpha`
- `w_kappa`
- `w_cp`

- `w_eps0`
- `w_al`
- `w_scd`
- `Xp`
- `Wp`
- `Pp`
- `Gp`
- `Objective`
- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`
Relative directory of target.
- `tempdir`
- `rundir`
`self.tempdir = os.path.join('temp',self.name)` *The directory in which the simulation is running - this can be updated.*
- `FF`
Need the forcefield (here for now)
- `xct`
Counts how often the objective function was computed.
- `gct`
Counts how often the gradient was computed.
- `hct`
Counts how often the Hessian was computed.
- `write_objective`
Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

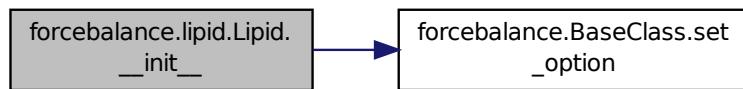
8.32.1 Detailed Description

Subclass of Target for lipid property matching.

Definition at line 51 of file lipid.py.

8.32.2 Constructor & Destructor Documentation

`def forcebalance.lipid.Lipid.__init__(self, options, tgt_opts, forcefield)` Definition at line 54 of file lipid.py.
 Here is the call graph for this function:



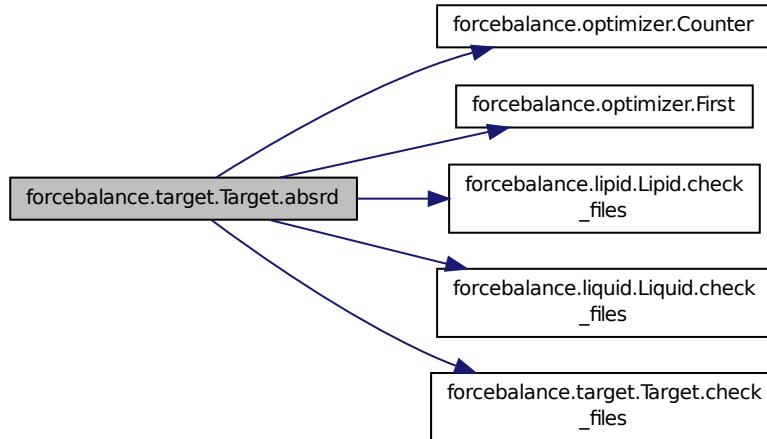
8.32.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.lipid.Lipid.check_files( self, there ) Definition at line 252 of file lipid.py.
```

```
def forcebalance.lipid.Lipid.get( self, mvals, AGrad = True, AHess = True ) Fitting of lipid bulk properties.
```

This is the current major direction of development for ForceBalance. Basically, fitting the QM energies / forces alone does not always give us the best simulation behavior. In many cases it makes more sense to try and reproduce some experimentally known data as well.

In order to reproduce experimentally known data, we need to run a simulation and compare the simulation result to experiment. The main challenge here is that the simulations are computationally intensive (i.e. they require energy and force evaluations), and furthermore the results are noisy. We need to run the simulations automatically and remotely (i.e. on clusters) and a good way to calculate the derivatives of the simulation results with respect to the parameter values.

This function contains some experimentally known values of the density and enthalpy of vaporization (Hvap) of lipid water. It launches the density and Hvap calculations on the cluster, and gathers the results / derivatives. The actual calculation of results / derivatives is done in a separate file.

After the results come back, they are gathered together to form an objective function.

Parameters

in	mvals	Mathematical parameter values
----	-------	-------------------------------

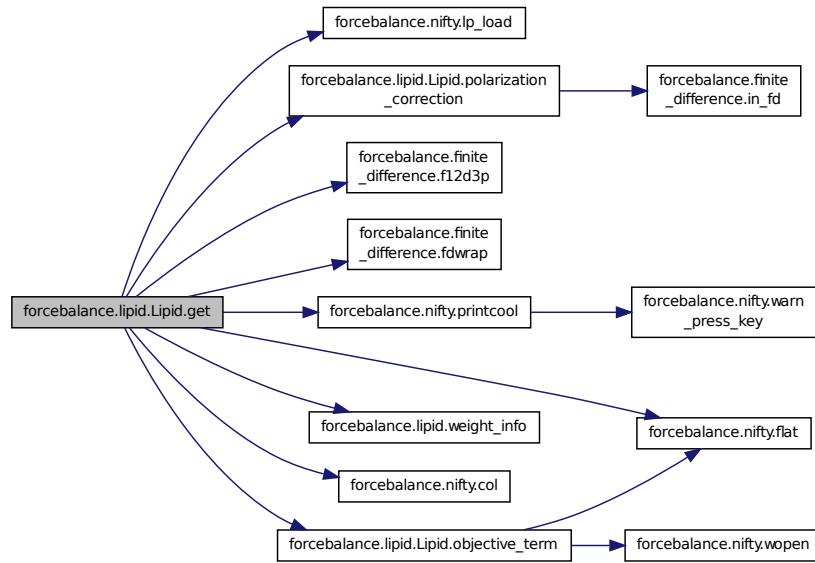
in	<i>AGrad</i>	Switch to turn on analytic gradient
in	<i>AHess</i>	Switch to turn on analytic Hessian

Returns

Answer Contribution to the objective function Fill in the weight matrix with MBAR weights where MBAR was run, and equal weights otherwise.

Definition at line 479 of file lipid.py.

Here is the call graph for this function:



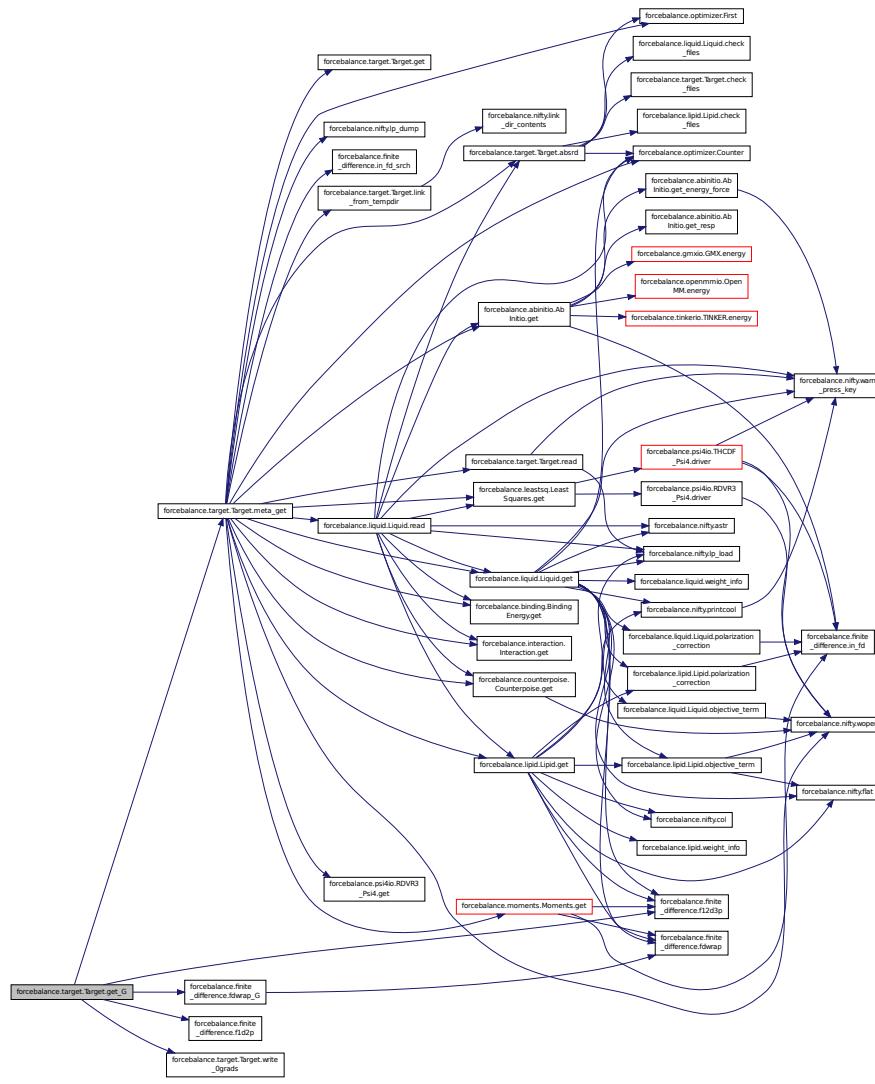
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1.pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



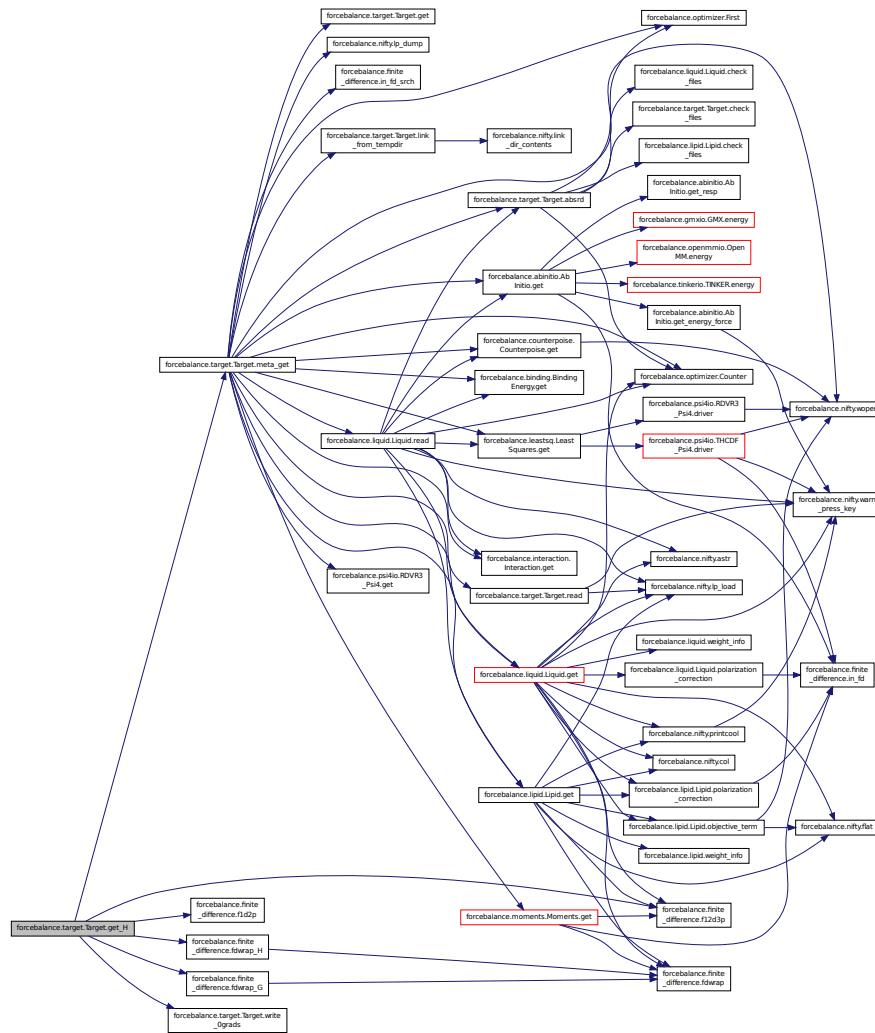
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2.pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

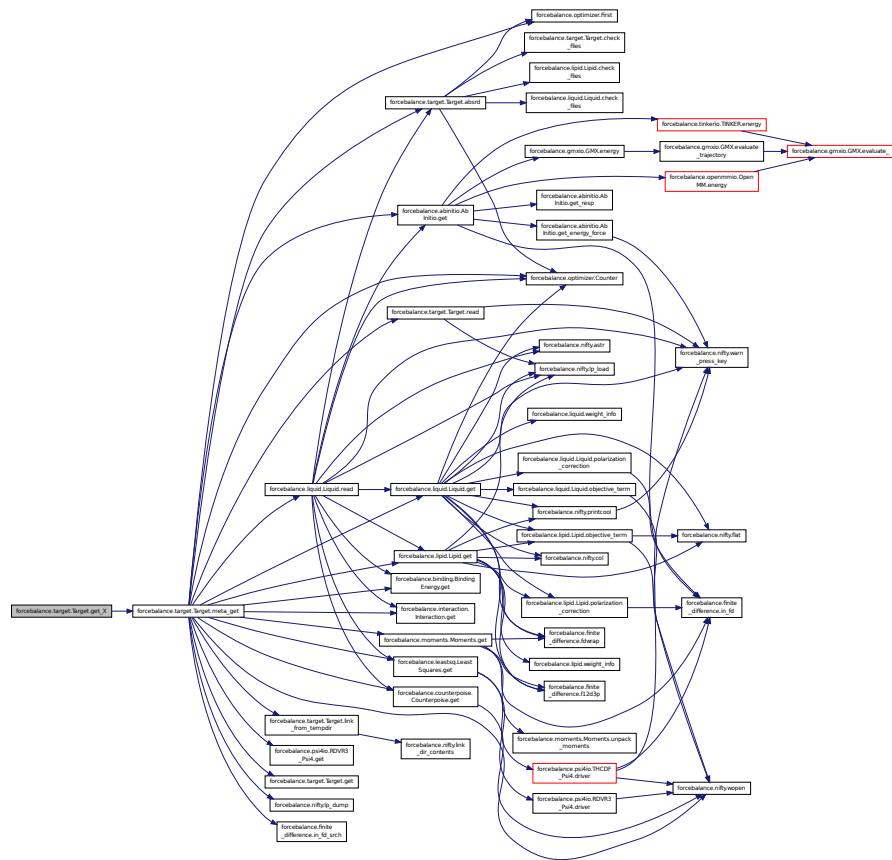
Here is the call graph for this function:



def forcebalance.target.Target.get.X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

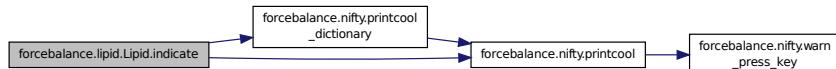
Definition at line 184 of file target.py.

Here is the call graph for this function:



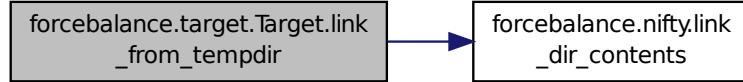
def forcebalance.lipid.Lipid.indicate (self) Definition at line 303 of file lipid.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

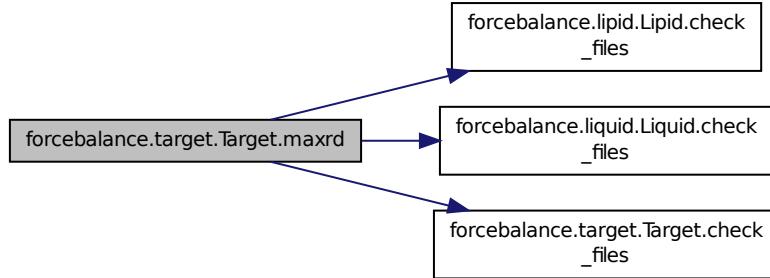
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

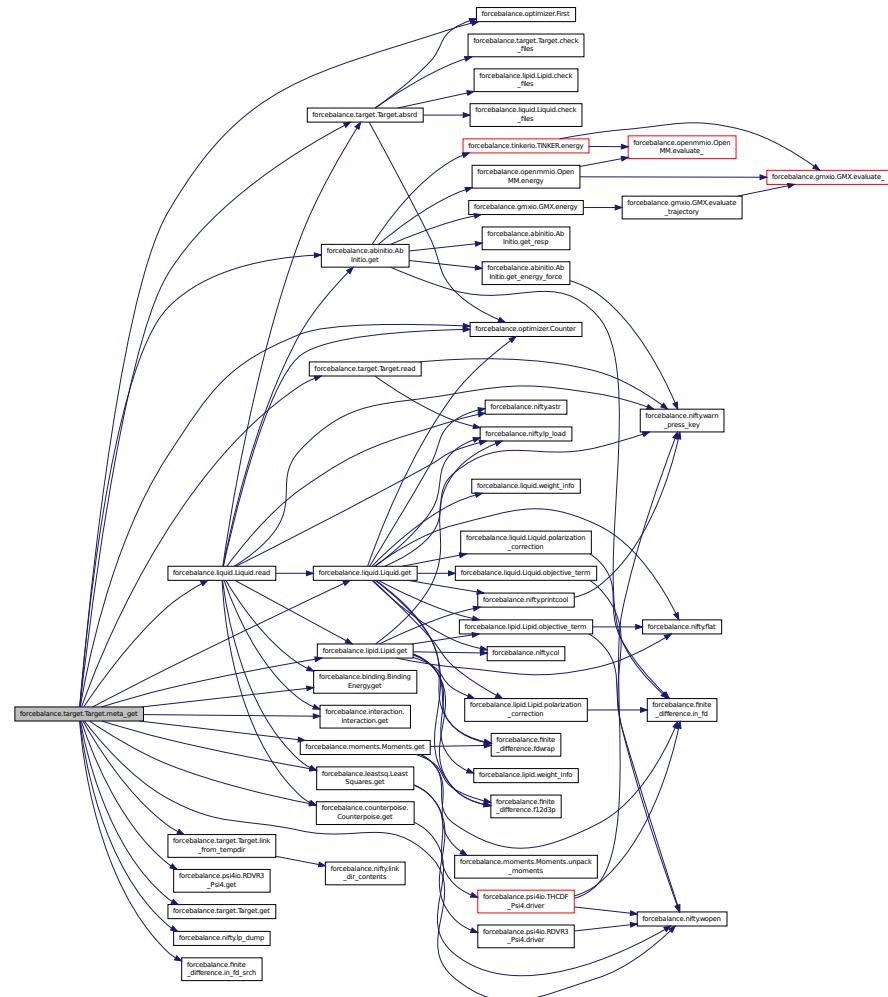


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

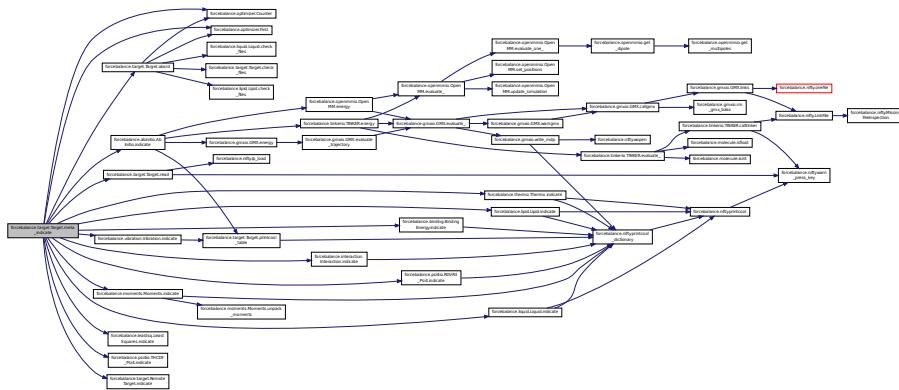
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

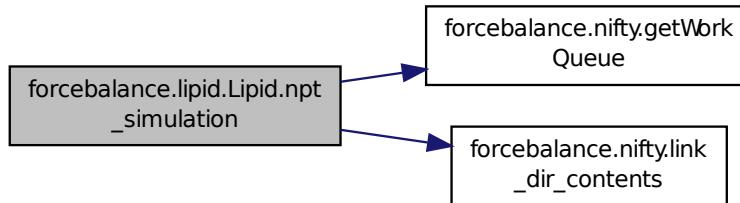
Here is the call graph for this function:



def forcebalance.lipid.Lipid.npt_simulation (self, temperature, pressure, simnum) Submit a NPT simulation to the Work Queue.

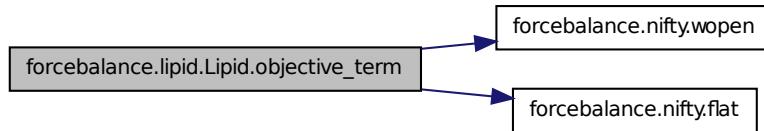
Definition at line 269 of file lipid.py.

Here is the call graph for this function:



def forcebalance.lipid.Lipid.objective_term (self, points, expname, calc, err, grad, name = "Quantity", SubAverage = False) Definition at line 330 of file lipid.py.

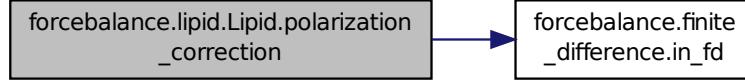
Here is the call graph for this function:



```
def forcebalance.lipid.Lipid.polarization_correction ( self, mvals )
```

Definition at line 287 of file lipid.py.

Here is the call graph for this function:

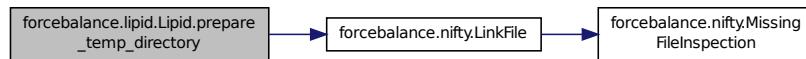


```
def forcebalance.lipid.Lipid.prepare_temp_directory ( self )
```

Prepare the temporary directory by copying in important files.

Definition at line 148 of file lipid.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table ( self, data = OrderedDict ([]), headings = [], banner = None, footnote = None, color = 0 )
```

[inherited] Print target information in an organized table format. Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

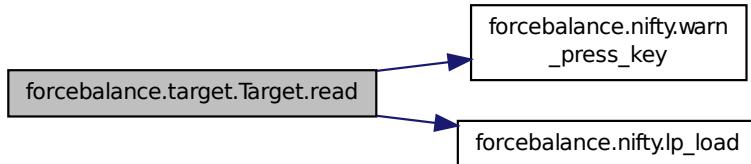
Here is the call graph for this function:



```
def forcebalance.target.Target.read ( self, mvals, AGrad = False, AHess = False ) [inherited]  
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
```

Definition at line 379 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.read_0grads ( self ) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.
```

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

```
def forcebalance.lipid.Lipid.read_data ( self ) Definition at line 155 of file lipid.py.
```

```
def forcebalance.target.Target.refresh_temp_directory ( self ) [inherited] Back up the temporary directory if desired, delete it and then create a new one.
```

Definition at line 321 of file target.py.

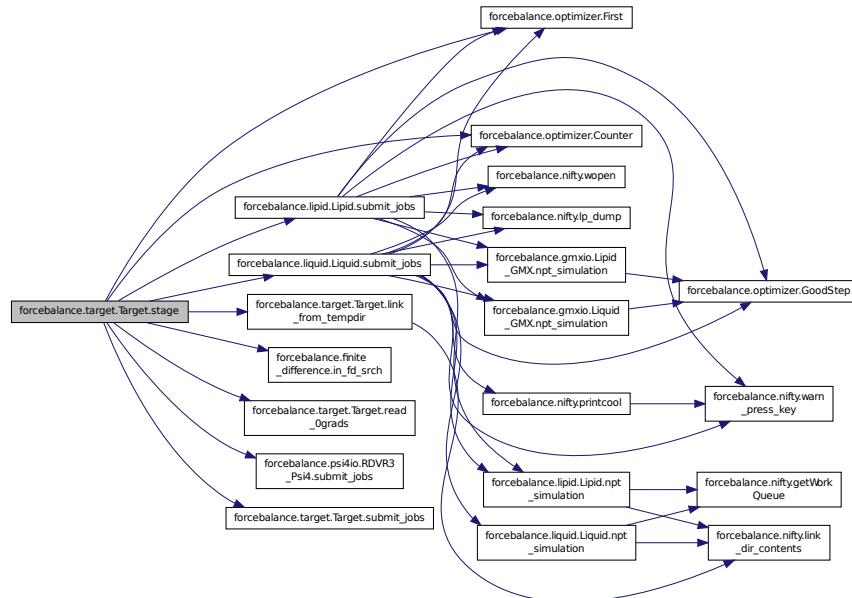
```
def forcebalance.BaseClass.set_option ( self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

```
def forcebalance.target.Target.stage ( self, mvals, AGrad = False, AHess = False, customdir = None ) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.
```

The 'get' method should not worry about the directory that it's running in.

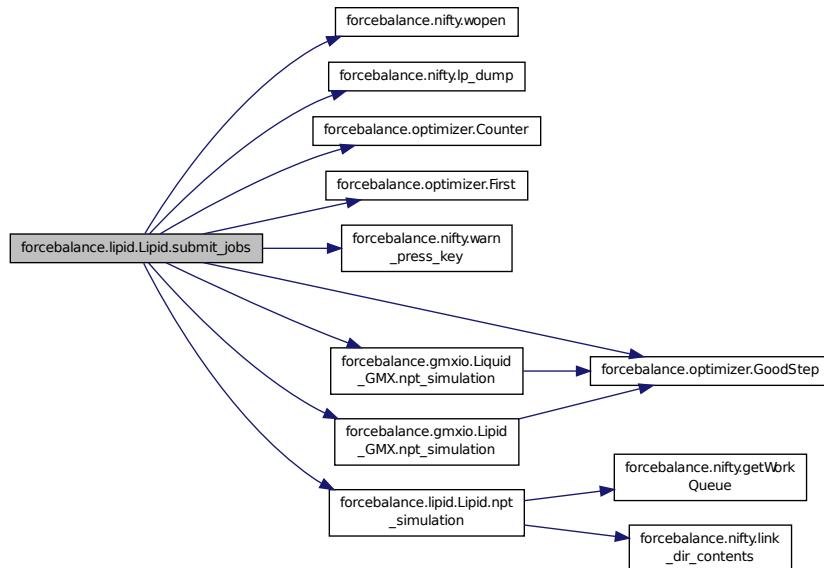
Definition at line 565 of file target.py.

Here is the call graph for this function:



def forcebalance.lipid.Lipid.submit_jobs (self, mvals, AGrad = True, AHess = True) Definition at line 414 of file lipid.py.

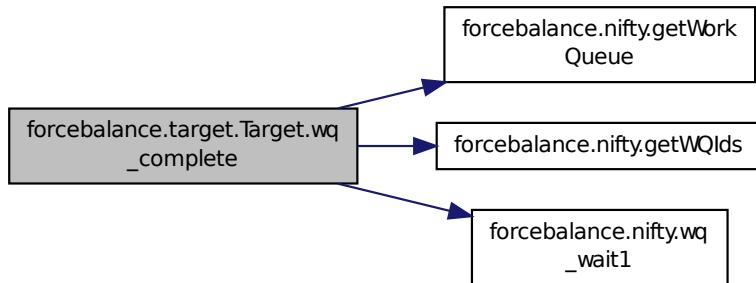
Here is the call graph for this function:



def forcebalance.target.Target.wq_complete (self) [inherited] This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.32.4 Member Data Documentation

forcebalance.lipid.Lipid.do_self.pol Definition at line 96 of file lipid.py.

forcebalance.lipid.Lipid.engname Definition at line 276 of file lipid.py.

forcebalance.lipid.Lipid.extra_output Definition at line 112 of file lipid.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.lipid.Lipid.gas_engine Read the reference data.

Definition at line 127 of file lipid.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.lipid.Lipid.Gp Definition at line 724 of file lipid.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.lipid.Lipid.Labels Definition at line 242 of file lipid.py.

forcebalance.lipid.Lipid.last_traj Definition at line 110 of file lipid.py.

forcebalance.lipid.Lipid.lipid_mol Definition at line 108 of file lipid.py.

forcebalance.lipid.Lipid.MBarEnergy Evaluated energies for all trajectories (i.e. all iterations and all temperatures), using all mvals
Definition at line 144 of file lipid.py.

forcebalance.lipid.Lipid.Objective Definition at line 726 of file lipid.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.
Dictionary of whether to call the derivatives.
Definition at line 127 of file target.py.

forcebalance.lipid.Lipid.PhasePoints Definition at line 238 of file lipid.py.

forcebalance.lipid.Lipid.Pp Definition at line 721 of file lipid.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.
Submit jobs to the Work Queue.
Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.
Definition at line 123 of file target.py.

forcebalance.lipid.Lipid.read_indicate Definition at line 129 of file lipid.py.

forcebalance.lipid.Lipid.read_objective Definition at line 132 of file lipid.py.

forcebalance.lipid.Lipid.RefData Definition at line 166 of file lipid.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number
The 'customdir' is customizable and can go below anything.
Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.
Definition at line 158 of file target.py.

forcebalance.lipid.Lipid.SavedMVal Saved force field mvals for all iterations.
Definition at line 140 of file lipid.py.

forcebalance.lipid.Lipid.SavedTraj Saved trajectories for all iterations and all temperatures.
Definition at line 142 of file lipid.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.
Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization
Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.lipid.Lipid.w_al Definition at line 698 of file lipid.py.

forcebalance.lipid.Lipid.w_alpha Definition at line 694 of file lipid.py.

forcebalance.lipid.Lipid.w_cp Definition at line 696 of file lipid.py.

forcebalance.lipid.Lipid.w_eps0 Definition at line 697 of file lipid.py.

forcebalance.lipid.Lipid.w_kappa Definition at line 695 of file lipid.py.

forcebalance.lipid.Lipid.w_rho Density.

Ignore enthalpy. Thermal expansion coefficient. Isothermal compressibility. Isobaric heat capacity. Static dielectric constant. Average area per lipid Deuterium order parameter Estimation of errors.

Definition at line 693 of file lipid.py.

forcebalance.lipid.Lipid.w_scd Definition at line 699 of file lipid.py.

forcebalance.lipid.Lipid.Wp Definition at line 719 of file lipid.py.

forcebalance.lipid.Lipid.write_indicate Definition at line 130 of file lipid.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

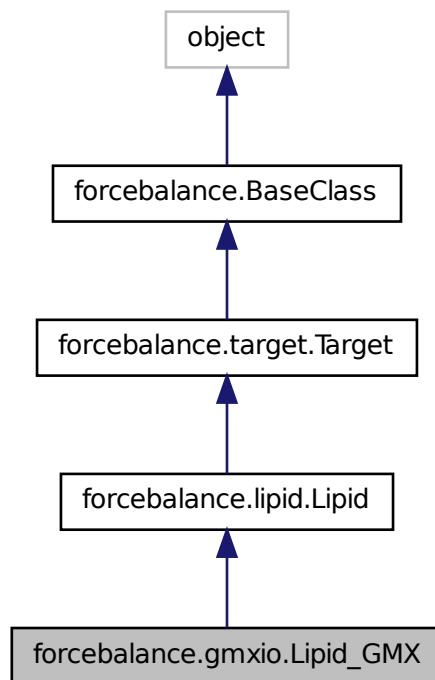
forcebalance.lipid.Lipid.Xp Definition at line 717 of file lipid.py.

The documentation for this class was generated from the following file:

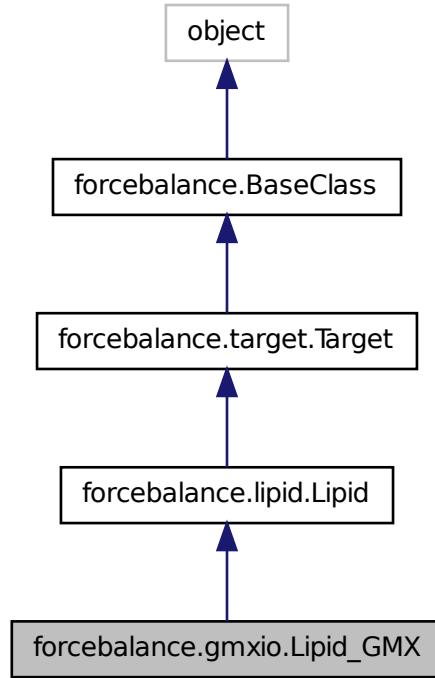
- [lipid.py](#)

8.33 forcebalance.gmxio.Lipid_GMX Class Reference

Inheritance diagram for forcebalance.gmxio.Lipid_GMX:



Collaboration diagram for forcebalance.gmxio.Lipid_GMX:



Public Member Functions

- def `__init__`
- def `npt_simulation`

Submit a NPT simulation to the Work Queue.
- def `prepare_temp_directory`

Prepare the temporary directory by copying in important files.
- def `read_data`
- def `check_files`
- def `polarization_correction`
- def `indicate`
- def `objective_term`
- def `submit_jobs`
- def `get`

Fitting of lipid bulk properties.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.

- def [get_G](#)
Computes the objective function contribution and its gradient.
- def [get_H](#)
Computes the objective function contribution and its gradient / Hessian.
- def [link_from_tempdir](#)
- def [refresh_temp_directory](#)
Back up the temporary directory if desired, delete it and then create a new one.
- def [read](#)
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def [absrd](#)
Supply the correct directory specified by user's "read" option.
- def [maxrd](#)
Supply the latest existing temp-directory containing valid data.
- def [meta_indicate](#)
Wrap around the indicate function, so it can print to screen and also to a file.
- def [meta_get](#)
Wrapper around the get function.
- def [stage](#)
Stages the directory for the target, and then launches Work Queue processes if any.
- def [wq_complete](#)
This method determines whether the Work Queue tasks for the current target have completed.
- def [printcool_table](#)
Print target information in an organized table format.
- def [__setattr__](#)
- def [set_option](#)

Public Attributes

- [engine_](#)
- [engname](#)
- [nptpx](#)
- [nptfiles](#)
- [scripts](#)
- [extra_output](#)
- [LfDict](#)
- [LfDict_New](#)
- [last_traj](#)
- [do_self_pol](#)
- [lipid_mol](#)
- [gas_engine](#)
Read the reference data.
- [read_indicate](#)
- [write_indicate](#)
- [read_objective](#)
- [SavedMVal](#)
Saved force field mvals for all iterations.
- [SavedTraj](#)
Saved trajectories for all iterations and all temperatures.

- **MBarEnergy**
Evaluated energies for all trajectories (i.e.
- **RefData**
- **PhasePoints**
- **Labels**
- **w_rho**
Density.
- **w_alpha**
- **w_kappa**
- **w_cp**
- **w_eps0**
- **w_al**
- **w_scd**
- **Xp**
- **Wp**
- **Pp**
- **Gp**
- **Objective**
- **rd**
Root directory of the whole project.
- **pgrad**
Iteration where we turn on zero-gradient skipping.
- **tempbase**
Relative directory of target.
- **tempdir**
- **rundir**
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

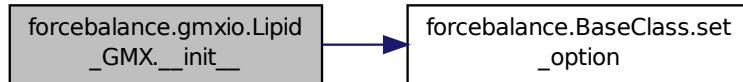
8.33.1 Detailed Description

Definition at line 1396 of file gmxio.py.

8.33.2 Constructor & Destructor Documentation

```
def forcebalance.gmxio.Lipid_GMX.__init__ ( self, options, tgt_opts, forcefield ) Definition at line 1397 of file gmxio.py.
```

Here is the call graph for this function:



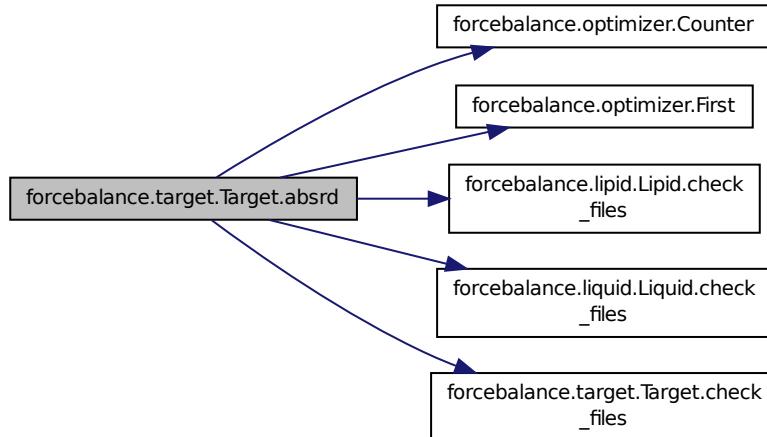
8.33.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.lipid.Lipid.check_files ( self, there ) [inherited] Definition at line 252 of file lipid.py.
```

```
def forcebalance.lipid.Lipid.get ( self, mvals, AGrad = True, AHess = True ) [inherited] Fitting of lipid bulk properties.
```

This is the current major direction of development for ForceBalance. Basically, fitting the QM energies / forces alone does not always give us the best simulation behavior. In many cases it makes more sense to try and reproduce some experimentally known data as well.

In order to reproduce experimentally known data, we need to run a simulation and compare the simulation result to experiment. The main challenge here is that the simulations are computationally intensive (i.e. they require energy and force evaluations), and furthermore the results are noisy. We need to run the simulations automatically and remotely (i.e. on clusters) and a good way to calculate the derivatives of the simulation results with respect to the parameter values.

This function contains some experimentally known values of the density and enthalpy of vaporization (H_{vap}) of lipid water. It launches the density and H_{vap} calculations on the cluster, and gathers the results / derivatives. The actual calculation of results / derivatives is done in a separate file.

After the results come back, they are gathered together to form an objective function.

Parameters

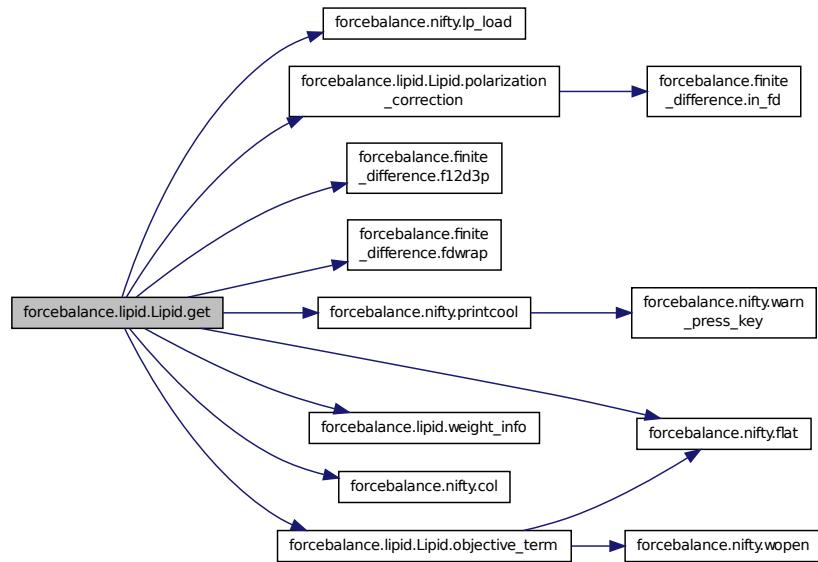
in	<i>mvals</i>	Mathematical parameter values
in	<i>AGrad</i>	Switch to turn on analytic gradient
in	<i>AHess</i>	Switch to turn on analytic Hessian

Returns

Answer Contribution to the objective function Fill in the weight matrix with MBAR weights where MBAR was run, and equal weights otherwise.

Definition at line 479 of file lipid.py.

Here is the call graph for this function:



def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

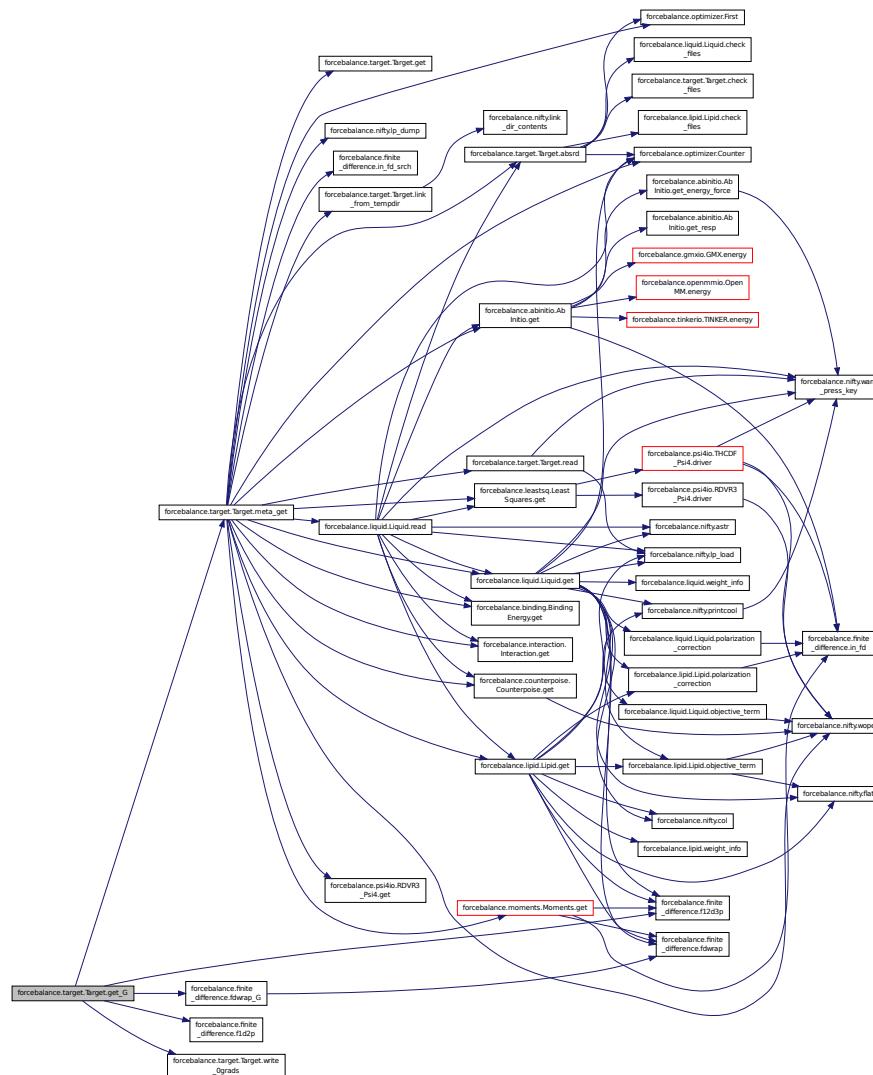
First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned

on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



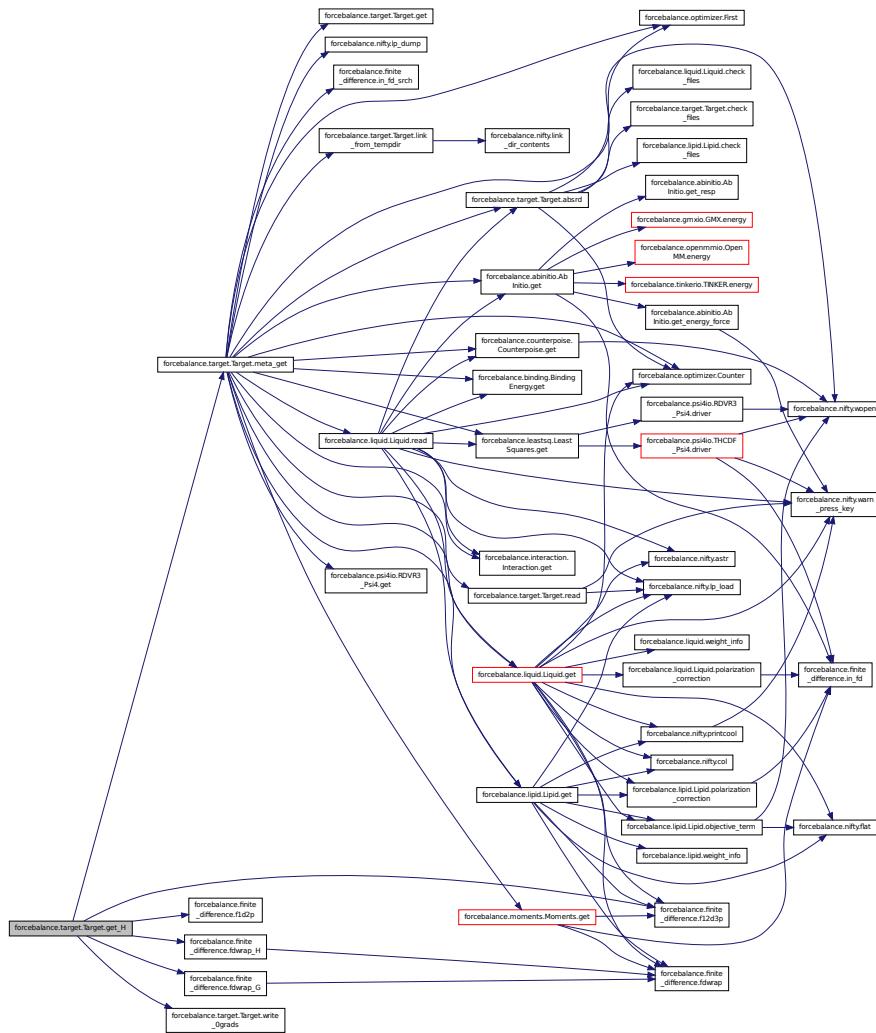
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

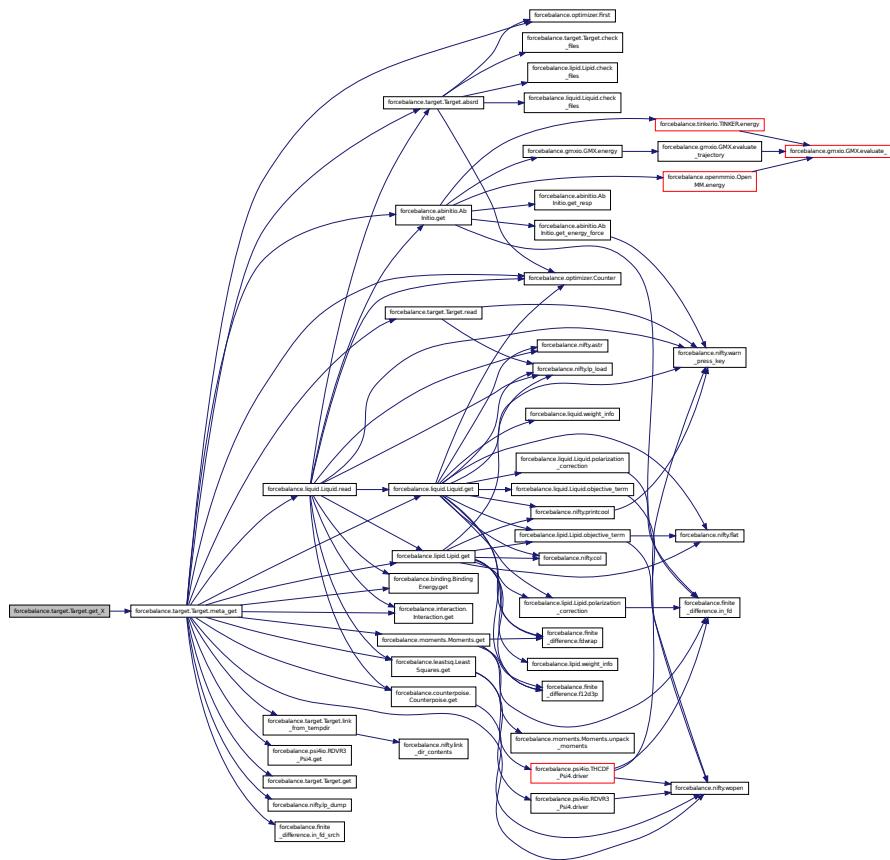
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

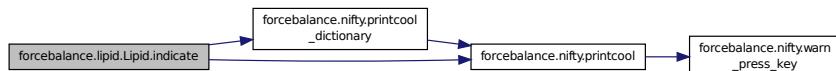
Definition at line 184 of file target.py.

Here is the call graph for this function:



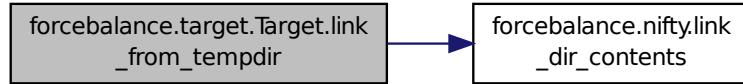
def forcebalance.lipid.Lipid.indicate(self) [inherited] Definition at line 303 of file lipid.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

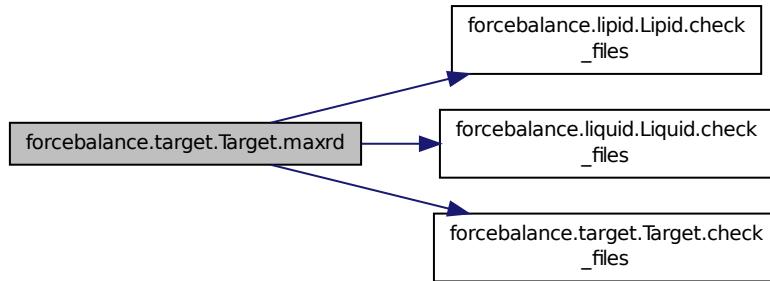
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

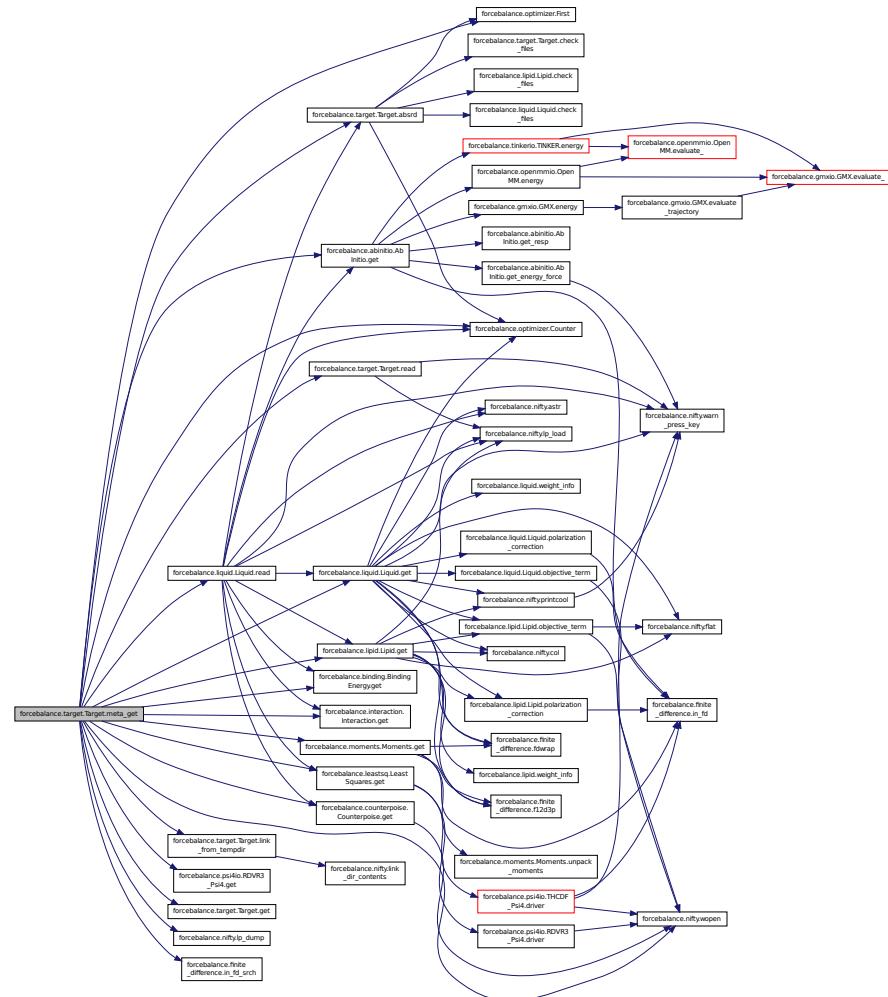


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

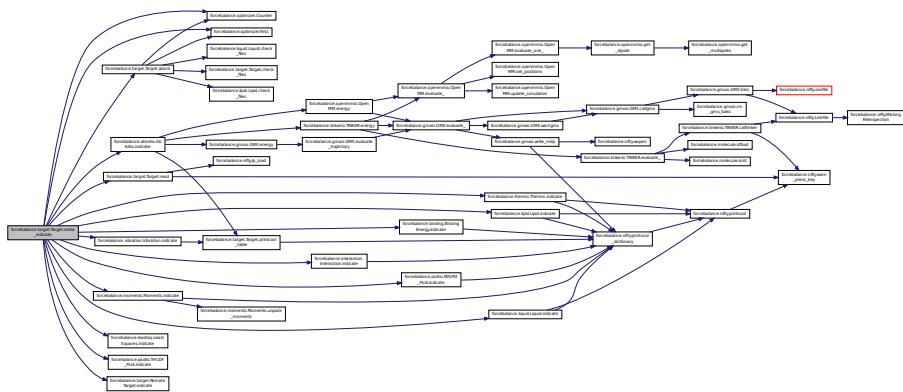
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

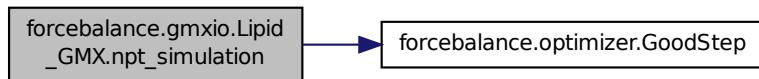
Here is the call graph for this function:



def forcebalance.gmxio.Lipid_GMX.npt_simulation (self, temperature, pressure, simnum) Submit a NPT simulation to the Work Queue.

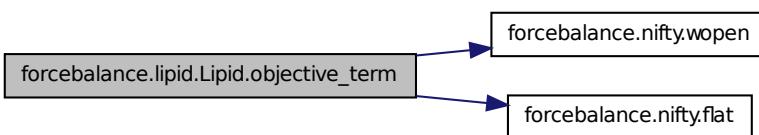
Definition at line 1434 of file gmxio.py.

Here is the call graph for this function:



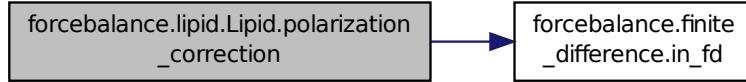
```
def forcebalance.lipid.Lipid.objective_term( self, points, expname, calc, err, grad, name = "Quantity",  
SubAverage = False ) [inherited] Definition at line 330 of file lipid.py.
```

Here is the call graph for this function:



def forcebalance.lipid.Lipid.polarization_correction (*self*, *mvals*) [inherited] Definition at line 287 of file lipid.py.

Here is the call graph for this function:



def forcebalance.lipid.Lipid.prepare_temp_directory (self) [inherited] Prepare the temporary directory by copying in important files.

Definition at line 148 of file lipid.py.

Here is the call graph for this function:



def forcebalance.target.Target.printcool_table (self, data = OrderedDict ([]), headings = [], banner = None, footnote = None, color = 0) [inherited] Print target information in an organized table format.

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

data	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
headings	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
banner	Optional heading line, which will be printed at the top in the title.
footnote	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

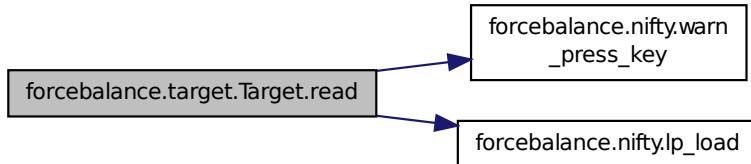
Here is the call graph for this function:



```
def forcebalance.target.Target.read ( self, mvals, AGrad = False, AHess = False ) [inherited]  
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
```

Definition at line 379 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.read_0grads ( self ) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.
```

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

```
def forcebalance.lipid.Lipid.read_data ( self ) [inherited] Definition at line 155 of file lipid.py.
```

```
def forcebalance.target.Target.refresh_temp_directory ( self ) [inherited] Back up the temporary directory if desired, delete it and then create a new one.
```

Definition at line 321 of file target.py.

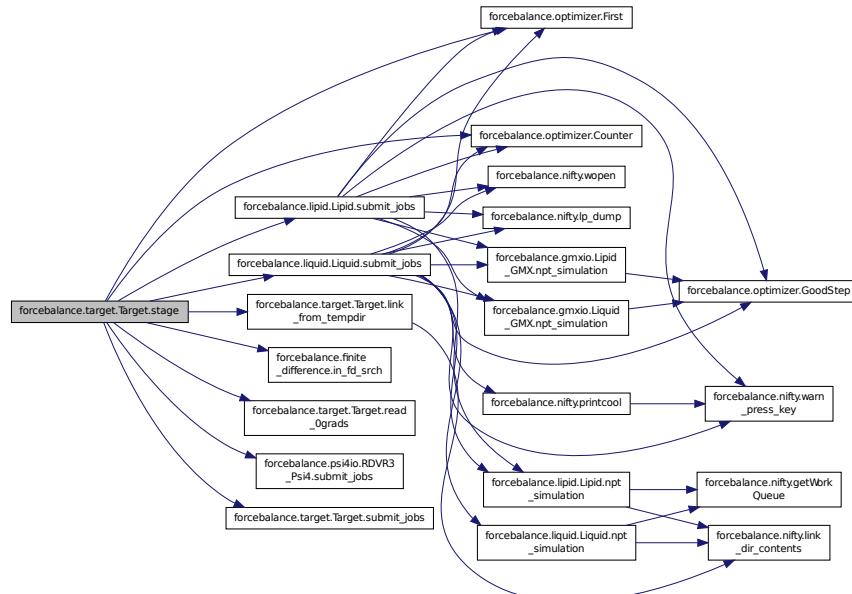
```
def forcebalance.BaseClass.set_option ( self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

```
def forcebalance.target.Target.stage ( self, mvals, AGrad = False, AHess = False, customdir = None ) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.
```

The 'get' method should not worry about the directory that it's running in.

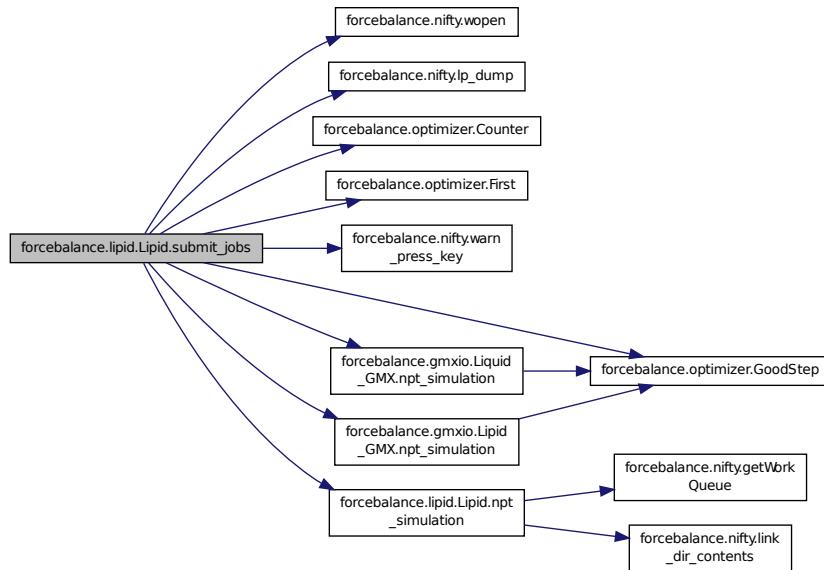
Definition at line 565 of file target.py.

Here is the call graph for this function:



def forcebalance.lipid.Lipid.submit_jobs (self, mvals, AGrad = True, AHess = True) [inherited]
Definition at line 414 of file lipid.py.

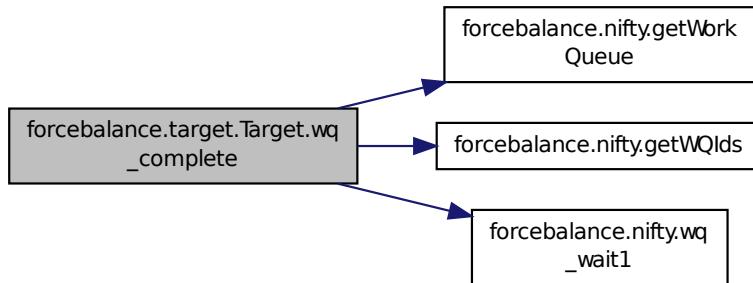
Here is the call graph for this function:



```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.write_0grads( self, Ans ) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

8.33.4 Member Data Documentation

`forcebalance.lipid.Lipid.do_self.pol` [inherited] Definition at line 96 of file lipid.py.

`forcebalance.gmxio.Lipid_GMX.engine` Definition at line 1407 of file gmxio.py.

`forcebalance.gmxio.Lipid_GMX.engname` Definition at line 1409 of file gmxio.py.

`forcebalance.gmxio.Lipid_GMX.extra_output` Definition at line 1424 of file gmxio.py.

`forcebalance.target.Target.FF` [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

`forcebalance.lipid.Lipid.gas_engine` [inherited] Read the reference data.

Definition at line 127 of file lipid.py.

`forcebalance.target.Target.gct` [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

`forcebalance.lipid.Lipid.Gp` [inherited] Definition at line 724 of file lipid.py.

`forcebalance.target.Target.hct` [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

`forcebalance.lipid.Lipid.Labels` [inherited] Definition at line 242 of file lipid.py.

forcebalance.gmxio.Lipid_GMX.last_traj Definition at line 1445 of file gmxio.py.

forcebalance.gmxio.Lipid_GMX.LfDict Definition at line 1429 of file gmxio.py.

forcebalance.gmxio.Lipid_GMX.LfDict_New Definition at line 1430 of file gmxio.py.

forcebalance.lipid.Lipid.lipid_mol [inherited] Definition at line 108 of file lipid.py.

forcebalance.lipid.Lipid.MBarEnergy [inherited] Evaluated energies for all trajectories (i.e. all iterations and all temperatures), using all mvals
Definition at line 144 of file lipid.py.

forcebalance.gmxio.Lipid_GMX.nptfiles Definition at line 1413 of file gmxio.py.

forcebalance.gmxio.Lipid_GMX.nptpx Definition at line 1411 of file gmxio.py.

forcebalance.lipid.Lipid.Objective [inherited] Definition at line 726 of file lipid.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.
Dictionary of whether to call the derivatives.
Definition at line 127 of file target.py.

forcebalance.lipid.Lipid.PhasePoints [inherited] Definition at line 238 of file lipid.py.

forcebalance.lipid.Lipid.Pp [inherited] Definition at line 721 of file lipid.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.
Submit jobs to the Work Queue.
Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.
Definition at line 123 of file target.py.

forcebalance.lipid.Lipid.read_indicate [inherited] Definition at line 129 of file lipid.py.

forcebalance.lipid.Lipid.read_objective [inherited] Definition at line 132 of file lipid.py.

forcebalance.lipid.Lipid.RefData [inherited] Definition at line 166 of file lipid.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number
The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.lipid.Lipid.SavedMVal [inherited] Saved force field mvals for all iterations.
Definition at line 140 of file lipid.py.

forcebalance.lipid.Lipid.SavedTraj [inherited] Saved trajectories for all iterations and all temperatures.
Definition at line 142 of file lipid.py.

forcebalance.gmxio.Lipid_GMX.scripts Definition at line 1416 of file gmxio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.
Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization
Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.lipid.Lipid.w_al [inherited] Definition at line 698 of file lipid.py.

forcebalance.lipid.Lipid.w_alpha [inherited] Definition at line 694 of file lipid.py.

forcebalance.lipid.Lipid.w_cp [inherited] Definition at line 696 of file lipid.py.

forcebalance.lipid.Lipid.w_eps0 [inherited] Definition at line 697 of file lipid.py.

forcebalance.lipid.Lipid.w_kappa [inherited] Definition at line 695 of file lipid.py.

forcebalance.lipid.Lipid.w_rho [inherited] Density.

Ignore enthalpy. Thermal expansion coefficient. Isothermal compressibility. Isobaric heat capacity. Static dielectric constant. Average area per lipid Deuterium order parameter Estimation of errors.
Definition at line 693 of file lipid.py.

forcebalance.lipid.Lipid.w_scd [inherited] Definition at line 699 of file lipid.py.

forcebalance.lipid.Lipid.Wp [inherited] Definition at line 719 of file lipid.py.

forcebalance.lipid.Lipid.write_indicate [inherited] Definition at line 130 of file lipid.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)
Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.
Definition at line 162 of file target.py.

forcebalance.lipid.Lipid.Xp [inherited] Definition at line 717 of file lipid.py.

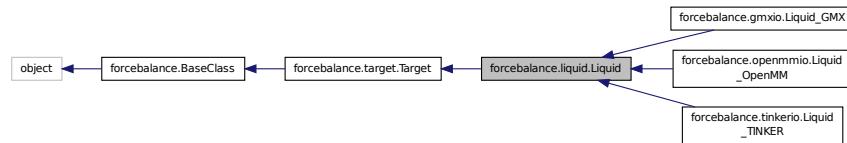
The documentation for this class was generated from the following file:

- [gmxio.py](#)

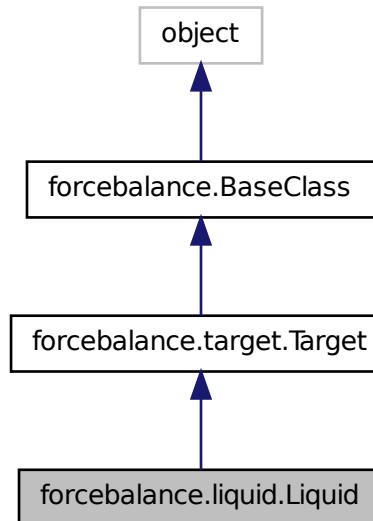
8.34 forcebalance.liquid.Liquid Class Reference

Subclass of Target for liquid property matching.

Inheritance diagram for forcebalance.liquid.Liquid:



Collaboration diagram for forcebalance.liquid.Liquid:



Public Member Functions

- def `_init_`
- def `prepare_temp_directory`

Prepare the temporary directory by copying in important files.
- def `read_data`
- def `check_files`
- def `npt_simulation`

Submit a NPT simulation to the Work Queue.
- def `polarization_correction`
- def `indicate`
- def `objective_term`

- def `submit_jobs`
- def `read`
Read in time series for all previous iterations.
- def `get`
Fitting of liquid bulk properties.
- def `get_X`
Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
Computes the objective function contribution and its gradient.
- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `do_self_pol`
- `liquid_mol`
- `gas_mol`
- `last_traj`
- `extra_output`
- `gas_engine`
Read the reference data.
- `read_indicate`
- `write_indicate`
- `SavedTraj`
Saved trajectories for all iterations and all temperatures.

- **MBarEnergy**
Evaluated energies for all trajectories (i.e.
- **AllResults**
Saved results for all iterations self.SavedMVals = [].
- **RefData**
- **PhasePoints**
- **Labels**
- **engname**
- **w_rho**
Density.
- **w_hvap**
- **w_alpha**
- **w_kappa**
- **w_cp**
- **w_eps0**
- **Xp**
- **Wp**
- **Pp**
- **Gp**
- **Objective**
- **rd**
Root directory of the whole project.
- **pgrad**
Iteration where we turn on zero-gradient skipping.
- **tempbase**
Relative directory of target.
- **tempdir**
- **rundir**
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

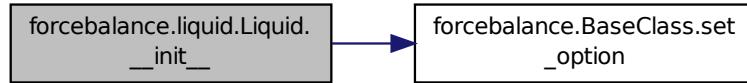
8.34.1 Detailed Description

Subclass of Target for liquid property matching.

Definition at line 51 of file liquid.py.

8.34.2 Constructor & Destructor Documentation

```
def forcebalance.liquid.Liquid.__init__( self, options, tgt_opts, forcefield ) Definition at line 54 of file liquid.py.  
Here is the call graph for this function:
```



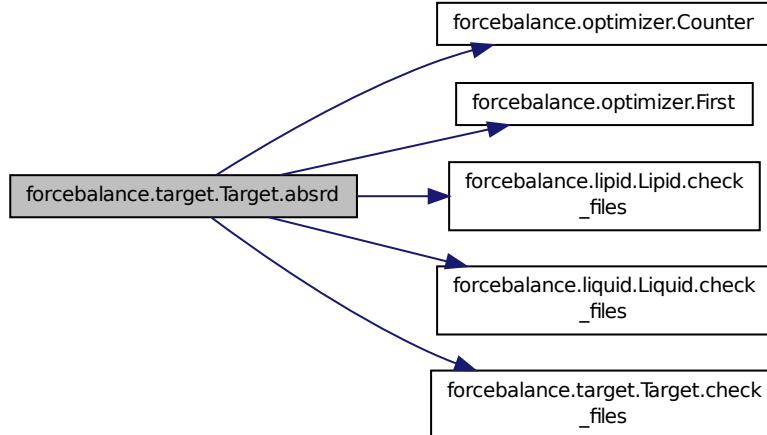
8.34.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.check_files( self, there ) Definition at line 253 of file liquid.py.
```

```
def forcebalance.liquid.Liquid.get( self, mvals, AGrad = True, AHess = True ) Fitting of liquid bulk properties.
```

This is the current major direction of development for ForceBalance. Basically, fitting the QM energies / forces alone does not always give us the best simulation behavior. In many cases it makes more sense to try and reproduce some experimentally known data as well.

In order to reproduce experimentally known data, we need to run a simulation and compare the simulation result to experiment. The main challenge here is that the simulations are computationally intensive (i.e. they require energy and force evaluations), and furthermore the results are noisy. We need to run the simulations automatically and remotely (i.e. on clusters) and a good way to calculate the derivatives of the simulation results with respect to the parameter values.

This function contains some experimentally known values of the density and enthalpy of vaporization (H_{vap}) of liquid water. It launches the density and H_{vap} calculations on the cluster, and gathers the results / derivatives. The actual calculation of results / derivatives is done in a separate file.

After the results come back, they are gathered together to form an objective function.

Parameters

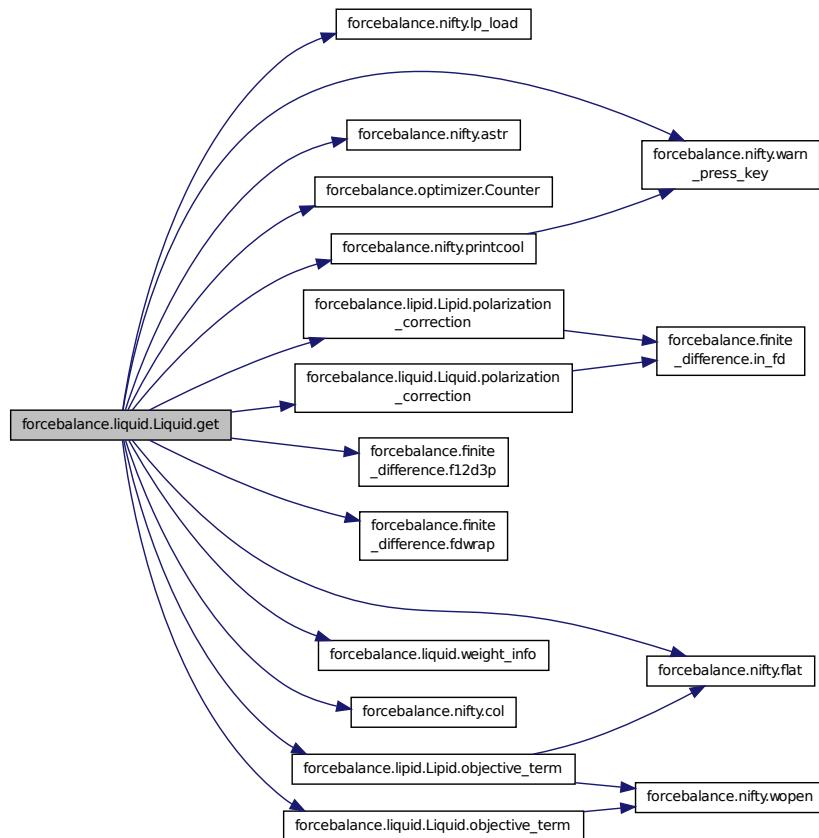
in	<i>mvals</i>	Mathematical parameter values
in	<i>AGrad</i>	Switch to turn on analytic gradient
in	<i>AHess</i>	Switch to turn on analytic Hessian

Returns

Answer Contribution to the objective function Fill in the weight matrix with MBAR weights where MBAR was run, and equal weights otherwise.

Definition at line 553 of file liquid.py.

Here is the call graph for this function:



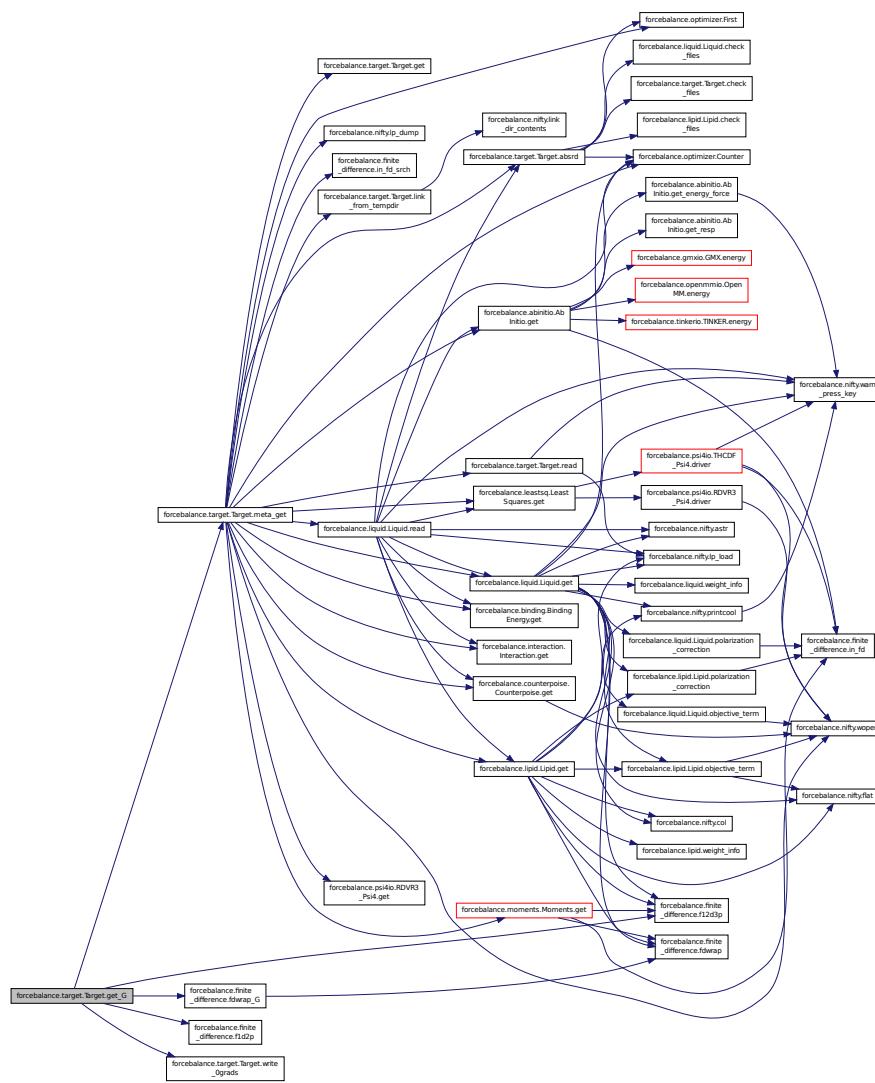
def forcebalance.target.Target.get_G(self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the `fd1_pids` and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

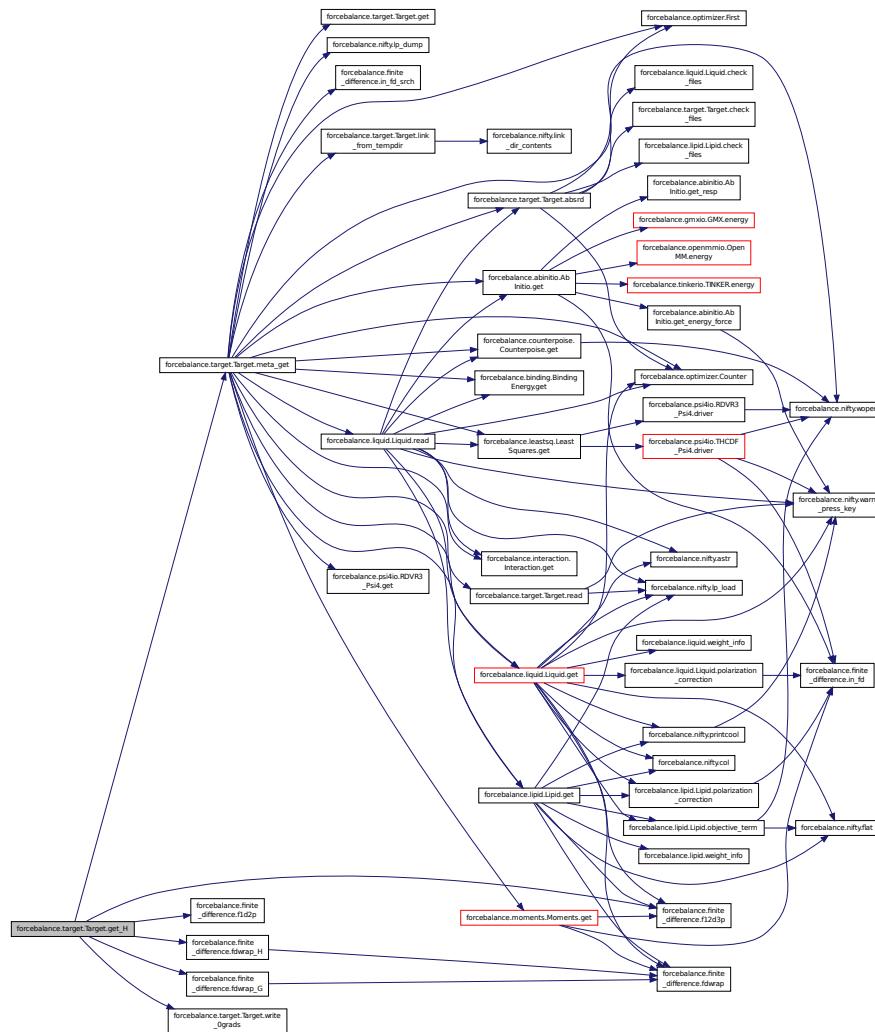
First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through

the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

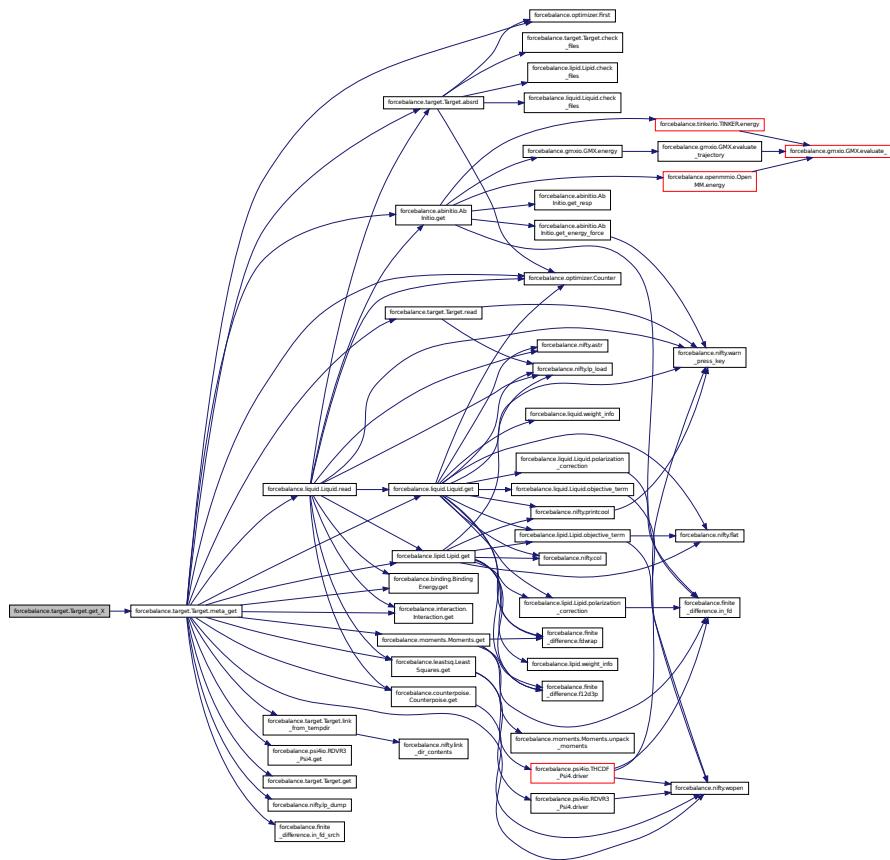
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

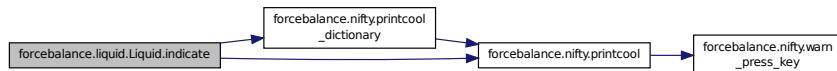
Definition at line 184 of file target.py.

Here is the call graph for this function:



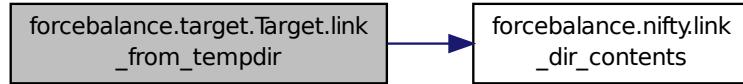
def forcebalance.liquid.Liquid.indicate (self) Definition at line 304 of file liquid.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

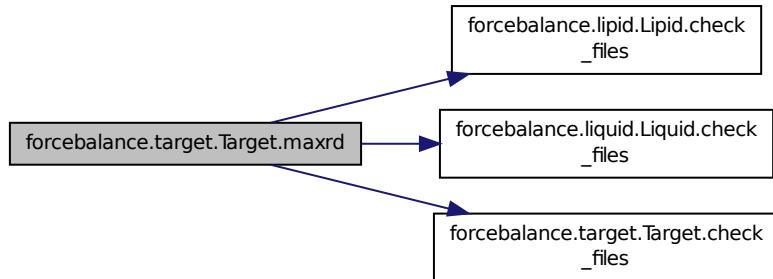
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

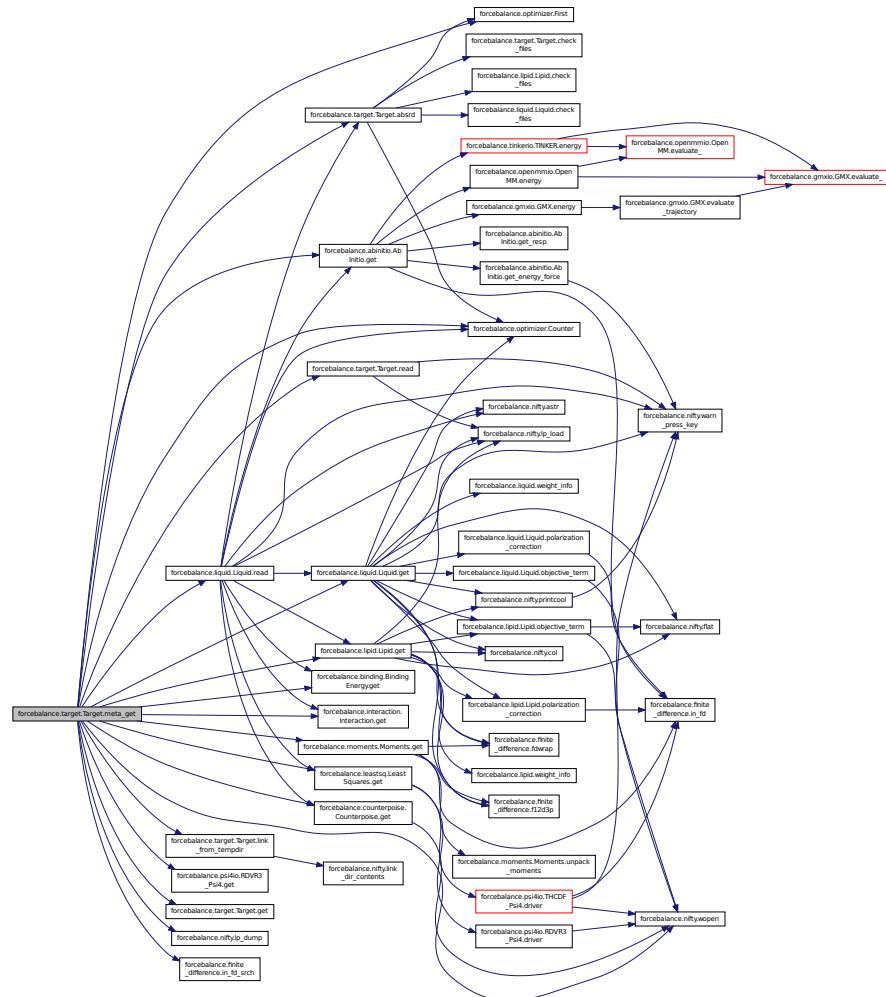


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

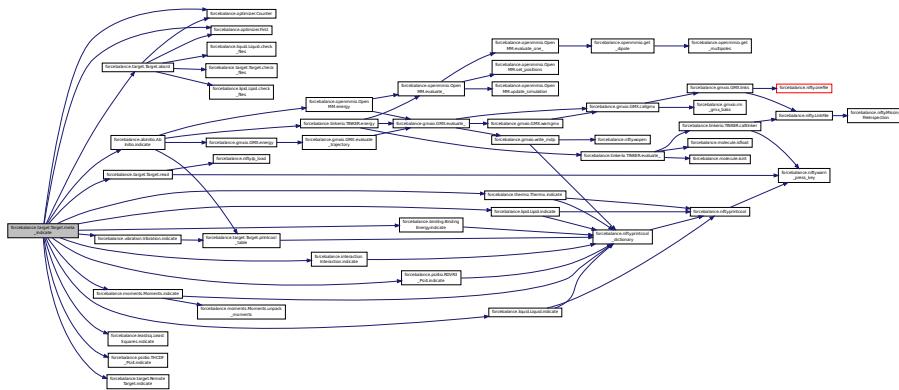
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

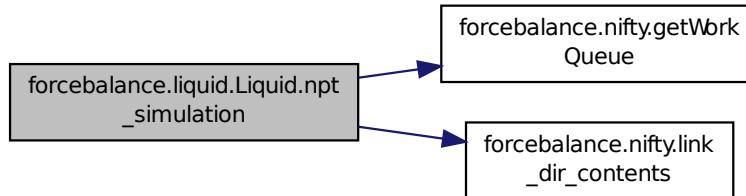
Here is the call graph for this function:



def forcebalance.liquid.Liquid.npt_simulation (self, temperature, pressure, simnum) Submit a NPT simulation to the Work Queue.

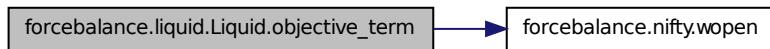
Definition at line 270 of file liquid.py.

Here is the call graph for this function:



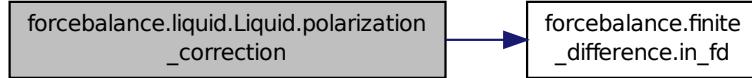
def forcebalance.liquid.Liquid.objective_term (self, points, expname, calc, err, grad, name = "Quantity", SubAverage = False) Definition at line 330 of file liquid.py.

Here is the call graph for this function:



def forcebalance.liquid.Liquid.polarization_correction (self, mvals) Definition at line 286 of file liquid.py.

Here is the call graph for this function:



def forcebalance.liquid.Liquid.prepare_temp_directory (self) Prepare the temporary directory by copying in important files.

Definition at line 155 of file liquid.py.

Here is the call graph for this function:



def forcebalance.target.Target.printcool_table (self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0) [inherited] Print target information in an organized table format.

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

data	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
headings	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
banner	Optional heading line, which will be printed at the top in the title.
footnote	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

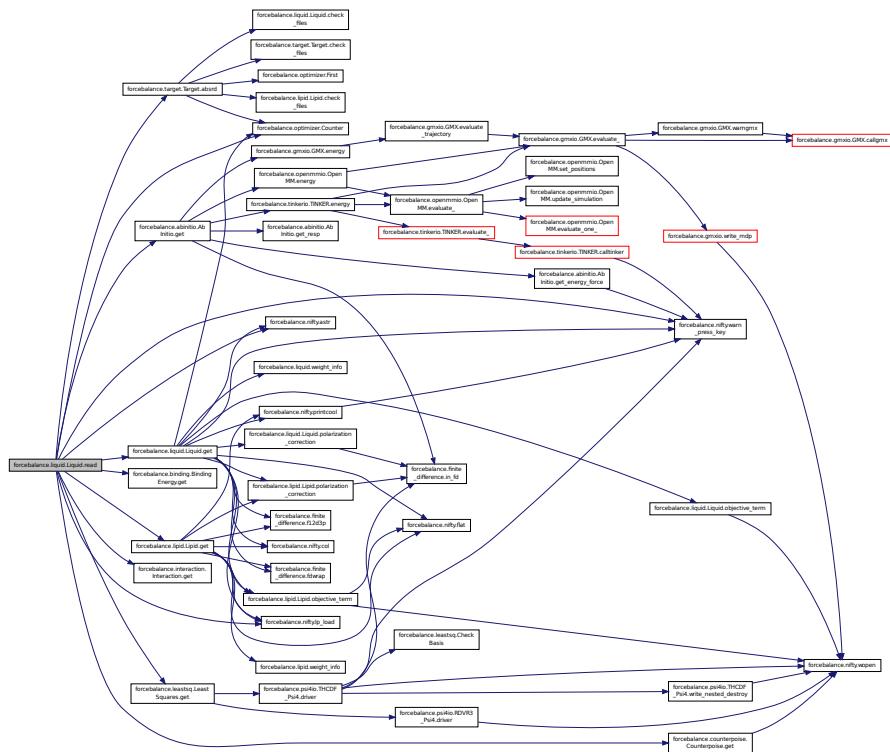
Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.read( self, mvals, AGrad = True, AHess = True ) Read in time series for all previous iterations.
```

Definition at line 447 of file liquid.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.read_0grads ( self ) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.
```

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.liquid.Liquid.read_data(self) Definition at line 162 of file liquid.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

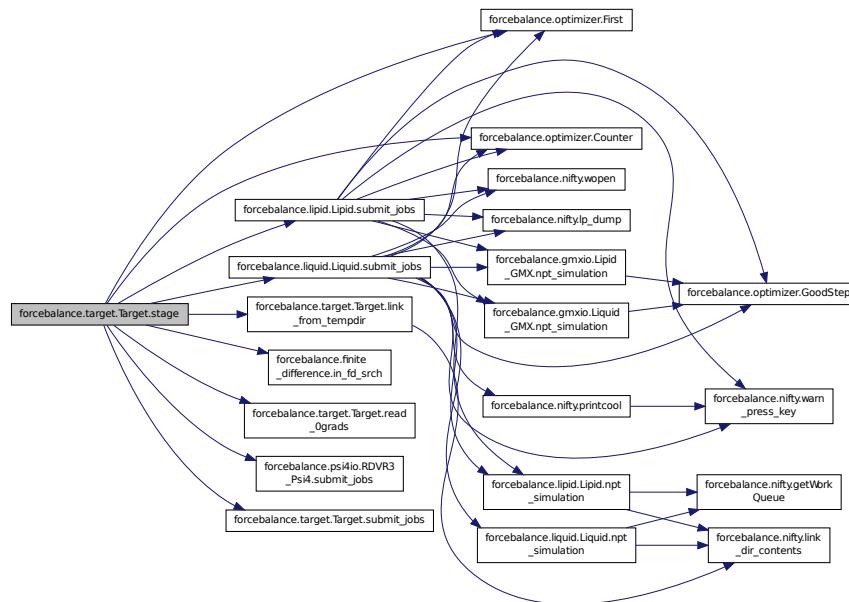
```
def forcebalance.BaseClass.set_option( self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

```
def forcebalance.target.Target.stage ( self, mvals, AGrad = False, AHess = False, customdir = None )  
[inherited] Stages the directory for the target, and then launches Work Queue processes if any.
```

The 'get' method should not worry about the directory that it's running in.

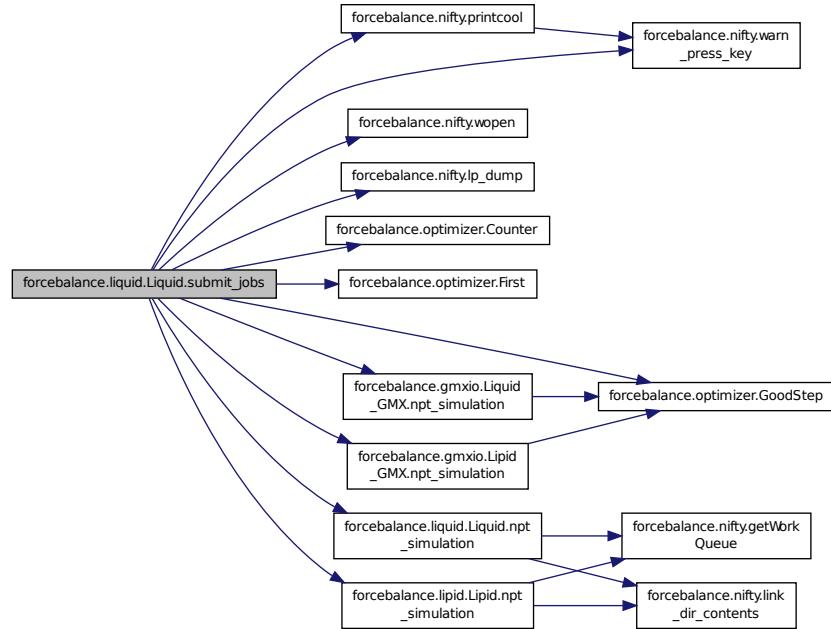
Definition at line 565 of file target.py.

Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.submit_jobs ( self, mvals, AGrad = True, AHess = True ) Definition at line  
409 of file liquid.py.
```

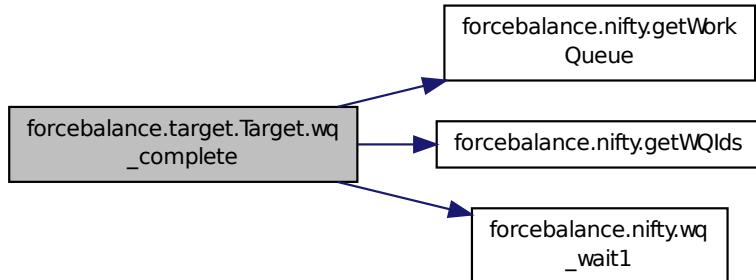
Here is the call graph for this function:



def forcebalance.target.Target.wq_complete(self) [inherited] This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_Ograds(self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.34.4 Member Data Documentation

forcebalance.liquid.Liquid.AllResults Saved results for all iterations self.SavedMVals = [].
Definition at line 151 of file liquid.py.

forcebalance.liquid.Liquid.do_self_pol Definition at line 98 of file liquid.py.

forcebalance.liquid.Liquid.engname Definition at line 275 of file liquid.py.

forcebalance.liquid.Liquid.extra_output Definition at line 118 of file liquid.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.liquid.Liquid.gas_engine Read the reference data.
Definition at line 133 of file liquid.py.

forcebalance.liquid.Liquid.gas_mol Definition at line 114 of file liquid.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.liquid.Liquid.Gp Definition at line 895 of file liquid.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.liquid.Liquid.Labels Definition at line 243 of file liquid.py.

forcebalance.liquid.Liquid.last_traj Definition at line 116 of file liquid.py.

forcebalance.liquid.Liquid.liquid_mol Definition at line 110 of file liquid.py.

forcebalance.liquid.Liquid.MBarEnergy Evaluated energies for all trajectories (i.e.
all iterations and all temperatures), using all mvals
Definition at line 148 of file liquid.py.

forcebalance.liquid.Liquid.Objective Definition at line 897 of file liquid.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.
Dictionary of whether to call the derivatives.
Definition at line 127 of file target.py.

forcebalance.liquid.Liquid.PhasePoints Definition at line 239 of file liquid.py.

forcebalance.liquid.Liquid.Pp Definition at line 892 of file liquid.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.liquid.Liquid.read_indicate Definition at line 135 of file liquid.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.liquid.Liquid.RefData Definition at line 173 of file liquid.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.liquid.Liquid.SavedTraj Saved trajectories for all iterations and all temperatures.

Definition at line 146 of file liquid.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.liquid.Liquid.w_alpha Definition at line 868 of file liquid.py.

forcebalance.liquid.Liquid.w_cp Definition at line 870 of file liquid.py.

forcebalance.liquid.Liquid.w_eps0 Definition at line 871 of file liquid.py.

forcebalance.liquid.Liquid.w_hvap Definition at line 867 of file liquid.py.

forcebalance.liquid.Liquid.w_kappa Definition at line 869 of file liquid.py.

forcebalance.liquid.Liquid.w_rho Density.

Enthalpy of vaporization. Thermal expansion coefficient. Isothermal compressibility. Isobaric heat capacity. Static dielectric constant. Estimation of errors.

Definition at line 866 of file liquid.py.

forcebalance.liquid.Liquid.Wp Definition at line 890 of file liquid.py.

forcebalance.liquid.Liquid.write_indicate Definition at line 136 of file liquid.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

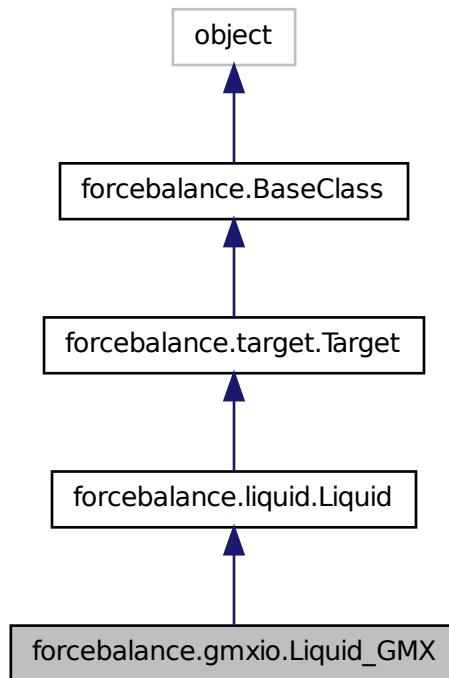
forcebalance.liquid.Liquid.Xp Definition at line 888 of file liquid.py.

The documentation for this class was generated from the following file:

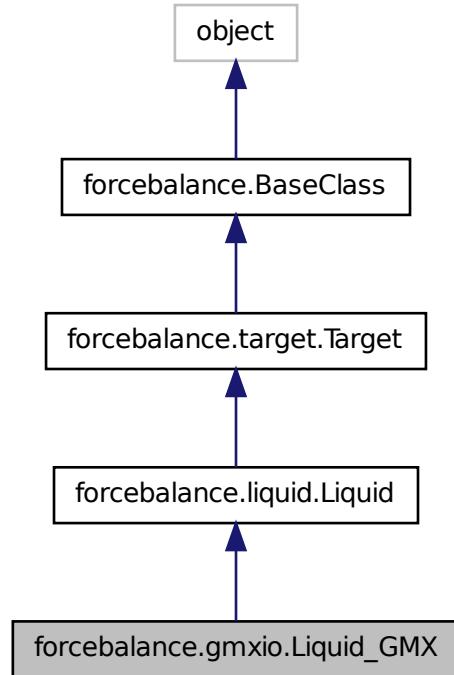
- [liquid.py](#)

8.35 forcebalance.gmxio.Liquid_GMX Class Reference

Inheritance diagram for forcebalance.gmxio.Liquid_GMX:



Collaboration diagram for forcebalance.gmxio.Liquid_GMX:



Public Member Functions

- def `__init__`
- def `npt_simulation`

Submit a NPT simulation to the Work Queue.
- def `prepare_temp_directory`

Prepare the temporary directory by copying in important files.
- def `read_data`
- def `check_files`
- def `polarization_correction`
- def `indicate`
- def `objective_term`
- def `submit_jobs`
- def `read`

Read in time series for all previous iterations.
- def `get`

Fitting of liquid bulk properties.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.

- def [write_Ograds](#)

Write a file to the target directory containing names of parameters that don't contribute to the gradient.

- def [get_G](#)

Computes the objective function contribution and its gradient.

- def [get_H](#)

Computes the objective function contribution and its gradient / Hessian.

- def [link_from_tempdir](#)

- def [refresh_temp_directory](#)

Back up the temporary directory if desired, delete it and then create a new one.

- def [absrd](#)

Supply the correct directory specified by user's "read" option.

- def [maxrd](#)

Supply the latest existing temp-directory containing valid data.

- def [meta_indicate](#)

Wrap around the indicate function, so it can print to screen and also to a file.

- def [meta_get](#)

Wrapper around the get function.

- def [stage](#)

Stages the directory for the target, and then launches Work Queue processes if any.

- def [wq_complete](#)

This method determines whether the Work Queue tasks for the current target have completed.

- def [printcool_table](#)

Print target information in an organized table format.

- def [__setattr__](#)

- def [set_option](#)

Public Attributes

- [engine_](#)

- [engname](#)

- [nptpx](#)

- [nptfiles](#)

- [gas_engine_args](#)

- [scripts](#)

- [extra_output](#)

- [LfDict](#)

- [LfDict_New](#)

- [last_traj](#)

- [do_self_pol](#)

- [liquid_mol](#)

- [gas_mol](#)

- [gas_engine](#)

Read the reference data.

- [read_indicate](#)

- [write_indicate](#)

- [SavedTraj](#)

Saved trajectories for all iterations and all temperatures.

- [MBarEnergy](#)

Evaluates energies for all trajectories (i.e.

- **AllResults**

Saved results for all iterations self.SavedMVals = [].

- **RefData**

- **PhasePoints**

- **Labels**

- **w_rho**

Density.

- **w_hvap**

- **w_alpha**

- **w_kappa**

- **w_cp**

- **w_eps0**

- **Xp**

- **Wp**

- **Pp**

- **Gp**

- **Objective**

- **rd**

Root directory of the whole project.

- **pgrad**

Iteration where we turn on zero-gradient skipping.

- **tempbase**

Relative directory of target.

- **tempdir**

- **rundir**

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

- **FF**

Need the forcefield (here for now)

- **xct**

Counts how often the objective function was computed.

- **gct**

Counts how often the gradient was computed.

- **hct**

Counts how often the Hessian was computed.

- **read_objective**

Whether to read objective.p from file when restarting an aborted run.

- **write_objective**

Whether to write objective.p at every iteration (true for all but remote.)

- **verbose_options**

- **PrintOptionDict**

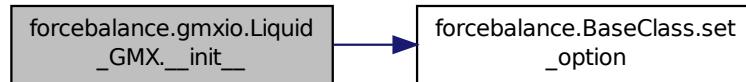
8.35.1 Detailed Description

Definition at line 1340 of file gmxio.py.

8.35.2 Constructor & Destructor Documentation

```
def forcebalance.gmxio.Liquid_GMX.__init__ ( self, options, tgt_opts, forcefield ) Definition at line 1341 of file gmxio.py.
```

Here is the call graph for this function:



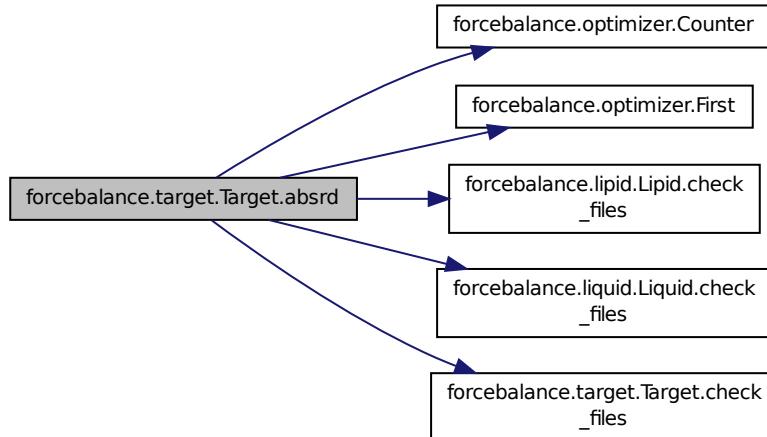
8.35.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.check_files ( self, there ) [inherited] Definition at line 253 of file liquid.py.
```

```
def forcebalance.liquid.Liquid.get ( self, mvals, AGrad = True, AHess = True ) [inherited] Fitting of liquid bulk properties.
```

This is the current major direction of development for ForceBalance. Basically, fitting the QM energies / forces alone does not always give us the best simulation behavior. In many cases it makes more sense to try and reproduce some experimentally known data as well.

In order to reproduce experimentally known data, we need to run a simulation and compare the simulation result to experiment. The main challenge here is that the simulations are computationally intensive (i.e. they require energy and force evaluations), and furthermore the results are noisy. We need to run the simulations automatically and remotely (i.e. on clusters) and a good way to calculate the derivatives of the simulation results with respect to the parameter values.

This function contains some experimentally known values of the density and enthalpy of vaporization (H_{vap}) of liquid water. It launches the density and H_{vap} calculations on the cluster, and gathers the results / derivatives. The actual calculation of results / derivatives is done in a separate file.

After the results come back, they are gathered together to form an objective function.

Parameters

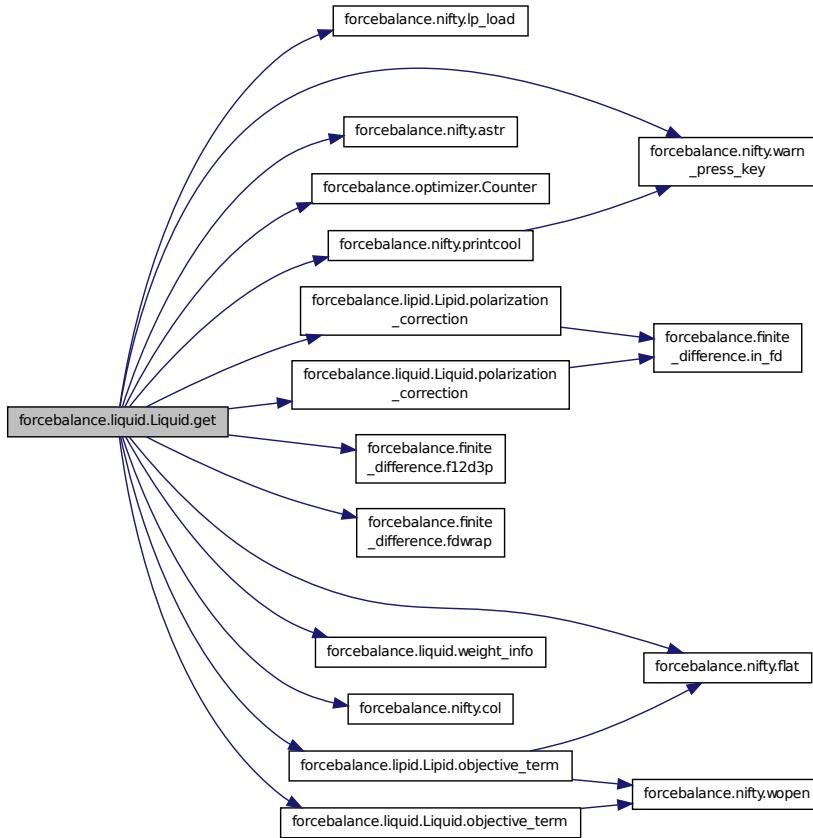
in	<i>mvals</i>	Mathematical parameter values
in	<i>AGrad</i>	Switch to turn on analytic gradient
in	<i>AHess</i>	Switch to turn on analytic Hessian

Returns

Answer Contribution to the objective function Fill in the weight matrix with MBAR weights where MBAR was run, and equal weights otherwise.

Definition at line 553 of file liquid.py.

Here is the call graph for this function:



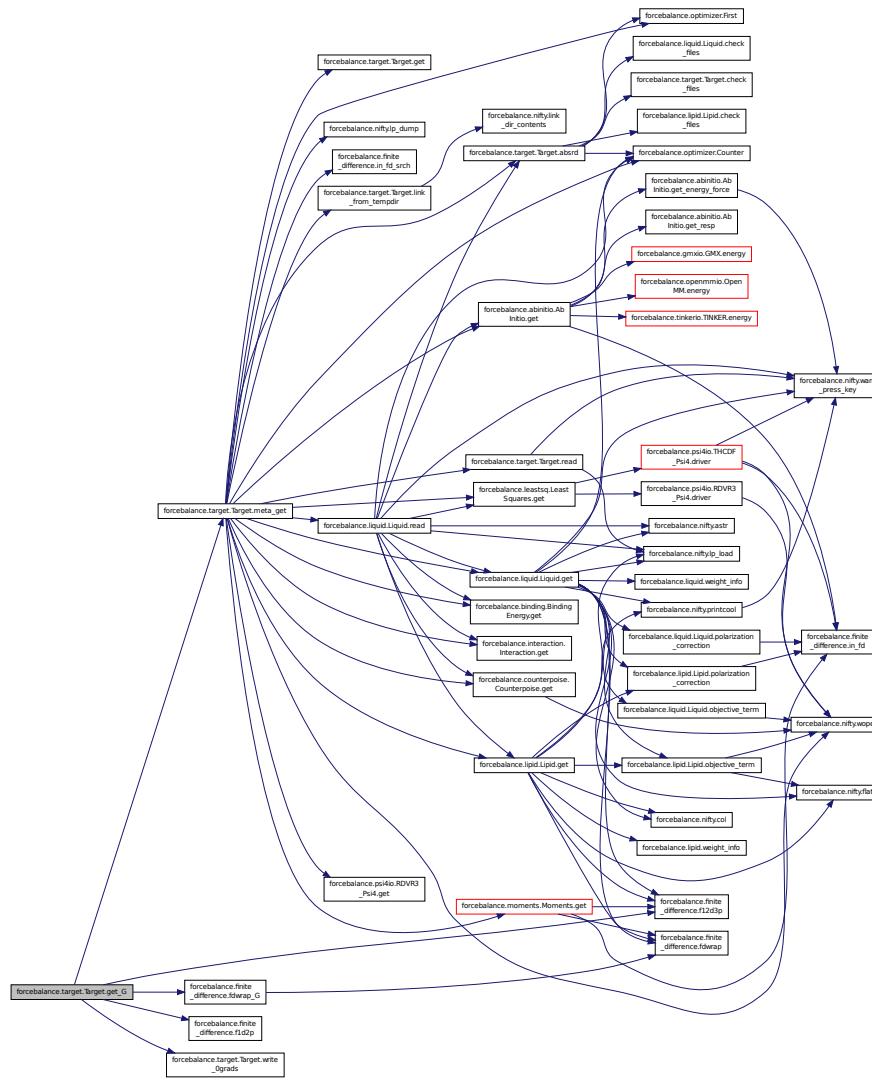
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



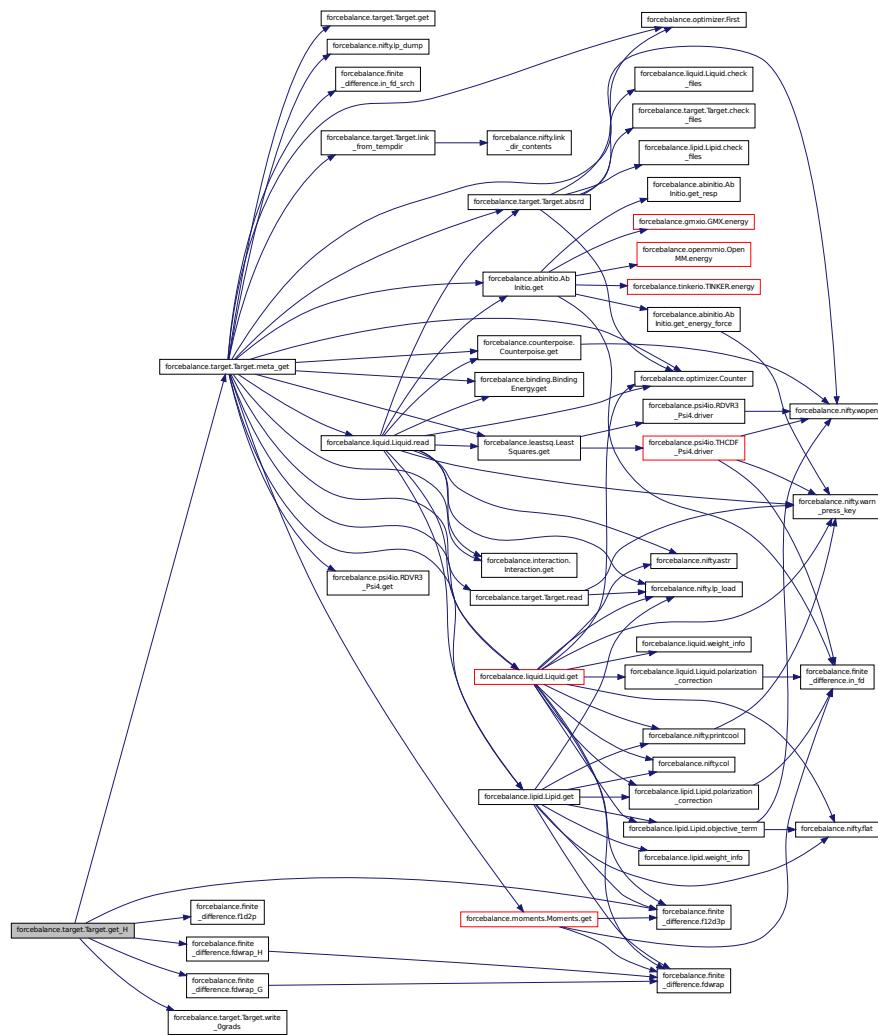
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

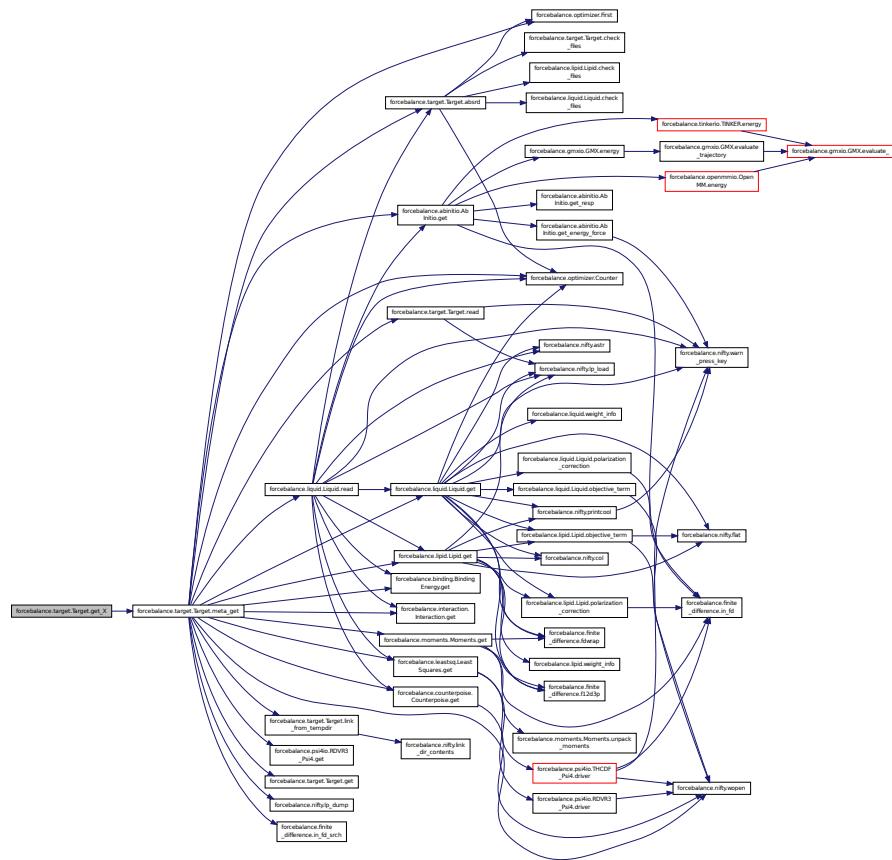
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

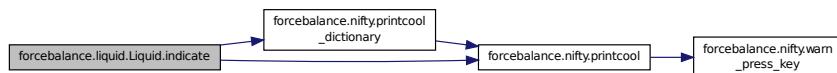
Definition at line 184 of file target.py.

Here is the call graph for this function:



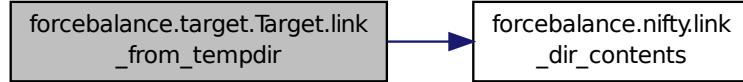
def forcebalance.liquid.Liquid.indicate (self) [inherited] Definition at line 304 of file liquid.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

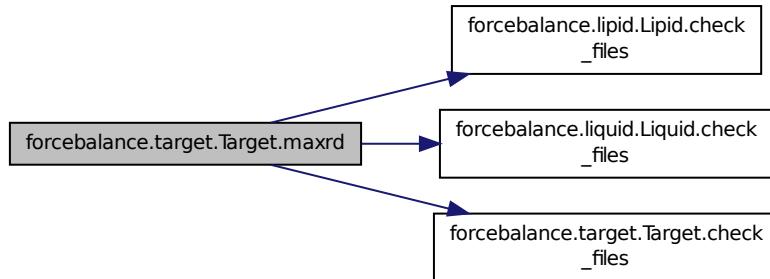
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

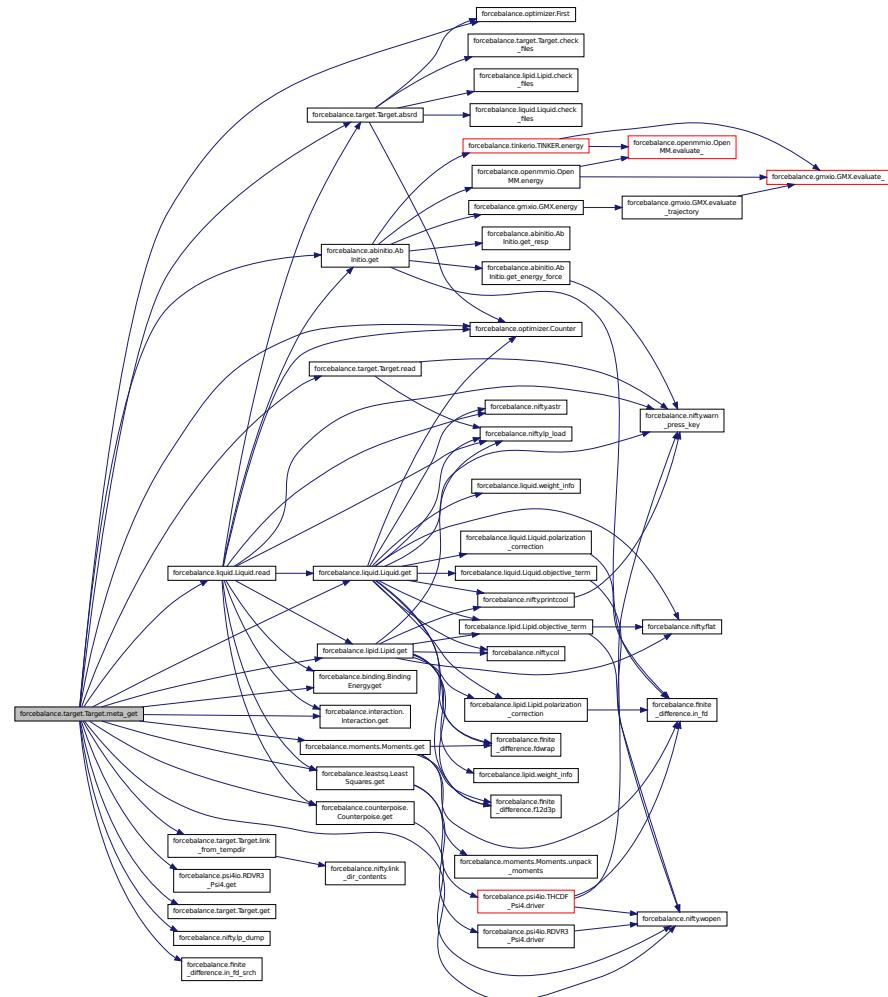


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

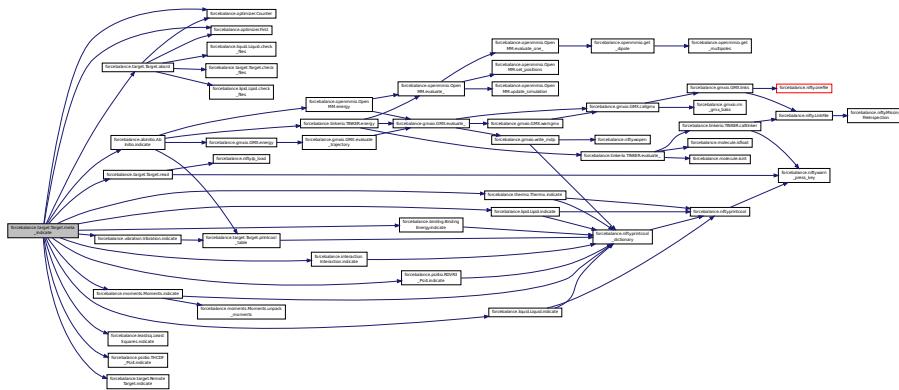
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

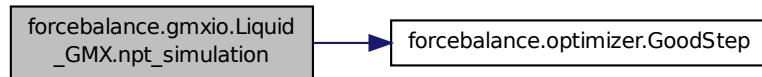
Here is the call graph for this function:



def forcebalance.gmxio.Liquid_GMX.npt.simulation (self, temperature, pressure, simnum) Submit a NPT simulation to the Work Queue.

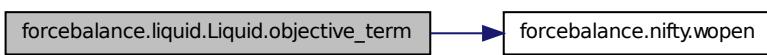
Definition at line 1383 of file gmxio.py.

Here is the call graph for this function:



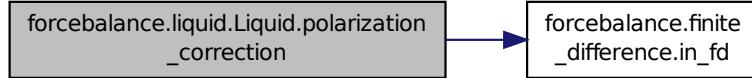
def forcebalance.liquid.Liquid.objective_term (self, points, expname, calc, err, grad, name = "Quantity", SubAverage = False) [inherited] Definition at line 330 of file liquid.py.

Here is the call graph for this function:



def forcebalance.liquid.Liquid.polarization_correction (self, mvals) [inherited] Definition at line 286 of file liquid.py.

Here is the call graph for this function:



def forcebalance.liquid.Liquid.prepare_temp_directory (self) [inherited] Prepare the temporary directory by copying in important files.

Definition at line 155 of file liquid.py.

Here is the call graph for this function:



def forcebalance.target.Target.printcool_table (self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0) [inherited] Print target information in an organized table format.

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

data	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
headings	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
banner	Optional heading line, which will be printed at the top in the title.
footnote	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

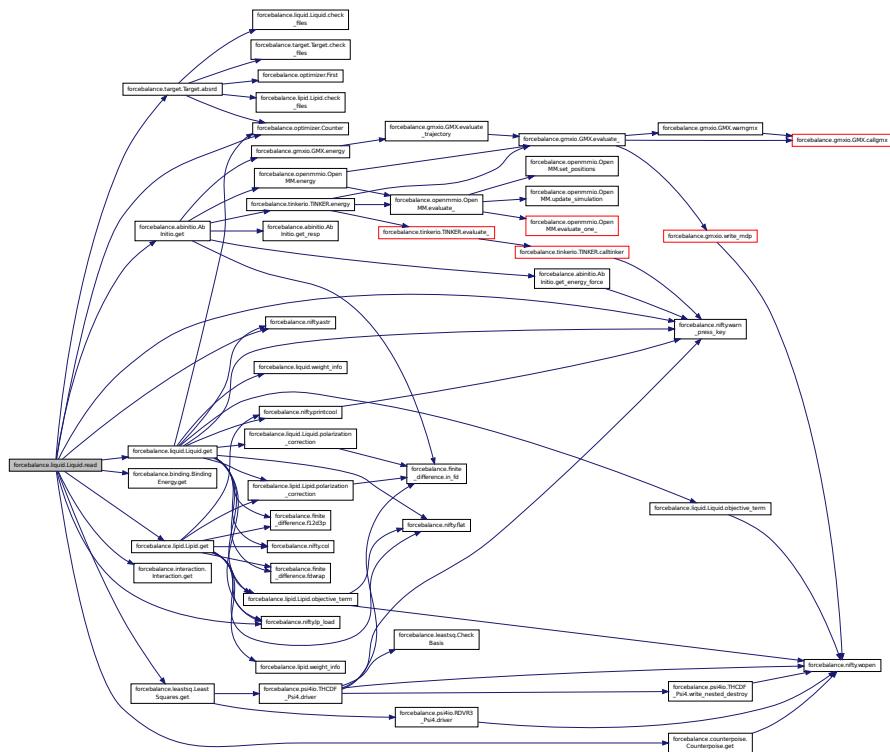
Here is the call graph for this function:



def forcebalance.liquid.Liquid.read (self, mvals, AGrad = True, AHess = True) [inherited] Read in time series for all previous iterations.

Definition at line 447 of file liquid.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.read_0grads ( self ) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.
```

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.liquid.Liquid.read_data (self) [inherited] Definition at line 162 of file liquid.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

```
def forcebalance.BaseClass.set_option( self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

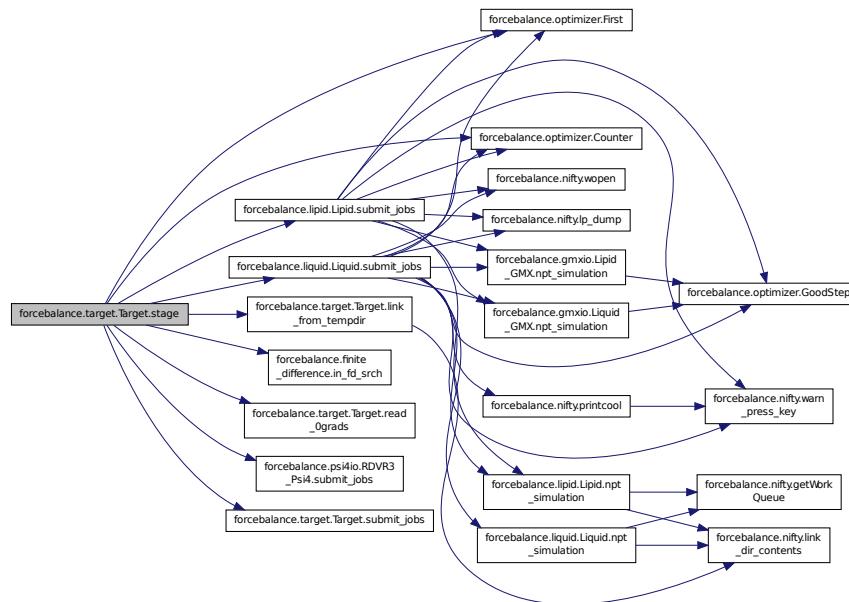
```
def forcebalance.target.Target.stage ( self, mvals, AGrad = False, AHess = False, customdir = None ) [inherited]
```

Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

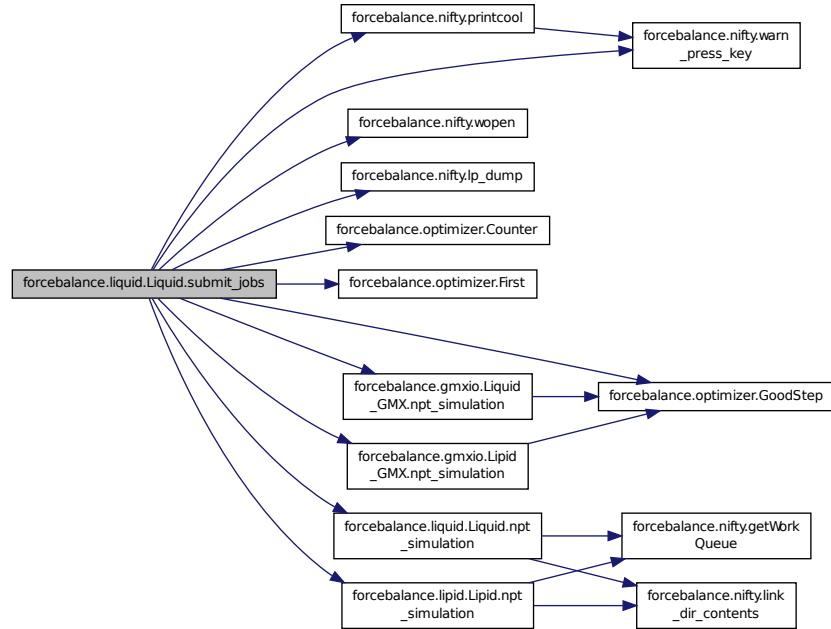
Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.submit_jobs ( self, mvals, AGrad = True, AHess = True ) [inherited]
```

Definition at line 409 of file liquid.py.

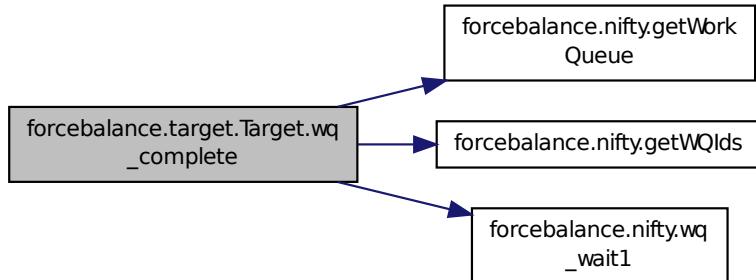
Here is the call graph for this function:



def forcebalance.target.Target.wq_complete(self) [inherited] This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_Ograds(self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.35.4 Member Data Documentation

forcebalance.liquid.Liquid.AllResults [inherited] Saved results for all iterations self.SavedMVals = [].
Definition at line 151 of file liquid.py.

forcebalance.liquid.Liquid.do_self_pol [inherited] Definition at line 98 of file liquid.py.

forcebalance.gmxio.Liquid_GMX.engine_ Definition at line 1353 of file gmxio.py.

forcebalance.gmxio.Liquid_GMX.engname Definition at line 1355 of file gmxio.py.

forcebalance.gmxio.Liquid_GMX.extra_output Definition at line 1373 of file gmxio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.liquid.Liquid.gas_engine [inherited] Read the reference data.
Definition at line 133 of file liquid.py.

forcebalance.gmxio.Liquid_GMX.gas_engine_args Definition at line 1362 of file gmxio.py.

forcebalance.liquid.Liquid.gas_mol [inherited] Definition at line 114 of file liquid.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.liquid.Liquid.Gp [inherited] Definition at line 895 of file liquid.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.liquid.Liquid.Labels [inherited] Definition at line 243 of file liquid.py.

forcebalance.gmxio.Liquid_GMX.last_traj Definition at line 1394 of file gmxio.py.

forcebalance.gmxio.Liquid_GMX.LfDict Definition at line 1378 of file gmxio.py.

forcebalance.gmxio.Liquid_GMX.LfDict_New Definition at line 1379 of file gmxio.py.

forcebalance.liquid.Liquid.liquid_mol [inherited] Definition at line 110 of file liquid.py.

forcebalance.liquid.Liquid.MBarEnergy [inherited] Evaluated energies for all trajectories (i.e.
all iterations and all temperatures), using all mvals
Definition at line 148 of file liquid.py.

forcebalance.gmxio.Liquid_GMX.nptfiles Definition at line 1359 of file gmxio.py.

forcebalance.gmxio.Liquid_GMX.nptpx Definition at line 1357 of file gmxio.py.

forcebalance.liquid.Liquid.Objective [inherited] Definition at line 897 of file liquid.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.liquid.Liquid.PhasePoints [inherited] Definition at line 239 of file liquid.py.

forcebalance.liquid.Liquid.Pp [inherited] Definition at line 892 of file liquid.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.liquid.Liquid.read_indicate [inherited] Definition at line 135 of file liquid.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.liquid.Liquid.RefData [inherited] Definition at line 173 of file liquid.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number. The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.liquid.Liquid.SavedTraj [inherited] Saved trajectories for all iterations and all temperatures.

Definition at line 146 of file liquid.py.

forcebalance.gmxio.Liquid_GMX.scripts Definition at line 1365 of file gmxio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.liquid.Liquid.w_alpha [inherited] Definition at line 868 of file liquid.py.

forcebalance.liquid.Liquid.w_cp [inherited] Definition at line 870 of file liquid.py.

forcebalance.liquid.Liquid.w_eps0 [inherited] Definition at line 871 of file liquid.py.

forcebalance.liquid.Liquid.w_hvap [inherited] Definition at line 867 of file liquid.py.

forcebalance.liquid.Liquid.w_kappa [inherited] Definition at line 869 of file liquid.py.

forcebalance.liquid.Liquid.w_rho [inherited] Density.

Enthalpy of vaporization. Thermal expansion coefficient. Isothermal compressibility. Isobaric heat capacity. Static dielectric constant. Estimation of errors.

Definition at line 866 of file liquid.py.

forcebalance.liquid.Liquid.Wp [inherited] Definition at line 890 of file liquid.py.

forcebalance.liquid.Liquid.write_indicate [inherited] Definition at line 136 of file liquid.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

forcebalance.liquid.Liquid.Xp [inherited] Definition at line 888 of file liquid.py.

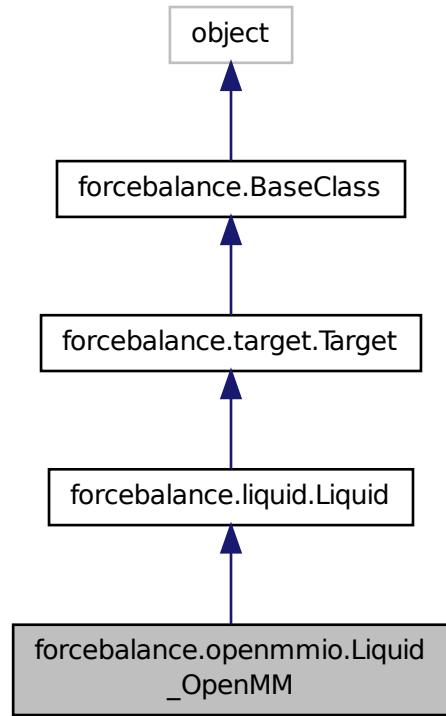
The documentation for this class was generated from the following file:

- [gmxio.py](#)

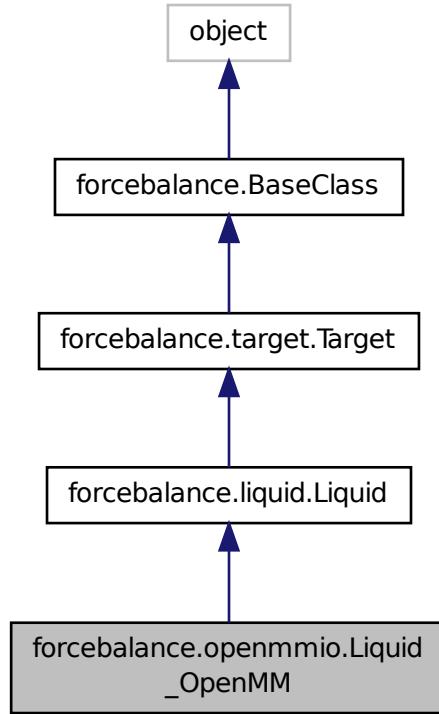
8.36 forcebalance.openmmio.Liquid_OpenMM Class Reference

Condensed phase property matching using [OpenMM](#).

Inheritance diagram for forcebalance.openmmio.Liquid_OpenMM:



Collaboration diagram for forcebalance.openmmio.Liquid_OpenMM:



Public Member Functions

- def `__init__`
- def `prepare_temp_directory`

Prepare the temporary directory by copying in important files.
- def `read_data`
- def `check_files`
- def `npt_simulation`

Submit a NPT simulation to the Work Queue.
- def `polarization_correction`
- def `indicate`
- def `objective_term`
- def `submit_jobs`
- def `read`

Read in time series for all previous iterations.
- def `get`

Fitting of liquid bulk properties.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.

- def [read_0grads](#)
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def [write_0grads](#)
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def [get_G](#)
Computes the objective function contribution and its gradient.
- def [get_H](#)
Computes the objective function contribution and its gradient / Hessian.
- def [link_from_tempdir](#)
- def [refresh_temp_directory](#)
Back up the temporary directory if desired, delete it and then create a new one.
- def [absrd](#)
Supply the correct directory specified by user's "read" option.
- def [maxrd](#)
Supply the latest existing temp-directory containing valid data.
- def [meta_indicate](#)
Wrap around the indicate function, so it can print to screen and also to a file.
- def [meta_get](#)
Wrapper around the get function.
- def [stage](#)
Stages the directory for the target, and then launches Work Queue processes if any.
- def [wq_complete](#)
This method determines whether the Work Queue tasks for the current target have completed.
- def [printcool_table](#)
Print target information in an organized table format.
- def [__setattr__](#)
- def [set_option](#)

Public Attributes

- [engine_](#)
- [engname](#)
- [nptpx](#)
- [nptfiles](#)
- [gas_engine_args](#)
- [scripts](#)
- [extra_output](#)
- [do_self_pol](#)
- [liquid_mol](#)
- [gas_mol](#)
- [last_traj](#)
- [gas_engine](#)
Read the reference data.
- [read_indicate](#)
- [write_indicate](#)
- [SavedTraj](#)
Saved trajectories for all iterations and all temperatures.
- [MBarEnergy](#)

- **AllResults**
Evaluates energies for all trajectories (i.e. Saved results for all iterations self.SavedMVals = []).
- **RefData**
- **PhasePoints**
- **Labels**
- **w_rho**
Density.
 - **w_hvap**
 - **w_alpha**
 - **w_kappa**
 - **w_cp**
 - **w_eps0**
 - **Xp**
 - **Wp**
 - **Pp**
 - **Gp**
 - **Objective**
 - **rd**
- **pgrad**
Root directory of the whole project.
- **tempbase**
Iteration where we turn on zero-gradient skipping.
- **tempdir**
Relative directory of target.
- **rundir**
`self.tempdir = os.path.join('temp',self.name)` *The directory in which the simulation is running - this can be updated.*
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

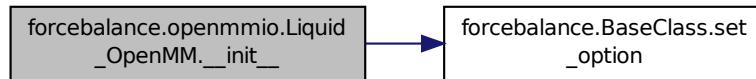
8.36.1 Detailed Description

Condensed phase property matching using OpenMM.
 Definition at line 1128 of file openmmio.py.

8.36.2 Constructor & Destructor Documentation

```
def forcebalance.openmmio.Liquid_OpenMM.__init__ ( self, options, tgt_opts, forcefield ) Definition at line  
1129 of file openmmio.py.
```

Here is the call graph for this function:



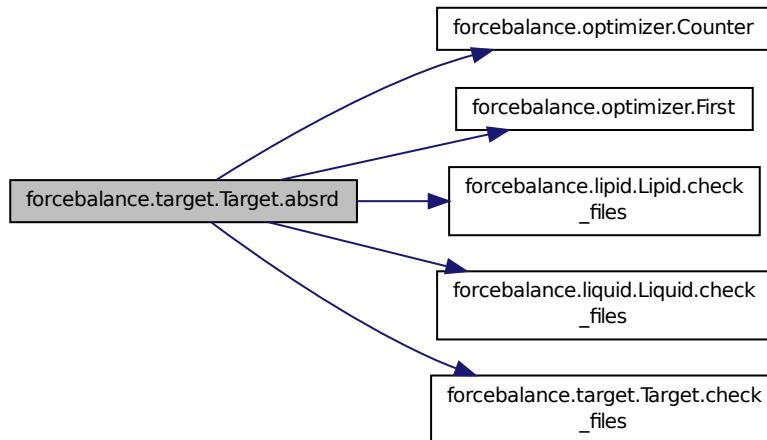
8.36.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory  
specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.check_files ( self, there ) [inherited] Definition at line 253 of file liquid.py.
```

```
def forcebalance.liquid.Liquid.get ( self, mvals, AGrad = True, AHess = True ) [inherited] Fitting  
of liquid bulk properties.
```

This is the current major direction of development for ForceBalance. Basically, fitting the QM energies / forces alone does not always give us the best simulation behavior. In many cases it makes more sense to try and reproduce some experimentally known data as well.

In order to reproduce experimentally known data, we need to run a simulation and compare the simulation result to experiment. The main challenge here is that the simulations are computationally intensive (i.e. they require energy and force evaluations), and furthermore the results are noisy. We need to run the simulations automatically and remotely (i.e. on clusters) and a good way to calculate the derivatives of the simulation results with respect to the parameter values.

This function contains some experimentally known values of the density and enthalpy of vaporization (H_{vap}) of liquid water. It launches the density and H_{vap} calculations on the cluster, and gathers the results / derivatives. The actual calculation of results / derivatives is done in a separate file.

After the results come back, they are gathered together to form an objective function.

Parameters

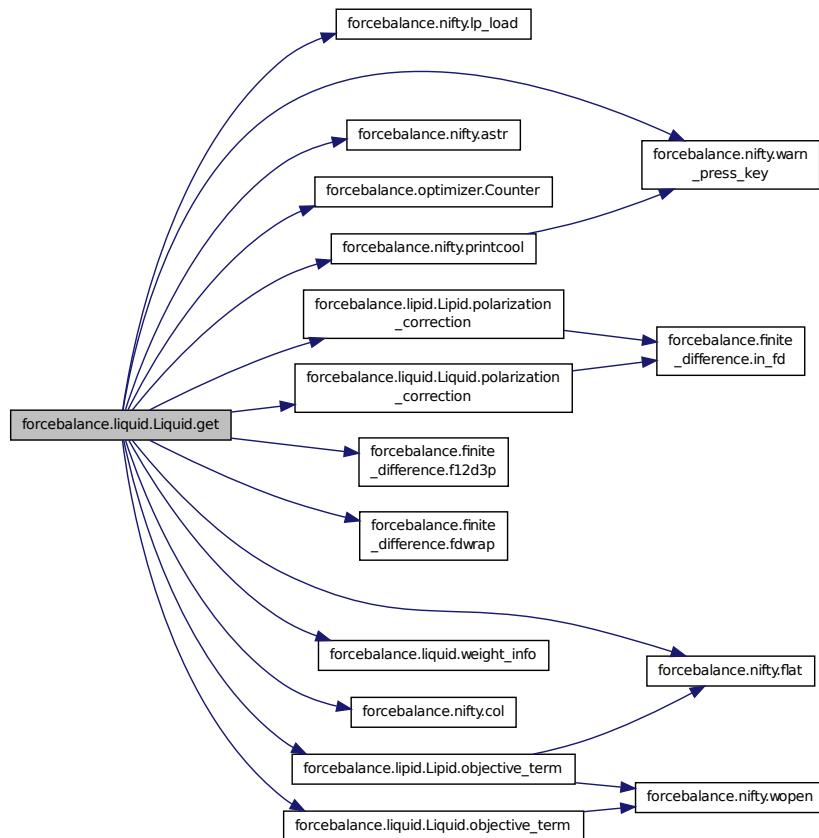
in	<i>mvals</i>	Mathematical parameter values
in	<i>AGrad</i>	Switch to turn on analytic gradient
in	<i>AHess</i>	Switch to turn on analytic Hessian

Returns

Answer Contribution to the objective function Fill in the weight matrix with MBAR weights where MBAR was run, and equal weights otherwise.

Definition at line 553 of file liquid.py.

Here is the call graph for this function:



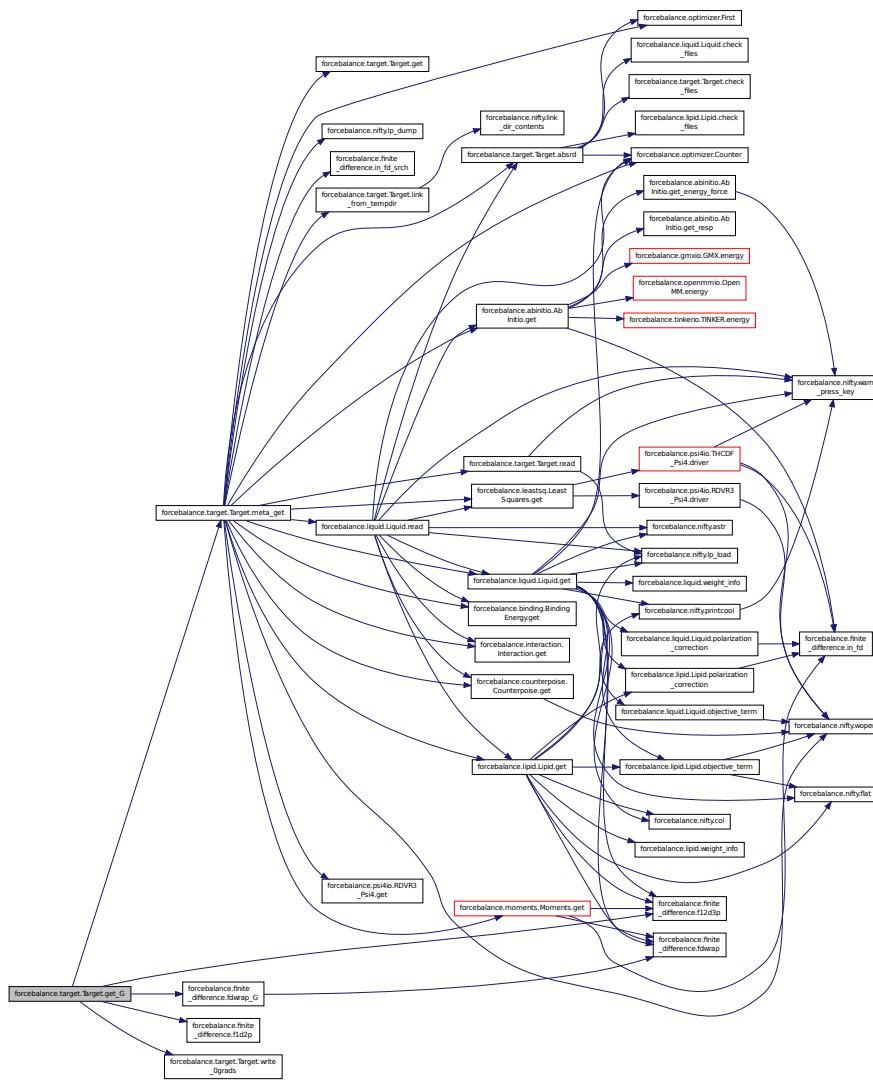
```
def forcebalance.target.Target.get_G ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.get_H ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient / Hessian.
```

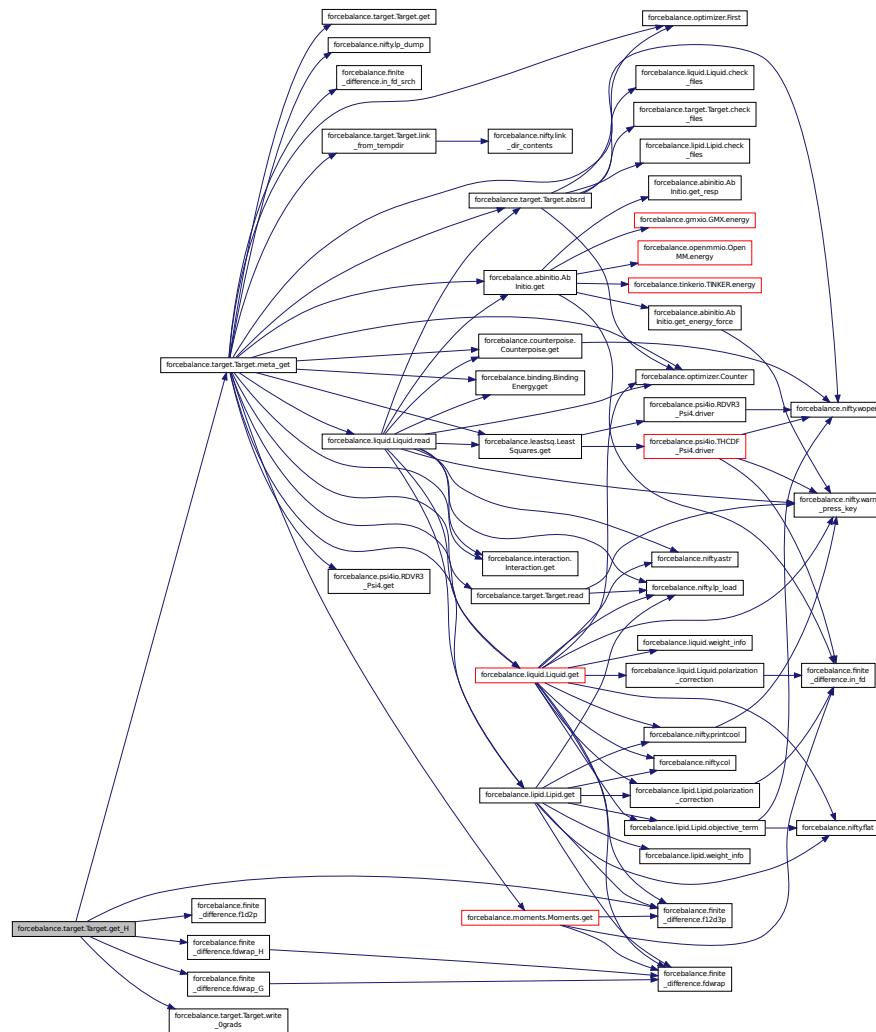
First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through

the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

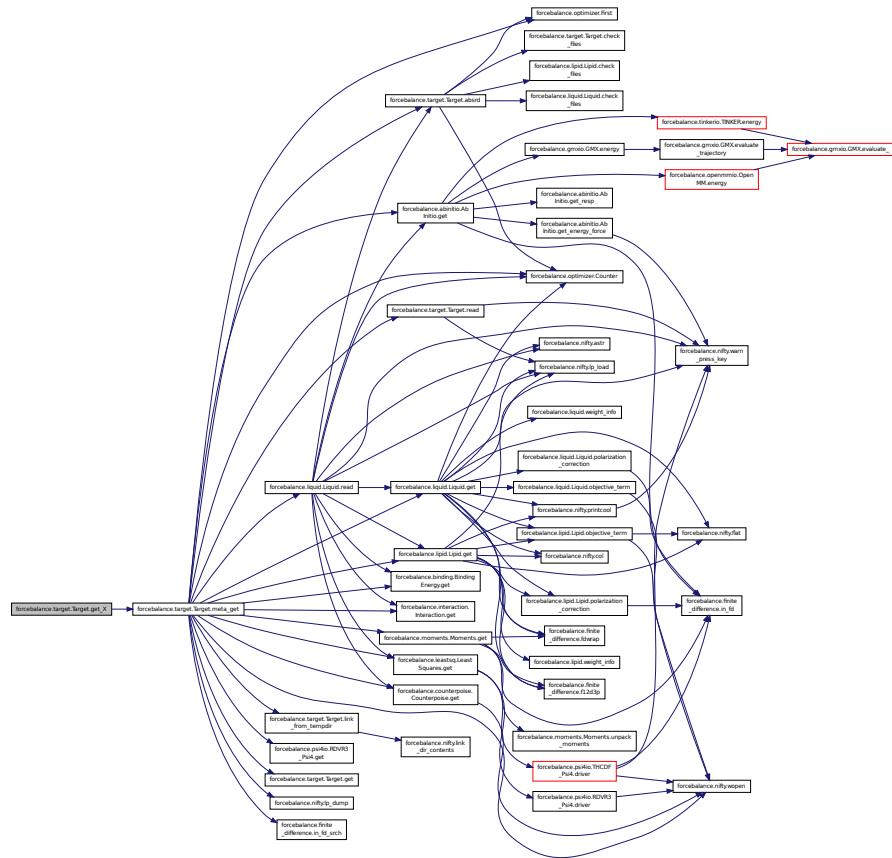
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

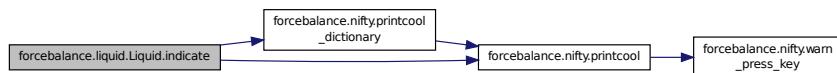
Definition at line 184 of file target.py.

Here is the call graph for this function:



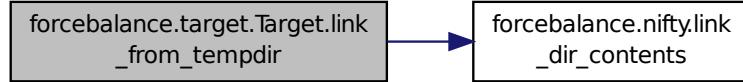
def forcebalance.liquid.Liquid.indicate (self) [inherited] Definition at line 304 of file liquid.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

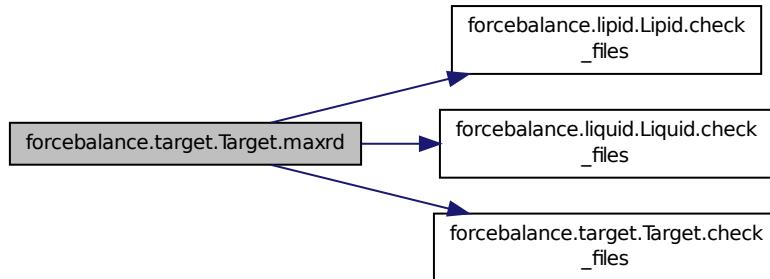
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

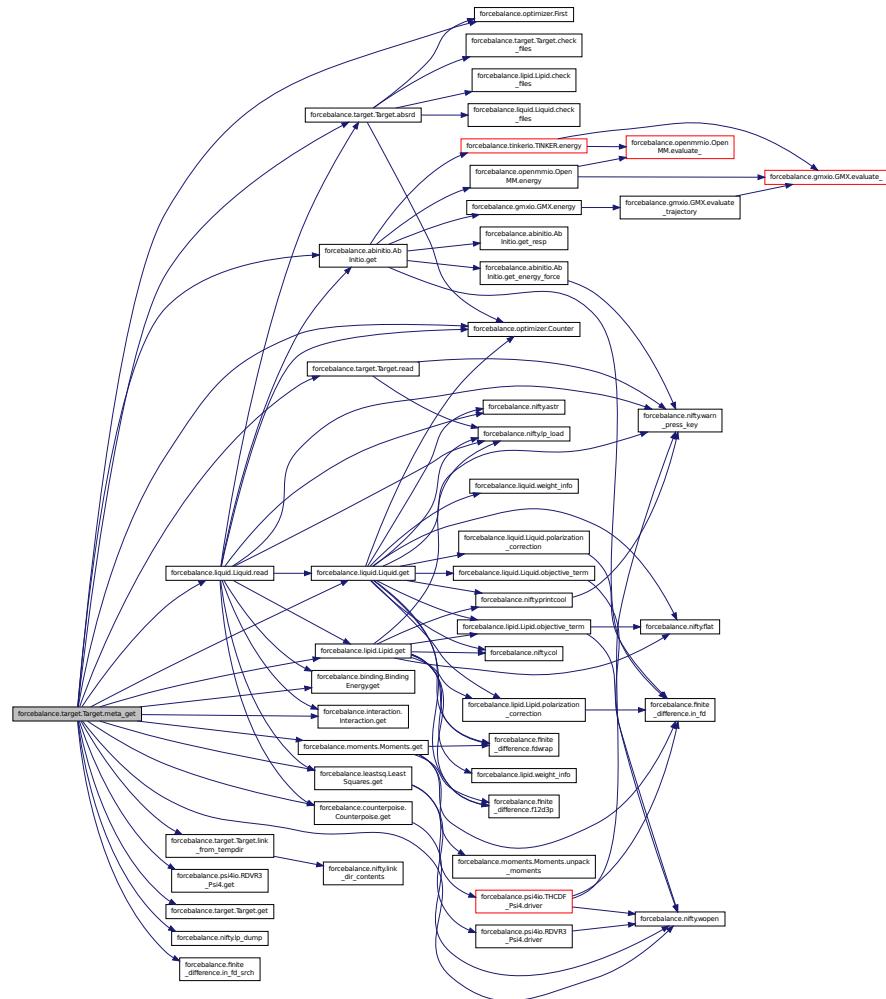


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

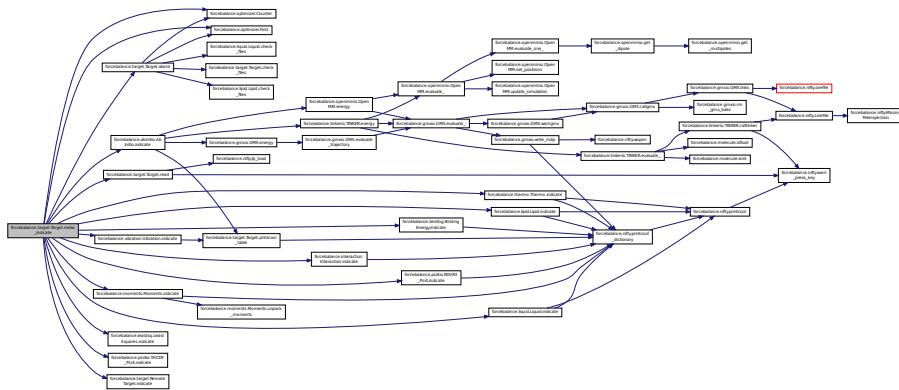
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:

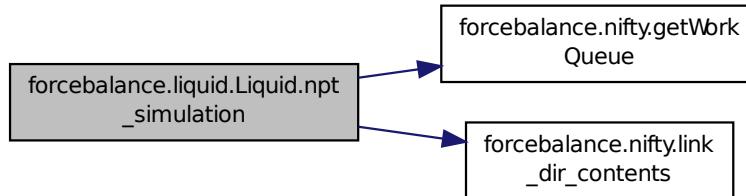


```
def forcebalance.liquid.Liquid.npt_simulation ( self, temperature, pressure, simnum ) [inherited]
```

Submit a NPT simulation to the Work Queue.

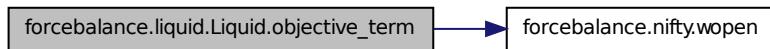
Definition at line 270 of file liquid.py.

Here is the call graph for this function:



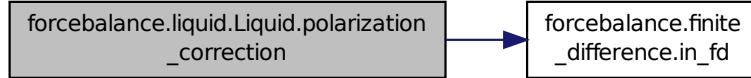
```
def forcebalance.liquid.Liquid.objective_term ( self, points, expname, calc, err, grad, name = "Quantity", SubAverage = False ) [inherited] Definition at line 330 of file liquid.py.
```

Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.polarization_correction ( self, mvals ) [inherited] Definition at line 286 of file liquid.py.
```

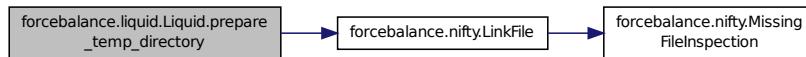
Here is the call graph for this function:



def forcebalance.liquid.Liquid.prepare_temp_directory (self) [inherited] Prepare the temporary directory by copying in important files.

Definition at line 155 of file liquid.py.

Here is the call graph for this function:



def forcebalance.target.Target.printcool_table (self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0) [inherited] Print target information in an organized table format.

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

data	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
headings	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
banner	Optional heading line, which will be printed at the top in the title.
footnote	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

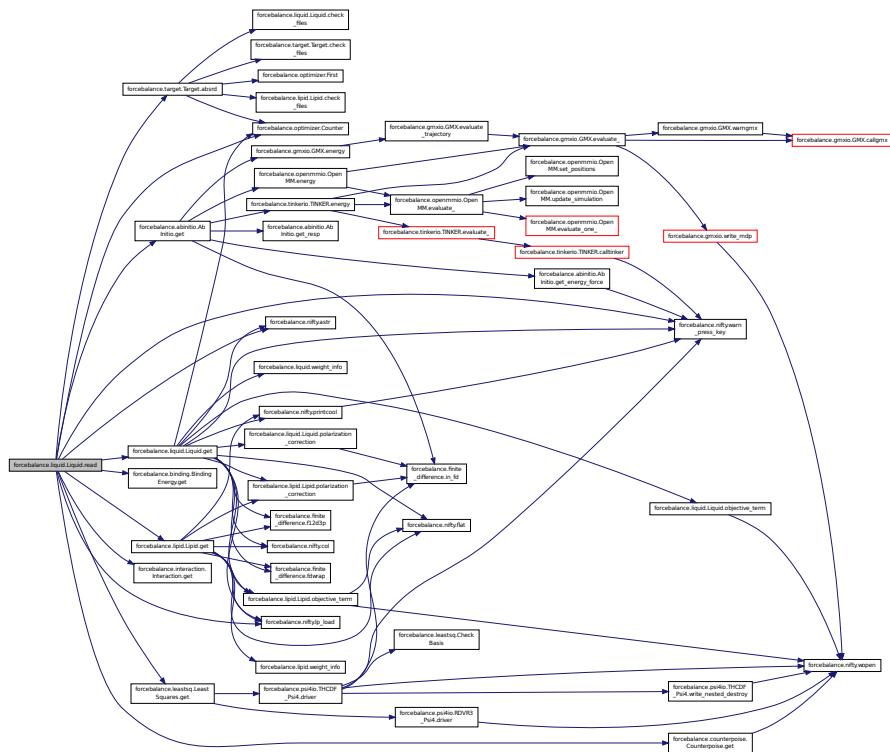
Here is the call graph for this function:



def forcebalance.liquid.Liquid.read (self, mvals, AGrad = True, AHess = True) [inherited] Read in time series for all previous iterations.

Definition at line 447 of file liquid.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.read_0grads ( self ) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.
```

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.liquid.Liquid.read_data (self) [inherited] Definition at line 162 of file liquid.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

```
def forcebalance.BaseClass.set_option( self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

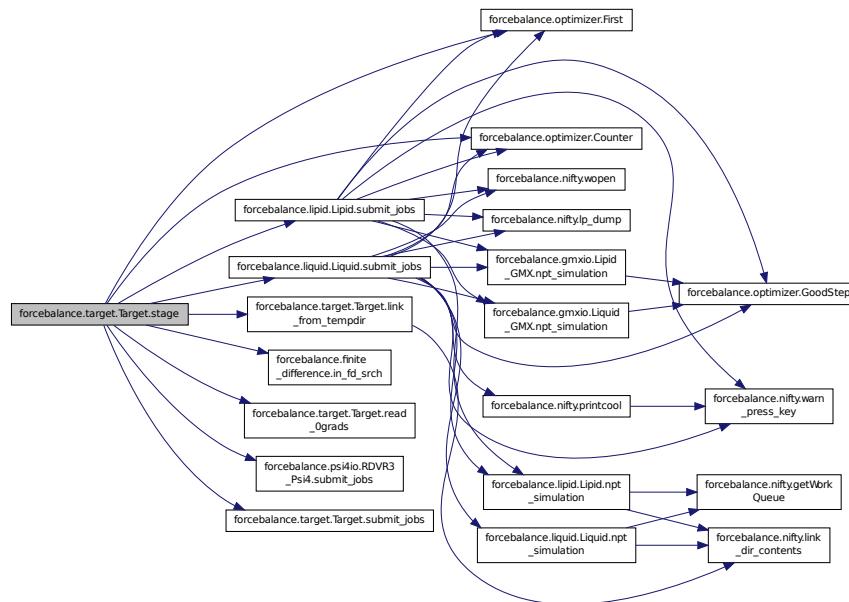
```
def forcebalance.target.Target.stage ( self, mvals, AGrad = False, AHess = False, customdir = None ) [inherited]
```

Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

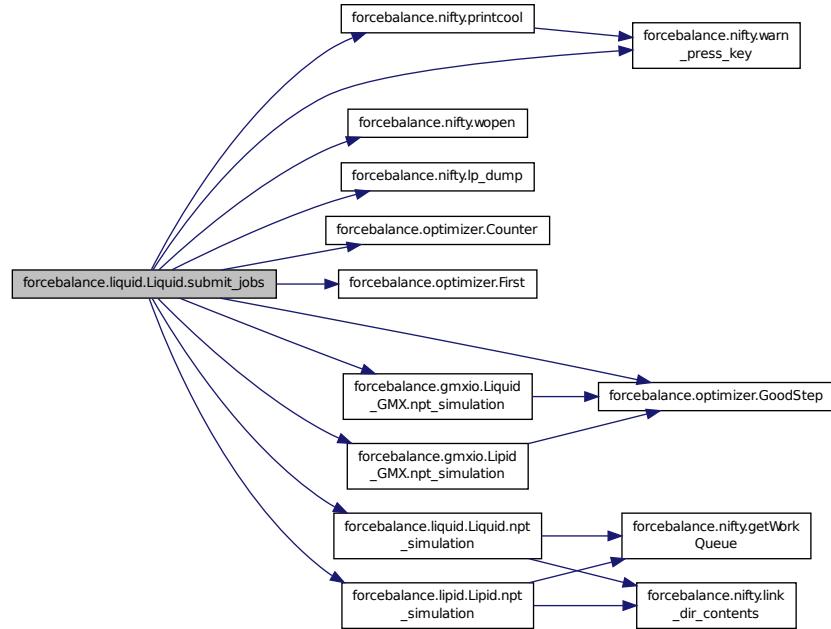
Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.submit_jobs ( self, mvals, AGrad = True, AHess = True ) [inherited]
```

Definition at line 409 of file liquid.py.

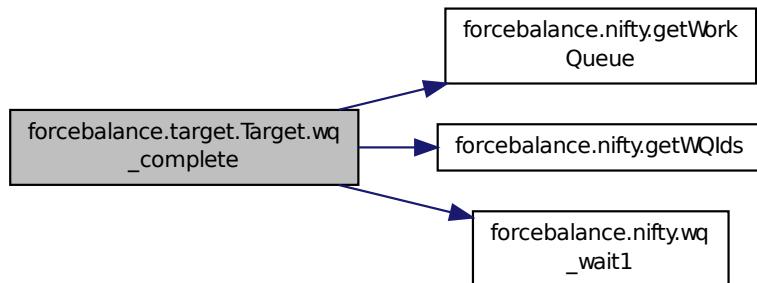
Here is the call graph for this function:



def forcebalance.target.Target.wq_complete(self) [inherited] This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_Ograds(self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.36.4 Member Data Documentation

forcebalance.liquid.Liquid.AllResults [inherited] Saved results for all iterations self.SavedMVals = [].
Definition at line 151 of file liquid.py.

forcebalance.liquid.Liquid.do_self_pol [inherited] Definition at line 98 of file liquid.py.

forcebalance.openmmio.Liquid_OpenMM.engine Definition at line 1147 of file openmmio.py.

forcebalance.openmmio.Liquid_OpenMM.engname Definition at line 1149 of file openmmio.py.

forcebalance.openmmio.Liquid_OpenMM.extra_output Definition at line 1162 of file openmmio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.liquid.Liquid.gas_engine [inherited] Read the reference data.
Definition at line 133 of file liquid.py.

forcebalance.openmmio.Liquid_OpenMM.gas_engine_args Definition at line 1155 of file openmmio.py.

forcebalance.liquid.Liquid.gas_mol [inherited] Definition at line 114 of file liquid.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.liquid.Liquid.Gp [inherited] Definition at line 895 of file liquid.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.liquid.Liquid.Labels [inherited] Definition at line 243 of file liquid.py.

forcebalance.liquid.Liquid.last_traj [inherited] Definition at line 116 of file liquid.py.

forcebalance.liquid.Liquid.liquid_mol [inherited] Definition at line 110 of file liquid.py.

forcebalance.liquid.Liquid.MBarEnergy [inherited] Evaluated energies for all trajectories (i.e. all iterations and all temperatures), using all mvals
Definition at line 148 of file liquid.py.

forcebalance.openmmio.Liquid_OpenMM.nptfiles Definition at line 1153 of file openmmio.py.

forcebalance.openmmio.Liquid_OpenMM.nptpfx Definition at line 1151 of file openmmio.py.

forcebalance.liquid.Liquid.Objective [inherited] Definition at line 897 of file liquid.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.
Dictionary of whether to call the derivatives.
Definition at line 127 of file target.py.

forcebalance.liquid.Liquid.PhasePoints [inherited] Definition at line 239 of file liquid.py.

forcebalance.liquid.Liquid.Pp [inherited] Definition at line 892 of file liquid.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.liquid.Liquid.read_indicate [inherited] Definition at line 135 of file liquid.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.liquid.Liquid.RefData [inherited] Definition at line 173 of file liquid.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.liquid.Liquid.SavedTraj [inherited] Saved trajectories for all iterations and all temperatures.

Definition at line 146 of file liquid.py.

forcebalance.openmmio.Liquid_OpenMM.scripts Definition at line 1157 of file openmmio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.liquid.Liquid.w_alpha [inherited] Definition at line 868 of file liquid.py.

forcebalance.liquid.Liquid.w_cp [inherited] Definition at line 870 of file liquid.py.

forcebalance.liquid.Liquid.w_eps0 [inherited] Definition at line 871 of file liquid.py.

forcebalance.liquid.Liquid.w_hvap [inherited] Definition at line 867 of file liquid.py.

forcebalance.liquid.Liquid.w_kappa [inherited] Definition at line 869 of file liquid.py.

forcebalance.liquid.Liquid.w_rho [inherited] Density.

Enthalpy of vaporization. Thermal expansion coefficient. Isothermal compressibility. Isobaric heat capacity. Static dielectric constant. Estimation of errors.

Definition at line 866 of file liquid.py.

forcebalance.liquid.Liquid.Wp [inherited] Definition at line 890 of file liquid.py.

forcebalance.liquid.Liquid.write_indicate [inherited] Definition at line 136 of file liquid.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

forcebalance.liquid.Liquid.Xp [inherited] Definition at line 888 of file liquid.py.

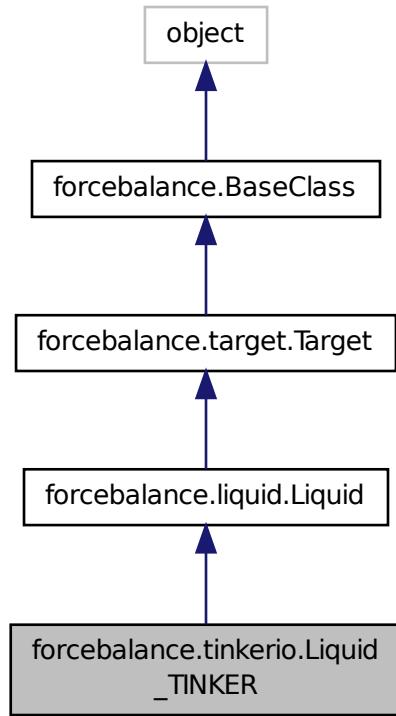
The documentation for this class was generated from the following file:

- [openmmio.py](#)

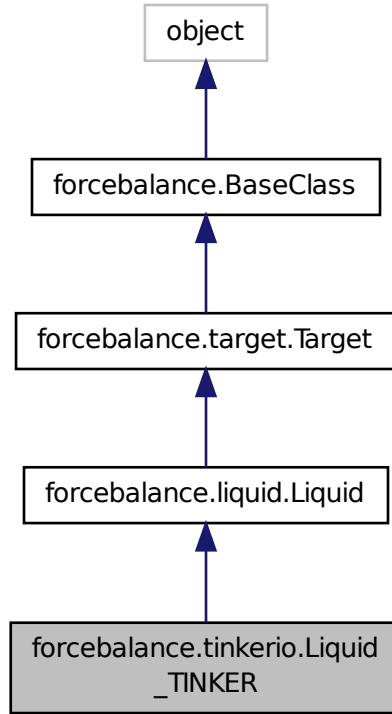
8.37 forcebalance.tinkerio.Liquid_TINKER Class Reference

Condensed phase property matching using [TINKER](#).

Inheritance diagram for forcebalance.tinkerio.Liquid_TINKER:



Collaboration diagram for forcebalance.tinkerio.Liquid_TINKER:



Public Member Functions

- def `__init__`
- def `npt_simulation`

Submit a NPT simulation to the Work Queue.
- def `prepare_temp_directory`

Prepare the temporary directory by copying in important files.
- def `read_data`
- def `check_files`
- def `polarization_correction`
- def `indicate`
- def `objective_term`
- def `submit_jobs`
- def `read`

Read in time series for all previous iterations.
- def `get`

Fitting of liquid bulk properties.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.

- def [read_0grads](#)
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def [write_0grads](#)
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def [get_G](#)
Computes the objective function contribution and its gradient.
- def [get_H](#)
Computes the objective function contribution and its gradient / Hessian.
- def [link_from_tempdir](#)
- def [refresh_temp_directory](#)
Back up the temporary directory if desired, delete it and then create a new one.
- def [absrd](#)
Supply the correct directory specified by user's "read" option.
- def [maxrd](#)
Supply the latest existing temp-directory containing valid data.
- def [meta_indicate](#)
Wrap around the indicate function, so it can print to screen and also to a file.
- def [meta_get](#)
Wrapper around the get function.
- def [stage](#)
Stages the directory for the target, and then launches Work Queue processes if any.
- def [wq_complete](#)
This method determines whether the Work Queue tasks for the current target have completed.
- def [printcool_table](#)
Print target information in an organized table format.
- def [__setattr__](#)
- def [set_option](#)

Public Attributes

- [engine_](#)
- [engname](#)
- [nptpx](#)
- [nptfiles](#)
- [gas_engine_args](#)
- [scripts](#)
- [extra_output](#)
- [DynDict](#)
- [DynDict_New](#)
- [last_traj](#)
- [do_self_pol](#)
- [liquid_mol](#)
- [gas_mol](#)
- [gas_engine](#)
Read the reference data.
- [read_indicate](#)
- [write_indicate](#)
- [SavedTraj](#)
Saved trajectories for all iterations and all temperatures.

- **MBarEnergy**
Evaluates energies for all trajectories (i.e.
- **AllResults**
Saved results for all iterations self.SavedMVals = [].
- **RefData**
- **PhasePoints**
- **Labels**
- **w_rho**
Density.
- **w_hvap**
- **w_alpha**
- **w_kappa**
- **w_cp**
- **w_eps0**
- **Xp**
- **Wp**
- **Pp**
- **Gp**
- **Objective**
- **rd**
Root directory of the whole project.
- **pgrad**
Iteration where we turn on zero-gradient skipping.
- **tempbase**
Relative directory of target.
- **tempdir**
- **rundir**
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

8.37.1 Detailed Description

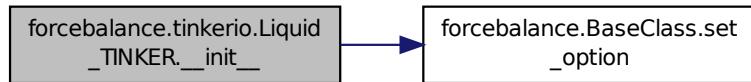
Condensed phase property matching using [TINKER](#).

Definition at line 1014 of file `tinkerio.py`.

8.37.2 Constructor & Destructor Documentation

```
def forcebalance.tinkerio.Liquid_TINKER.__init__ ( self, options, tgt_opts, forcefield ) Definition at line 1015  
of file tinkerio.py.
```

Here is the call graph for this function:



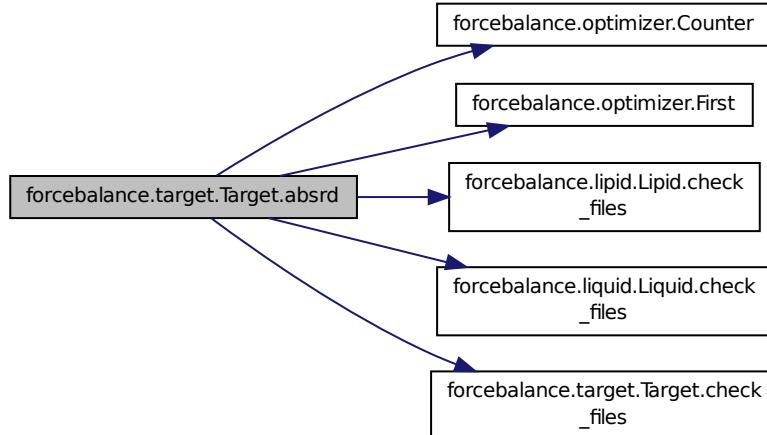
8.37.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory  
specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.check_files ( self, there ) [inherited] Definition at line 253 of file liquid.py.
```

```
def forcebalance.liquid.Liquid.get ( self, mvals, AGrad = True, AHess = True ) [inherited] Fitting  
of liquid bulk properties.
```

This is the current major direction of development for ForceBalance. Basically, fitting the QM energies / forces alone does not always give us the best simulation behavior. In many cases it makes more sense to try and reproduce some experimentally known data as well.

In order to reproduce experimentally known data, we need to run a simulation and compare the simulation result to experiment. The main challenge here is that the simulations are computationally intensive (i.e. they require energy and force evaluations), and furthermore the results are noisy. We need to run the simulations automatically and remotely (i.e. on clusters) and a good way to calculate the derivatives of the simulation results with respect to the parameter values.

This function contains some experimentally known values of the density and enthalpy of vaporization (H_{vap}) of liquid water. It launches the density and H_{vap} calculations on the cluster, and gathers the results / derivatives. The actual calculation of results / derivatives is done in a separate file.

After the results come back, they are gathered together to form an objective function.

Parameters

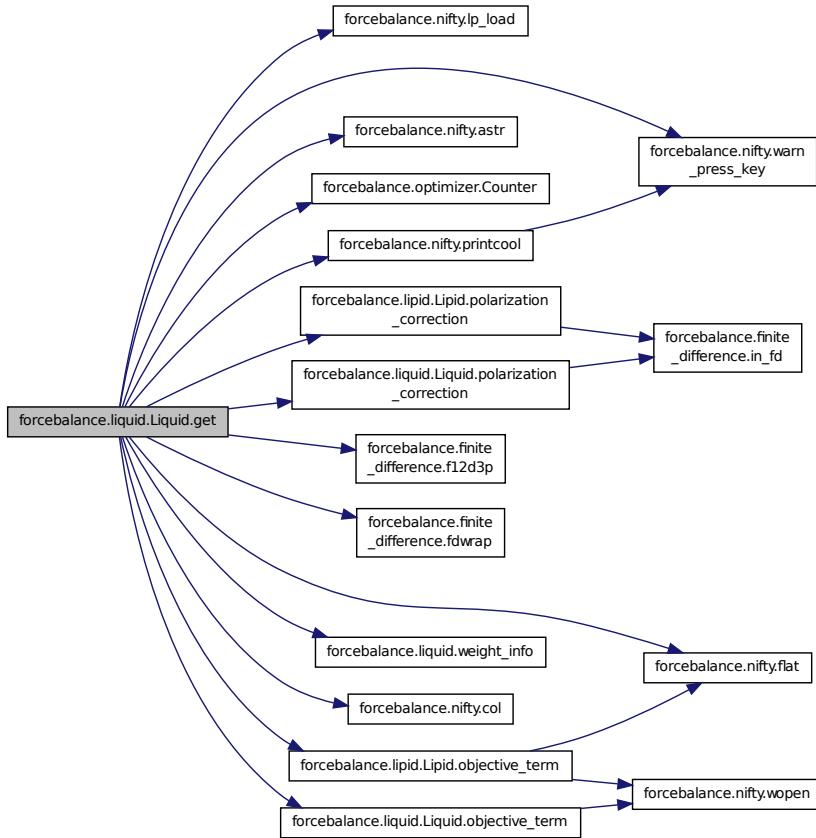
in	<i>mvals</i>	Mathematical parameter values
in	<i>AGrad</i>	Switch to turn on analytic gradient
in	<i>AHess</i>	Switch to turn on analytic Hessian

Returns

Answer Contribution to the objective function Fill in the weight matrix with MBAR weights where MBAR was run, and equal weights otherwise.

Definition at line 553 of file liquid.py.

Here is the call graph for this function:



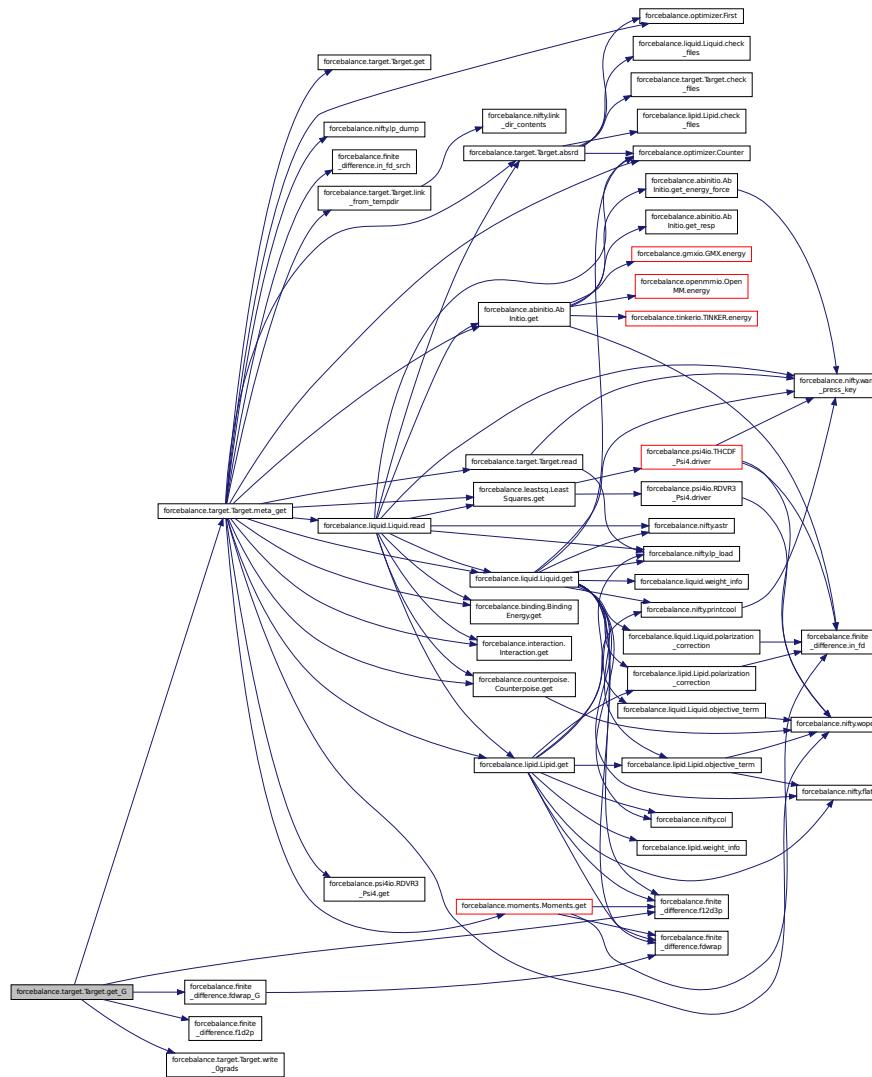
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the `fd1.pids` and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



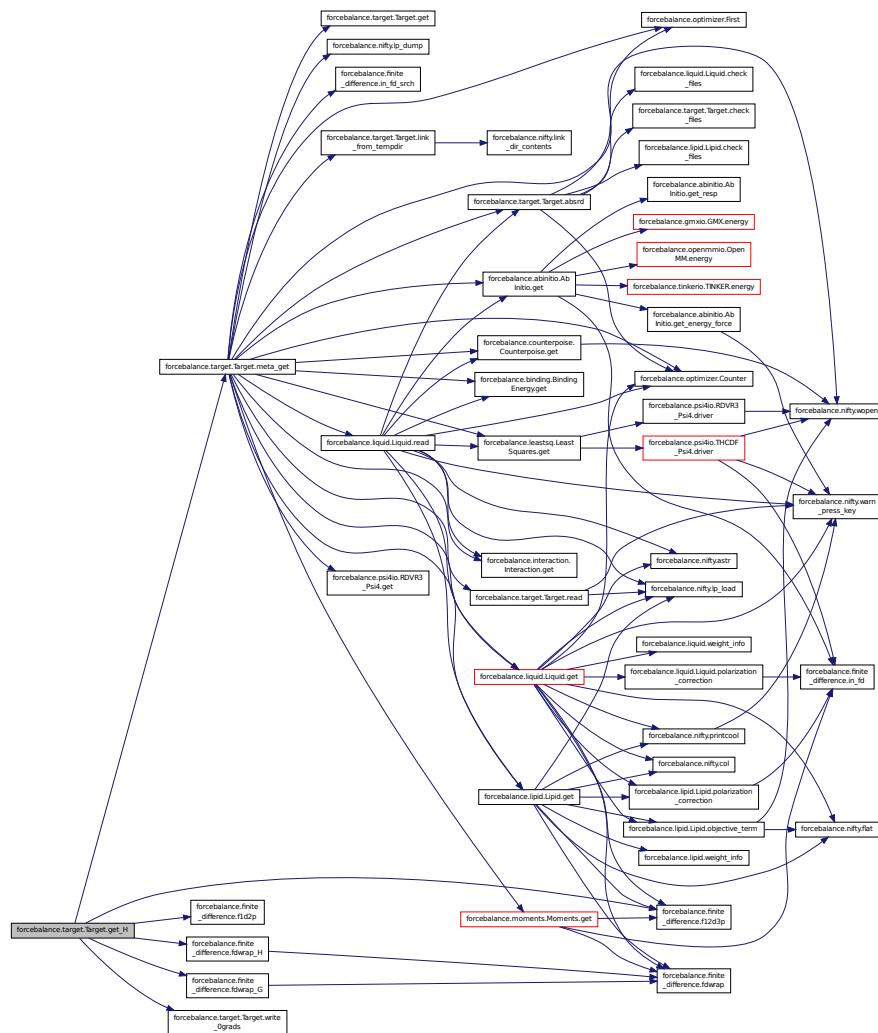
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

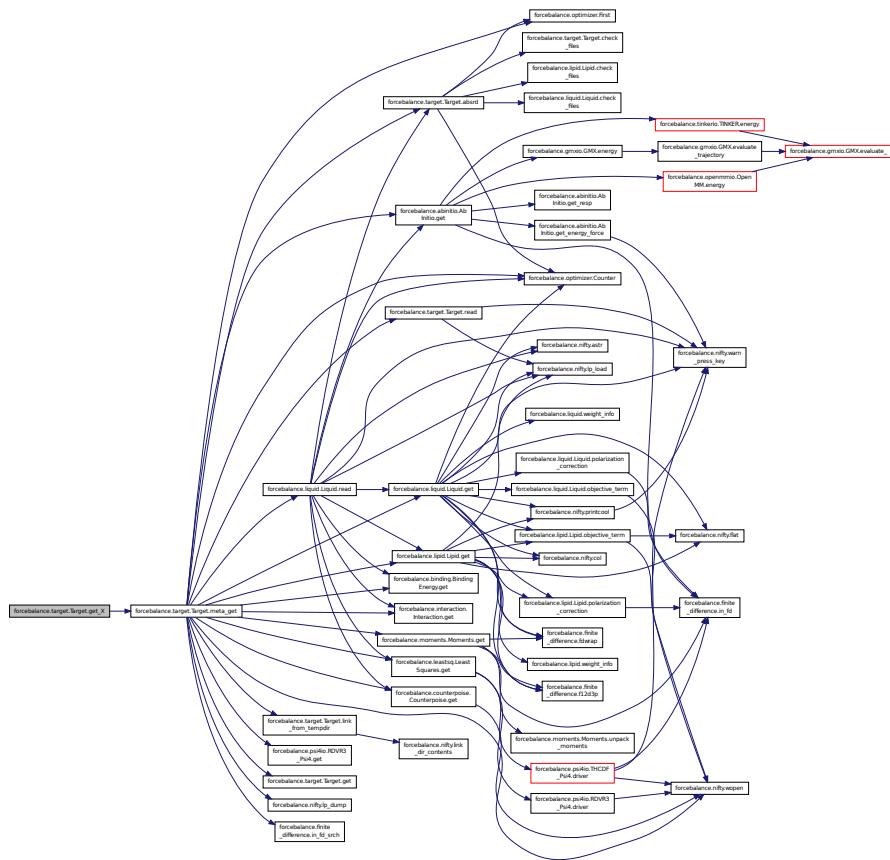
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

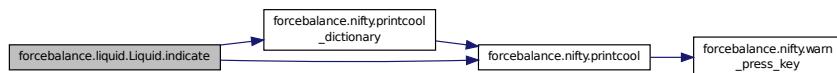
Definition at line 184 of file target.py.

Here is the call graph for this function:



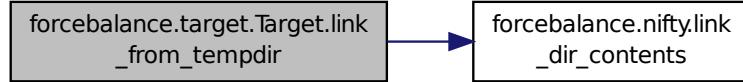
def forcebalance.liquid.Liquid.indicate (self) [inherited] Definition at line 304 of file liquid.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

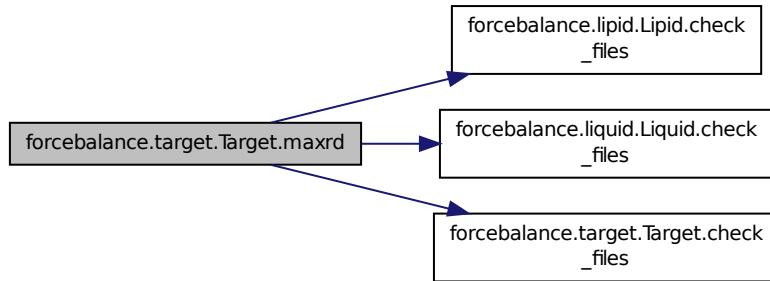
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

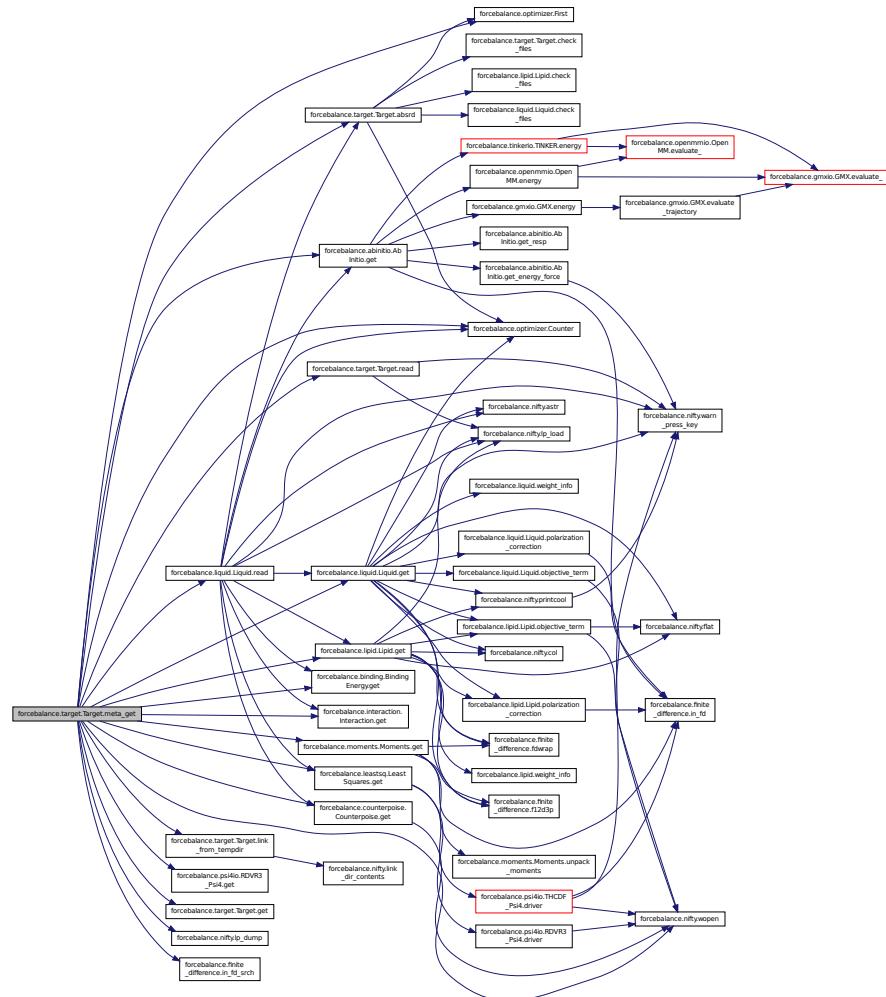


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

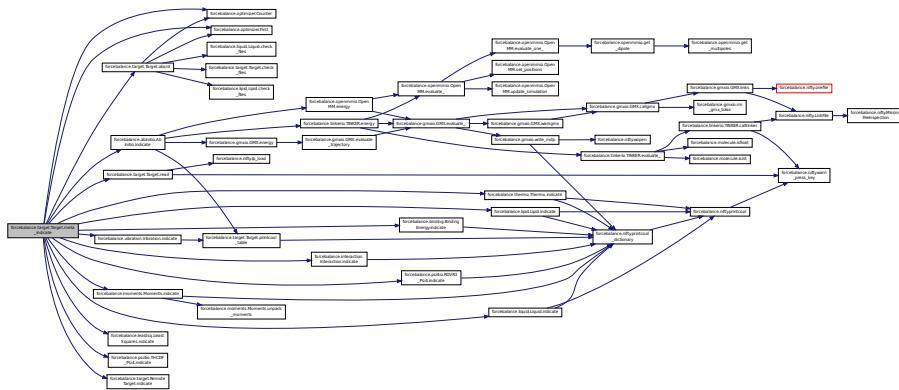
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

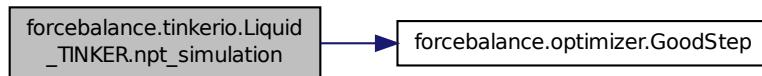
Here is the call graph for this function:



def forcebalance.tinkerio.Liquid_TINKER.npt_simulation (self, temperature, pressure, simnum) Submit a NPT simulation to the Work Queue.

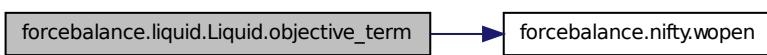
Definition at line 1052 of file tinkerio.py.

Here is the call graph for this function:



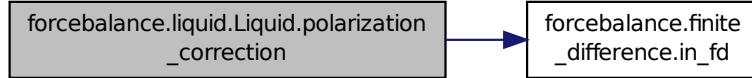
def forcebalance.liquid.Liquid.objective_term (self, points, expname, calc, err, grad, name = "Quantity", SubAverage = False) [inherited] Definition at line 330 of file liquid.py.

Here is the call graph for this function:



def forcebalance.liquid.Liquid.polarization.correction (self, mvals) [inherited] Definition at line 286 of file liquid.py.

Here is the call graph for this function:



def forcebalance.liquid.Liquid.prepare_temp_directory (self) [inherited] Prepare the temporary directory by copying in important files.

Definition at line 155 of file liquid.py.

Here is the call graph for this function:



def forcebalance.target.Target.printcool_table (self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0) [inherited] Print target information in an organized table format.

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

data	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
headings	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
banner	Optional heading line, which will be printed at the top in the title.
footnote	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

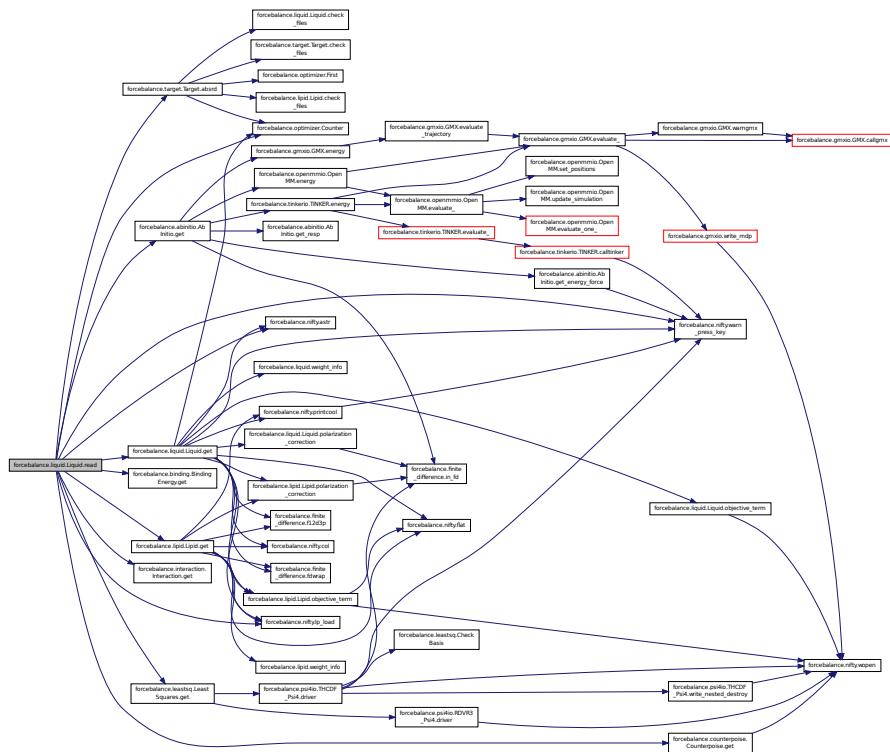
Here is the call graph for this function:



def forcebalance.liquid.Liquid.read (self, mvals, AGrad = True, AHess = True) [inherited] Read in time series for all previous iterations.

Definition at line 447 of file liquid.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.read_0grads ( self ) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.
```

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.liquid.Liquid.read_data (self) [inherited] Definition at line 162 of file liquid.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

```
def forcebalance.BaseClass.set_option( self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

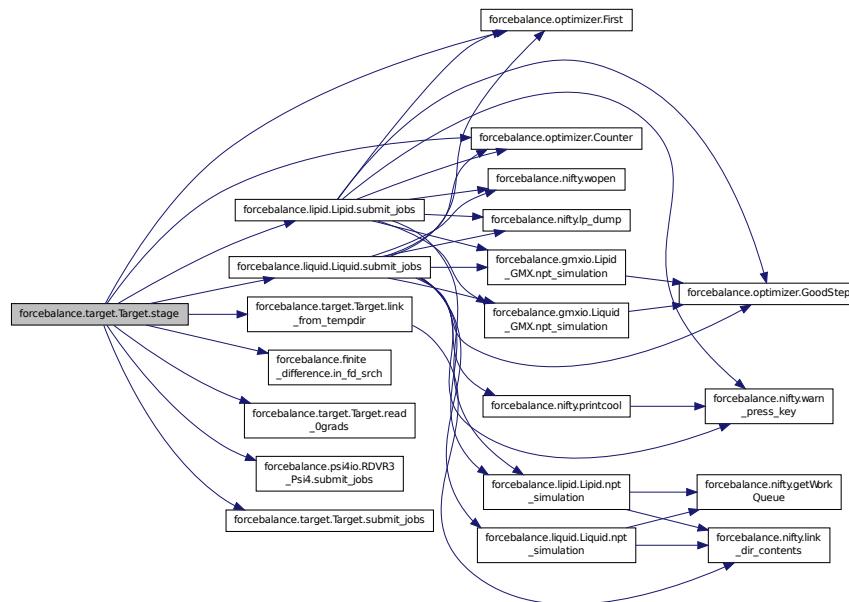
```
def forcebalance.target.Target.stage ( self, mvals, AGrad = False, AHess = False, customdir = None ) [inherited]
```

Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

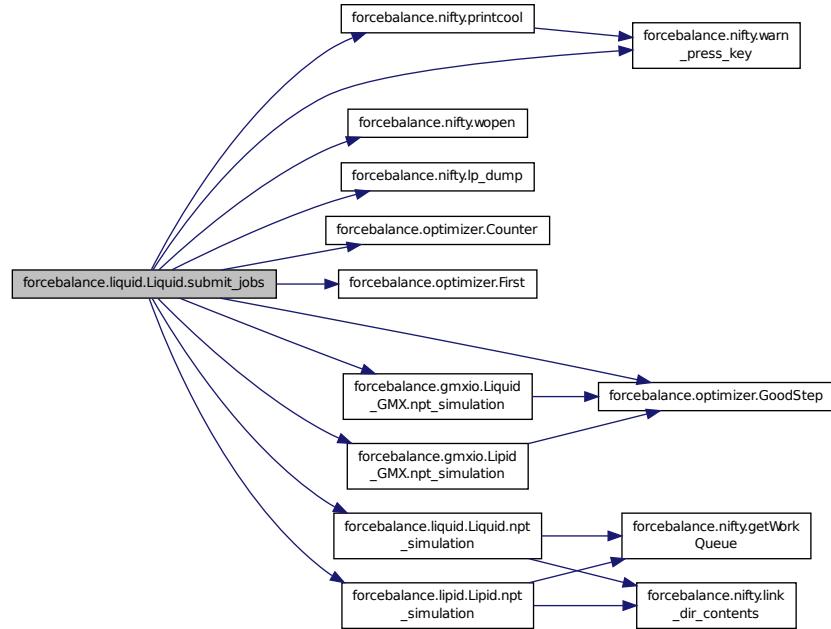
Here is the call graph for this function:



```
def forcebalance.liquid.Liquid.submit_jobs ( self, mvals, AGrad = True, AHess = True ) [inherited]
```

Definition at line 409 of file liquid.py.

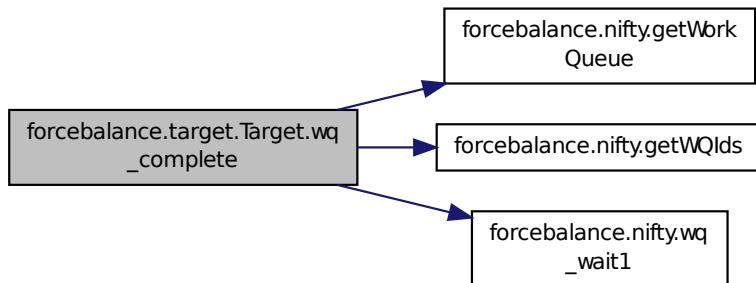
Here is the call graph for this function:



def forcebalance.target.Target.wq_complete(self) [inherited] This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_Ograds(self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.37.4 Member Data Documentation

forcebalance.liquid.Liquid.AllResults [inherited] Saved results for all iterations self.SavedMVals = [].
Definition at line 151 of file liquid.py.

forcebalance.liquid.Liquid.do_self_pol [inherited] Definition at line 98 of file liquid.py.

forcebalance.tinkerio.Liquid_TINKER.DynDict Definition at line 1047 of file tinkerio.py.

forcebalance.tinkerio.Liquid_TINKER.DynDict_New Definition at line 1048 of file tinkerio.py.

forcebalance.tinkerio.Liquid_TINKER.engine_ Definition at line 1025 of file tinkerio.py.

forcebalance.tinkerio.Liquid_TINKER.engname Definition at line 1027 of file tinkerio.py.

forcebalance.tinkerio.Liquid_TINKER.extra_output Definition at line 1043 of file tinkerio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.liquid.Liquid.gas_engine [inherited] Read the reference data.
Definition at line 133 of file liquid.py.

forcebalance.tinkerio.Liquid_TINKER.gas_engine_args Definition at line 1033 of file tinkerio.py.

forcebalance.liquid.Liquid.gas_mol [inherited] Definition at line 114 of file liquid.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.liquid.Liquid.Gp [inherited] Definition at line 895 of file liquid.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.liquid.Liquid.Labels [inherited] Definition at line 243 of file liquid.py.

forcebalance.tinkerio.Liquid_TINKER.last_traj Definition at line 1063 of file tinkerio.py.

forcebalance.liquid.Liquid.liquid_mol [inherited] Definition at line 110 of file liquid.py.

forcebalance.liquid.Liquid.MBarEnergy [inherited] Evaluated energies for all trajectories (i.e.
all iterations and all temperatures), using all mvals
Definition at line 148 of file liquid.py.

forcebalance.tinkerio.Liquid_TINKER.nptfiles Definition at line 1031 of file tinkerio.py.

forcebalance.tinkerio.Liquid_TINKER.nptpfx Definition at line 1029 of file tinkerio.py.

forcebalance.liquid.Liquid.Objective [inherited] Definition at line 897 of file liquid.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.liquid.Liquid.PhasePoints [inherited] Definition at line 239 of file liquid.py.

forcebalance.liquid.Liquid.Pp [inherited] Definition at line 892 of file liquid.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.liquid.Liquid.read_indicate [inherited] Definition at line 135 of file liquid.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.liquid.Liquid.RefData [inherited] Definition at line 173 of file liquid.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.liquid.Liquid.SavedTraj [inherited] Saved trajectories for all iterations and all temperatures.

Definition at line 146 of file liquid.py.

forcebalance.tinkerio.Liquid_TINKER.scripts Definition at line 1035 of file tinkerio.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.liquid.Liquid.w_alpha [inherited] Definition at line 868 of file liquid.py.

forcebalance.liquid.Liquid.w_cp [inherited] Definition at line 870 of file liquid.py.

forcebalance.liquid.Liquid.w_eps0 [inherited] Definition at line 871 of file liquid.py.

forcebalance.liquid.Liquid.w_hvap [inherited] Definition at line 867 of file liquid.py.

forcebalance.liquid.Liquid.w_kappa [inherited] Definition at line 869 of file liquid.py.

forcebalance.liquid.Liquid.w_rho [inherited] Density.
Enthalpy of vaporization. Thermal expansion coefficient. Isothermal compressibility. Isobaric heat capacity. Static dielectric constant. Estimation of errors.
Definition at line 866 of file liquid.py.

forcebalance.liquid.Liquid.Wp [inherited] Definition at line 890 of file liquid.py.

forcebalance.liquid.Liquid.write_indicate [inherited] Definition at line 136 of file liquid.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)
Definition at line 174 of file target.py.

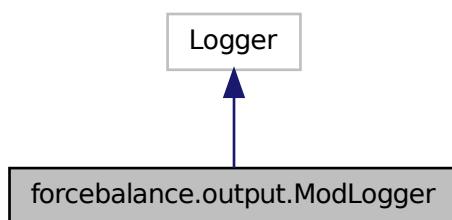
forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.
Definition at line 162 of file target.py.

forcebalance.liquid.Liquid.Xp [inherited] Definition at line 888 of file liquid.py.
The documentation for this class was generated from the following file:

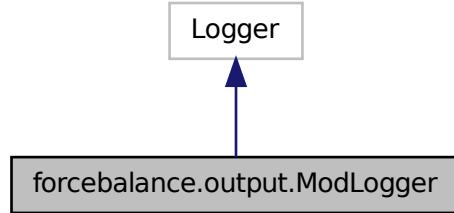
- [tinkerio.py](#)

8.38 forcebalance.output.ModLogger Class Reference

Inheritance diagram for forcebalance.output.ModLogger:



Collaboration diagram for forcebalance.output.ModLogger:



Public Member Functions

- def [error](#)

8.38.1 Detailed Description

Definition at line 82 of file output.py.

8.38.2 Member Function Documentation

def forcebalance.output.ModLogger.error (self, msg, args, kwargs) Definition at line 83 of file output.py.

The documentation for this class was generated from the following file:

- [output.py](#)

8.39 forcebalance.Mol2.mol2 Class Reference

This is to manage one [mol2](#) series of lines on the form:

Public Member Functions

- def [__init__](#)
- def [__repr__](#)
- def [out](#)
- def [set_mol_name](#)
 bond identifier (integer, starting from 1)
- def [set_num_atoms](#)
 number of atoms (integer)
- def [set_num_bonds](#)
 number of bonds (integer)
- def [set_num_subst](#)
 number of substructures (integer)
- def [set_num_feat](#)
 number of features (integer)
- def [set_num_sets](#)

- def `set_mol_type`
`bond identifier (integer, starting from 1)`
- def `set_charge_type`
`bond identifier (integer, starting from 1)`
- def `parse`
`Parse a series of text lines, and setup compound information.`
- def `get_atom`
`return the atom instance given its atom identifier`
- def `get_bonded_atoms`
`return a dictionary of atom instances bonded to the atom, and their types`
- def `set_donor_acceptor_atoms`
`modify atom types to specify donor, acceptor, or both`

Public Attributes

- `mol_name`
- `num_atoms`
- `num_bonds`
- `num_subst`
- `num_feat`
- `num_sets`
- `mol_type`
- `charge_type`
- `comments`
- `atoms`
- `bonds`

8.39.1 Detailed Description

This is to manage one `mol2` series of lines on the form:

```
@<TRIPOS>MOLECULE
CDK2.xray.inhl.1E9H
34 37 0 0 0
SMALL
GASTEIGER
Energy = 0

@<TRIPOS>ATOM
 1 C1          5.4790   42.2880   49.5910 C.ar     1  <1>      0.0424
 2 C2          4.4740   42.6430   50.5070 C.ar     1  <1>      0.0447
@<TRIPOS>BOND
 1    1    2    ar
 2    1    6    ar
```

Definition at line 288 of file Mol2.py.

8.39.2 Constructor & Destructor Documentation

`def forcebalance.Mol2.mol2.__init__ (self, data)` Definition at line 289 of file Mol2.py.

8.39.3 Member Function Documentation

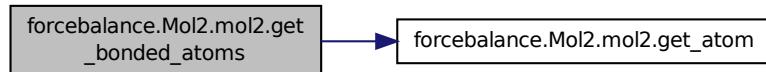
`def forcebalance.Mol2.mol2.__repr__ (self)` Definition at line 305 of file Mol2.py.

```
def forcebalance.Mol2.mol2.get_atom( self, id )  return the atom instance given its atom identifier  
Definition at line 461 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2.get_bonded_atoms( self, id )  return a dictionary of atom instances bonded to the  
atom, and their types
```

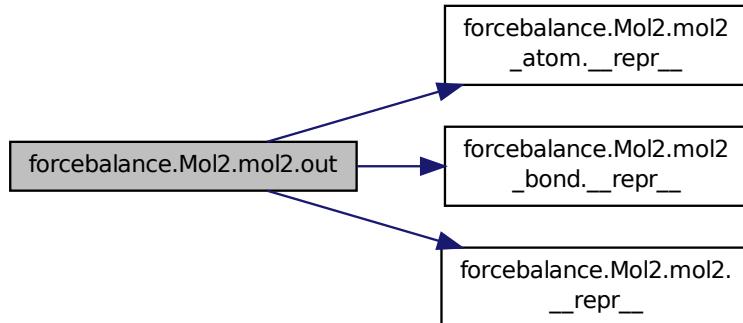
Definition at line 475 of file Mol2.py.

Here is the call graph for this function:



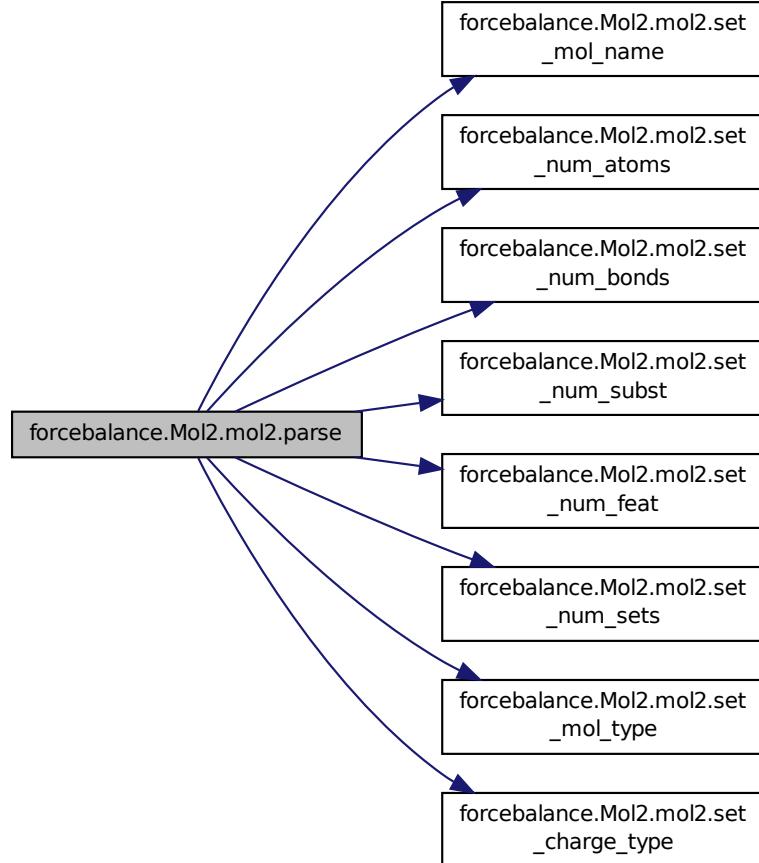
```
def forcebalance.Mol2.mol2.out( self, f=sys.stdout )  Definition at line 325 of file Mol2.py.
```

Here is the call graph for this function:



```
def forcebalance.Mol2.mol2.parse( self, data )  Parse a series of text lines, and setup compound information.  
Definition at line 405 of file Mol2.py.
```

Here is the call graph for this function:



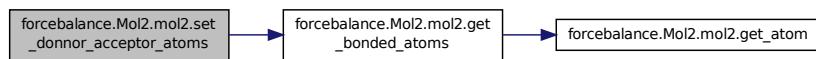
```
def forcebalance.Mol2.mol2.set_charge_type ( self, charge_type = None ) bond identifier (integer, starting from 1)
```

Definition at line 395 of file Mol2.py.

```
def forcebalance.Mol2.mol2.set_donor_acceptor_atoms ( self, verbose = 0 ) modify atom types to specify donor, acceptor, or both
```

Definition at line 490 of file Mol2.py.

Here is the call graph for this function:



```
def forcebalance.Mol2.mol2.set.mol_name ( self, mol_name = None ) bond identifier (integer, starting from 1)
Definition at line 332 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2.set.mol_type ( self, mol_type = None ) bond identifier (integer, starting from 1)
Definition at line 386 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2.set.num_atoms ( self, num_atoms = None ) number of atoms (integer)
Definition at line 341 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2.set.num_bonds ( self, num_bonds = None ) number of bonds (integer)
Definition at line 350 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2.set.num_feat ( self, num_feat = None ) number of features (integer)
Definition at line 368 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2.set.num_sets ( self, num_sets = None ) number of sets (integer)
Definition at line 377 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2.set.num_subst ( self, num_subst = None ) number of substructures (integer)
Definition at line 359 of file Mol2.py.
```

8.39.4 Member Data Documentation

forcebalance.Mol2.mol2.atoms Definition at line 300 of file Mol2.py.

forcebalance.Mol2.mol2.bonds Definition at line 301 of file Mol2.py.

forcebalance.Mol2.mol2.charge_type Definition at line 297 of file Mol2.py.

forcebalance.Mol2.mol2.comments Definition at line 298 of file Mol2.py.

forcebalance.Mol2.mol2.mol_name Definition at line 290 of file Mol2.py.

forcebalance.Mol2.mol2.mol_type Definition at line 296 of file Mol2.py.

forcebalance.Mol2.mol2.num_atoms Definition at line 291 of file Mol2.py.

forcebalance.Mol2.mol2.num_bonds Definition at line 292 of file Mol2.py.

forcebalance.Mol2.mol2.num_feat Definition at line 294 of file Mol2.py.

forcebalance.Mol2.mol2.num_sets Definition at line 295 of file Mol2.py.

forcebalance.Mol2.mol2.num_subst Definition at line 293 of file Mol2.py.
The documentation for this class was generated from the following file:

- [Mol2.py](#)

8.40 forcebalance.Mol2.mol2_atom Class Reference

This is to manage [mol2](#) atomic lines on the form: 1 C1 5.4790 42.2880 49.5910 C.ar 1 <1> 0.0424.

Public Member Functions

- def `_init_`
if data is passed, it will be installed
- def `parse`
split the text line into a series of properties
- def `_repr_`
assemble the properties as a text line, and return it
- def `set_atom_id`
atom identifier (integer, starting from 1)
- def `set_atom_name`
The name of the atom (string)
- def `set_crds`
the coordinates of the atom
- def `set_atom_type`
The mol2 type of the atom.
- def `set_subst_id`
substructure identifier
- def `set_subst_name`
substructure name
- def `set_charge`
atomic charge
- def `set_status_bit`
Never to use (in theory)

Public Attributes

- `atom_id`
- `atom_name`
- `x`
- `y`
- `z`
- `atom_type`
- `subst_id`
- `subst_name`
- `charge`
- `status_bit`

8.40.1 Detailed Description

This is to manage mol2 atomic lines on the form: 1 C1 5.4790 42.2880 49.5910 C.ar 1 <1> 0.0424.
Definition at line 32 of file Mol2.py.

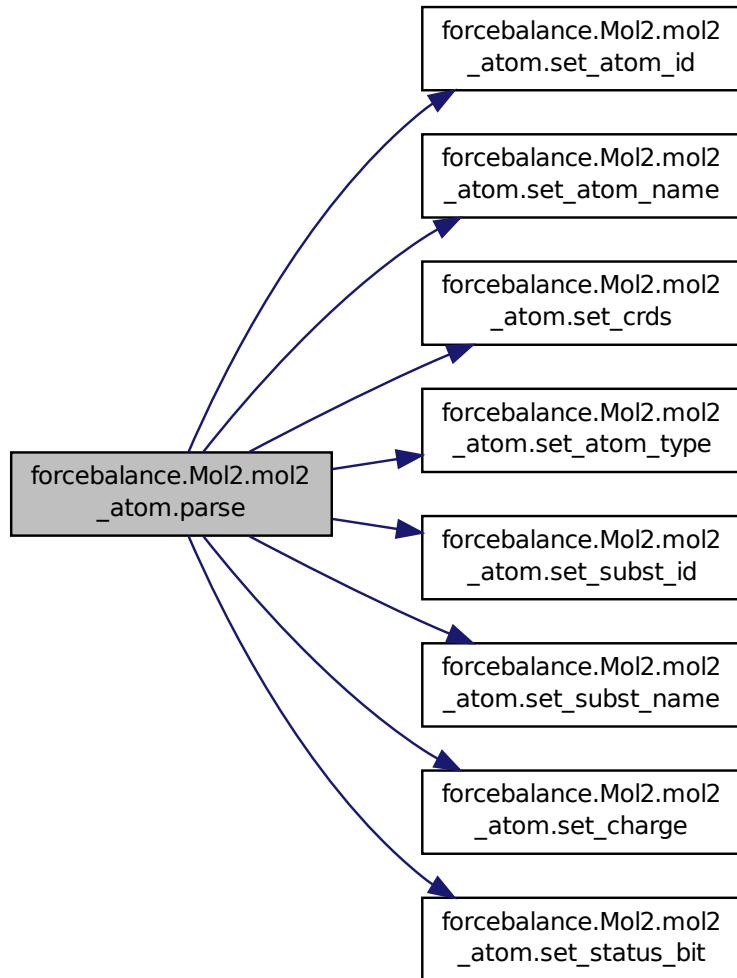
8.40.2 Constructor & Destructor Documentation

`def forcebalance.Mol2.mol2_atom.__init__(self, data = None)` if data is passed, it will be installed
Definition at line 37 of file Mol2.py.

8.40.3 Member Function Documentation

`def forcebalance.Mol2.mol2_atom.__repr__(self)` assemble the properties as a text line, and return it
Definition at line 78 of file Mol2.py.

```
def forcebalance.Mol2.mol2_atom.parse( self, data ) split the text line into a series of properties
Definition at line 56 of file Mol2.py.
Here is the call graph for this function:
```



```
def forcebalance.Mol2.mol2_atom.set_atom_id( self, atom_id = None ) atom identifier (integer, starting from 1)
Definition at line 90 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2_atom.set_atom_name( self, atom_name = None ) The name of the atom (string)
Definition at line 99 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2_atom.set_atom_type( self, atom_type = None ) The mol2 type of the atom.
Definition at line 119 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2_atom.set_charge( self, charge = None ) atomic charge
Definition at line 146 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2_atom.set_crds( self, x = None, y = None, z = None ) the coordinates of the
atom
Definition at line 108 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2_atom.set_status_bit( self, status_bit = None ) Never to use (in theory)
Definition at line 155 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2_atom.set_subst_id( self, subst_id = None ) substructure identifier
Definition at line 128 of file Mol2.py.
```

```
def forcebalance.Mol2.mol2_atom.set_subst_name( self, subst_name = None ) substructure name
Definition at line 137 of file Mol2.py.
```

8.40.4 Member Data Documentation

forcebalance.Mol2.mol2_atom.atom_id Definition at line 38 of file Mol2.py.

forcebalance.Mol2.mol2_atom.atom_name Definition at line 39 of file Mol2.py.

forcebalance.Mol2.mol2_atom.atom_type Definition at line 43 of file Mol2.py.

forcebalance.Mol2.mol2_atom.charge Definition at line 46 of file Mol2.py.

forcebalance.Mol2.mol2_atom.status_bit Definition at line 47 of file Mol2.py.

forcebalance.Mol2.mol2_atom.subst_id Definition at line 44 of file Mol2.py.

forcebalance.Mol2.mol2_atom.subst_name Definition at line 45 of file Mol2.py.

forcebalance.Mol2.mol2_atom.x Definition at line 40 of file Mol2.py.

forcebalance.Mol2.mol2_atom.y Definition at line 41 of file Mol2.py.

forcebalance.Mol2.mol2_atom.z Definition at line 42 of file Mol2.py.

The documentation for this class was generated from the following file:

- [Mol2.py](#)

8.41 forcebalance.Mol2.mol2_bond Class Reference

This is to manage mol2 bond lines on the form: 1 1 2 ar.

Public Member Functions

- def `__init__`
if data is passed, it will be installed
- def `__repr__`
- def `parse`
split the text line into a series of properties
- def `set_bond_id`
bond identifier (integer, starting from 1)
- def `set_origin_atom_id`
the origin atom identifier (integer)
- def `set_target_atom_id`
the target atom identifier (integer)
- def `set_bond_type`
bond type (string) one of: 1 = single 2 = double 3 = triple am = amide ar = aromatic du = dummy un = unknown nc = not connected
- def `set_status_bit`
Never to use (in theory)

Public Attributes

- `bond_id`
- `origin_atom_id`
- `target_atom_id`
- `bond_type`
- `status_bit`

8.41.1 Detailed Description

This is to manage mol2 bond lines on the form: 1 1 2 ar.

Definition at line 172 of file Mol2.py.

8.41.2 Constructor & Destructor Documentation

`def forcebalance.Mol2.mol2_bond.__init__(self, data = None)` if data is passed, it will be installed

Definition at line 177 of file Mol2.py.

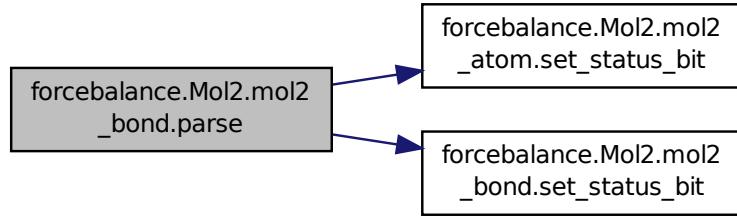
8.41.3 Member Function Documentation

`def forcebalance.Mol2.mol2_bond.__repr__(self)` Definition at line 186 of file Mol2.py.

`def forcebalance.Mol2.mol2_bond.parse(self, data)` split the text line into a series of properties

Definition at line 197 of file Mol2.py.

Here is the call graph for this function:



def forcebalance.Mol2.mol2.bond.set_bond_id (self, bond_id = None) bond identifier (integer, starting from 1)
Definition at line 214 of file Mol2.py.

def forcebalance.Mol2.mol2.bond.set_bond_type (self, bond_type = None) bond type (string) one of: 1 = single 2 = double 3 = triple am = amide ar = aromatic du = dummy un = unknown nc = not connected
Definition at line 250 of file Mol2.py.

def forcebalance.Mol2.mol2.bond.set_origin_atom_id (self, origin_atom_id = None) the origin atom identifier (integer)
Definition at line 223 of file Mol2.py.

def forcebalance.Mol2.mol2.bond.set_status_bit (self, status_bit = None) Never to use (in theory)
Definition at line 259 of file Mol2.py.

def forcebalance.Mol2.mol2.bond.set_target_atom_id (self, target_atom_id = None) the target atom identifier (integer)
Definition at line 232 of file Mol2.py.

8.41.4 Member Data Documentation

forcebalance.Mol2.mol2.bond.bond_id Definition at line 178 of file Mol2.py.

forcebalance.Mol2.mol2.bond.bond_type Definition at line 181 of file Mol2.py.

forcebalance.Mol2.mol2.bond.origin_atom_id Definition at line 179 of file Mol2.py.

forcebalance.Mol2.mol2.bond.status_bit Definition at line 206 of file Mol2.py.

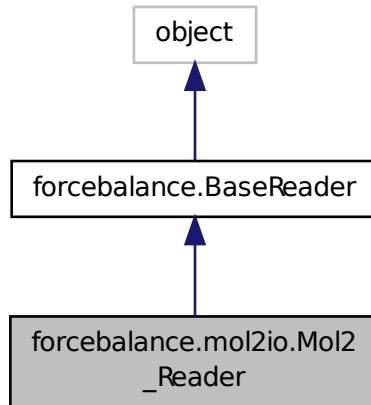
forcebalance.Mol2.mol2.bond.target_atom_id Definition at line 180 of file Mol2.py.
The documentation for this class was generated from the following file:

- [Mol2.py](#)

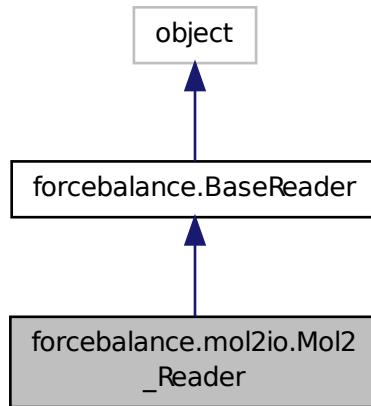
8.42 forcebalance.mol2io.Mol2_Reader Class Reference

Finite state machine for parsing Mol2 force field file.

Inheritance diagram for forcebalance.mol2io.Mol2_Reader:



Collaboration diagram for forcebalance.mol2io.Mol2_Reader:



Public Member Functions

- def `__init__`
- def `feed`
- def `Split`

- def [Whites](#)
- def [build_pid](#)
Returns the parameter type (e.g.

Public Attributes

- [pdict](#)
The parameter dictionary (defined in this file)
- [atom](#)
The atom numbers in the interaction (stored in the parser)
- [itype](#)
- [suffix](#)
- [ln](#)
- [adict](#)
The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.
- [molatom](#)
The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.
- [Molecules](#)
- [AtomTypes](#)

8.42.1 Detailed Description

Finite state machine for parsing [Mol2](#) force field file.
(just for parameterizing the charges)
Definition at line 22 of file mol2io.py.

8.42.2 Constructor & Destructor Documentation

def forcebalance.mol2io.Mol2_Reader.__init__ (self, fnm) Definition at line 24 of file mol2io.py.

8.42.3 Member Function Documentation

def forcebalance.BaseReader.build_pid (self, pfid) [inherited] Returns the parameter type (e.g. K in BONDSK) based on the current interaction type.
Both the 'pdict' dictionary (see [gmxio.pdict](#)) and the interaction type 'state' (here, BONDS) are needed to get the parameter type.
If, however, 'pdict' does not contain the ptype value, a suitable substitute is simply the field number.
Note that if the interaction type state is not set, then it defaults to the file name, so a generic parameter ID is 'filename.line_num.field_num'
Definition at line 124 of file __init__.py.

def forcebalance.mol2io.Mol2_Reader.feed (self, line) Definition at line 32 of file mol2io.py.

def forcebalance.BaseReader.Split (self, line) [inherited] Definition at line 99 of file __init__.py.

def forcebalance.BaseReader.Whites (self, line) [inherited] Definition at line 102 of file __init__.py.

8.42.4 Member Data Documentation

forcebalance.BaseReader.adict [inherited] The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.
Definition at line 89 of file __init__.py.

forcebalance.mol2io.Mol2_Reader.atom The atom numbers in the interaction (stored in the parser)
Definition at line 30 of file mol2io.py.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file __init__.py.

forcebalance.mol2io.Mol2_Reader.itype Definition at line 36 of file mol2io.py.

forcebalance.BaseReader.In [inherited] Definition at line 84 of file __init__.py.

forcebalance.BaseReader.molatom [inherited] The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

self.molecdict = OrderedDict() The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.

Definition at line 94 of file __init__.py.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file __init__.py.

forcebalance.mol2io.Mol2_Reader.pdict The parameter dictionary (defined in this file)

Definition at line 28 of file mol2io.py.

forcebalance.mol2io.Mol2_Reader.suffix Definition at line 44 of file mol2io.py.

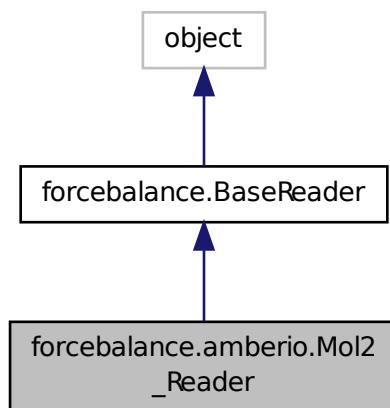
The documentation for this class was generated from the following file:

- [mol2io.py](#)

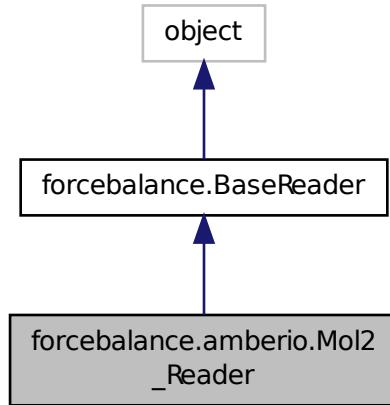
8.43 forcebalance.amberio.Mol2_Reader Class Reference

Finite state machine for parsing Mol2 force field file.

Inheritance diagram for forcebalance.amberio.Mol2_Reader:



Collaboration diagram for forcebalance.amberio.Mol2_Reader:



Public Member Functions

- def `_init_`
- def `feed`
- def `Split`
- def `Whites`
- def `build_pid`

Returns the parameter type (e.g.

Public Attributes

- `pdict`
The parameter dictionary (defined in this file)
- `atom`
The atom numbers in the interaction (stored in the parser)
- `atomnames`
The mol2 file provides a list of atom names.
- `section`
The section that we're in.
- `mol`
- `itype`
- `suffix`
- `molatom`
- `In`
- `adict`
The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.
- `Molecules`
- `AtomTypes`

8.43.1 Detailed Description

Finite state machine for parsing Mol2 force field file.
(just for parameterizing the charges)
Definition at line 43 of file amberio.py.

8.43.2 Constructor & Destructor Documentation

def forcebalance.amberio.Mol2_Reader.__init__ (self, fnm) Definition at line 45 of file amberio.py.

8.43.3 Member Function Documentation

def forcebalance.BaseReader.build_pid (self, pfd) [inherited] Returns the parameter type (e.g. K in BONDSK) based on the current interaction type.
Both the 'pdict' dictionary (see gmlio.pdict) and the interaction type 'state' (here, BONDS) are needed to get the parameter type.
If, however, 'pdict' does not contain the ptype value, a suitable substitute is simply the field number.
Note that if the interaction type state is not set, then it defaults to the file name, so a generic parameter ID is 'filename.line.num.field.num'
Definition at line 124 of file __init__.py.

def forcebalance.amberio.Mol2_Reader.feed (self, line) Definition at line 59 of file amberio.py.

def forcebalance.BaseReader.Split (self, line) [inherited] Definition at line 99 of file __init__.py.

def forcebalance.BaseReader.Whites (self, line) [inherited] Definition at line 102 of file __init__.py.

8.43.4 Member Data Documentation

forcebalance.BaseReader.adict [inherited] The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.
Definition at line 89 of file __init__.py.

forcebalance.amberio.Mol2_Reader.atom The atom numbers in the interaction (stored in the parser)
Definition at line 51 of file amberio.py.

forcebalance.amberio.Mol2_Reader.atomnames The mol2 file provides a list of atom names.
Definition at line 53 of file amberio.py.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file __init__.py.

forcebalance.amberio.Mol2_Reader.itype Definition at line 64 of file amberio.py.

forcebalance.BaseReader.In [inherited] Definition at line 84 of file __init__.py.

forcebalance.amberio.Mol2_Reader.mol Definition at line 57 of file amberio.py.

forcebalance.amberio.Mol2_Reader.molatom Definition at line 95 of file amberio.py.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file __init__.py.

forcebalance.amberio.Mol2.Reader.pdict The parameter dictionary (defined in this file)
Definition at line 49 of file amberio.py.

forcebalance.amberio.Mol2.Reader.section The section that we're in.
Definition at line 55 of file amberio.py.

forcebalance.amberio.Mol2.Reader.suffix Definition at line 93 of file amberio.py.
The documentation for this class was generated from the following file:

- [amberio.py](#)

8.44 forcebalance.Mol2.mol2_set Class Reference

Public Member Functions

- def [__init__](#)

A collection is organized as a dictionnary of compounds self.num_compounds : the number of compounds self.compounds : the dictionnary of compounds data : the data to setup the set subset: it is possible to specify a subset of the compounds to load, based on their mol.name identifiers.

- def [parse](#)

parse a list of lines, detect compounds, load them only load the subset if specified.

Public Attributes

- [num_compounds](#)
- [comments](#)
- [compounds](#)

8.44.1 Detailed Description

Definition at line 568 of file Mol2.py.

8.44.2 Constructor & Destructor Documentation

def forcebalance.Mol2.mol2_set.__init__ (self, data = None, subset = None) A collection is organized as a dictionnary of compounds self.num_compounds : the number of compounds self.compounds : the dictionnary of compounds data : the data to setup the set subset: it is possible to specify a subset of the compounds to load, based on their mol.name identifiers.

Definition at line 577 of file Mol2.py.

8.44.3 Member Function Documentation

def forcebalance.Mol2.mol2_set.parse (self, data, subset = None) parse a list of lines, detect compounds, load them only load the subset if specified.

Definition at line 621 of file Mol2.py.

8.44.4 Member Data Documentation

forcebalance.Mol2.mol2_set.comments Definition at line 579 of file Mol2.py.

forcebalance.Mol2.mol2_set.compounds Definition at line 580 of file Mol2.py.

forcebalance.Mol2.mol2.set.num_compounds Definition at line 578 of file Mol2.py.

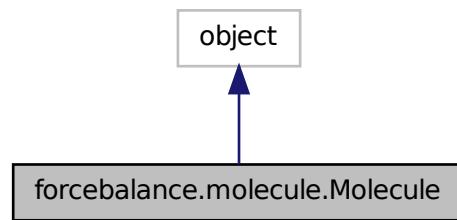
The documentation for this class was generated from the following file:

- [Mol2.py](#)

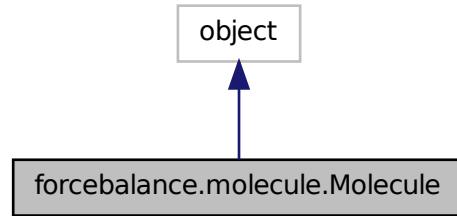
8.45 forcebalance.molecule.Molecule Class Reference

Lee-Ping's general file format conversion class.

Inheritance diagram for forcebalance.molecule.Molecule:



Collaboration diagram for forcebalance.molecule.Molecule:



Public Member Functions

- def [__len__](#)
Return the number of frames in the trajectory.
- def [__getattr__](#)
Whenever we try to get a class attribute, it first tries to get the attribute from the Data dictionary.
- def [__setattr__](#)
Whenever we try to get a class attribute, it first tries to get the attribute from the Data dictionary.
- def [__getitem__](#)
The [Molecule](#) class has list-like behavior, so we can get slices of it.

- def `__delitem__`
`Similarly, in order to delete a frame, we simply perform item deletion on framewise variables.`
- def `__iter__`
`List-like behavior for looping over trajectories.`
- def `_add__`
`Add method for Molecule objects.`
- def `_iadd__`
`Add method for Molecule objects.`
- def `repair`
`Attempt to repair trivial issues that would otherwise break the object.`
- def `append`
- def `__init__`
`To create the Molecule object, we simply define the table of file reading/writing functions and read in a file if it is provided.`
- def `require`
- def `write`
- def `center_of_mass`
- def `radius_of_gyration`
- def `rigid_water`
`If one atom is oxygen and the next two are hydrogen, make the water molecule rigid.`
- def `load_frames`
- def `edit_qcrems`
`Edit Q-Chem rem variables with a dictionary.`
- def `add_quantum`
- def `add_virtual_site`
`Add a virtual site to the system.`
- def `replace_peratom`
`Replace all of the data for a certain attribute in the system from orig to want.`
- def `replace_peratom_conditional`
`Replace all of the data for a attribute key2 from orig to want, contingent on key1 being equal to cond.`
- def `atom_select`
`Return a copy of the object with certain atoms selected.`
- def `atom_stack`
`Return a copy of the object with another molecule object appended.`
- def `align_by_moments`
`Align molecules using the moment of inertia.`
- def `align`
`Align molecules.`
- def `build_topology`
`A bare-bones implementation of the bond graph capability in the nanoreactor code.`
- def `find_angles`
`Return a list of 3-tuples corresponding to all of the angles in the system.`
- def `find_dihedrals`
`Return a list of 4-tuples corresponding to all of the dihedral angles in the system.`
- def `measure_dihedrals`
`Return a series of dihedral angles, given four atom indices numbered from zero.`
- def `all_pairwise_rmsd`
`Find pairwise RMSD (super slow, not like the one in MSMBuilder.)`

- def `pathwise_rmsd`
Find RMSD between frames along path.
- def `ref_rmsd`
Find RMSD to a reference frame.
- def `align_center`
- def `openmm_positions`
Returns the Cartesian coordinates in the `Molecule` object in a list of OpenMM-compatible positions, so it is possible to type `simulation.context.setPositions(Mol.openmm_positions()[0])` or something like that.
- def `openmm_boxes`
Returns the periodic box vectors in the `Molecule` object in a list of OpenMM-compatible boxes, so it is possible to type `simulation.context.setPeriodicBoxVectors(Mol.openmm_boxes()[0])` or something like that.
- def `split`
Split the molecule object into a number of separate files (chunks), either by specifying the number of frames per chunk or the number of chunks.
- def `read_xyz`
.xyz files can be TINKER formatted which is why we have the try/except here.
- def `read_xyz0`
Parse a .xyz file which contains several xyz coordinates, and return their elements.
- def `read_mdcrd`
Parse an AMBER .mdcrd file.
- def `read_qdata`
- def `read_mol2`
- def `read_dcd`
- def `read_com`
Parse a Gaussian .com file and return a SINGLE-ELEMENT list of xyz coordinates (no multiple file support)
- def `read_arc`
Read a TINKER .arc file.
- def `read_gro`
Read a GROMACS .gro file.
- def `read_charmm`
Read a CHARMM .cor (or .crd) file.
- def `read_qcin`
Read a Q-Chem input file.
- def `read_pdb`
Loads a PDB and returns a dictionary containing its data.
- def `read_qcesp`
- def `read_qcout`
Q-Chem output file reader, adapted for our parser.
- def `write_qcin`
- def `write_xyz`
- def `write_molproq`
- def `write_mdcrd`
- def `write_arc`
- def `write_gro`
- def `write_dcd`
- def `write_pdb`
Save to a PDB.
- def `write_qdata`

Text quantum data format.

- def [require_resid](#)
- def [require_resname](#)
- def [require_boxes](#)

Public Attributes

- [Read_Tab](#)

The table of file readers.

- [Write_Tab](#)

The table of file writers.

- [Funnel](#)

A funnel dictionary that takes redundant file types and maps them down to a few.

- [positive_resid](#)

Creates entries like 'gromacs' : 'gromacs' and 'xyz' : 'xyz' in the Funnel.

- [built_bonds](#)

- [Data](#)

- [comms](#)

Read in stuff if we passed in a file name, otherwise return an empty instance.

- [topology](#)

Make sure the comment line isn't too long for i in range(len(self.comms)): self.comms[i] = self.comms[i][:-100] if len(self.comms[i]) > 100 else self.comms[i] Attempt to build the topology for small systems.

- [molecules](#)

- [fout](#)

Fill in comments.

- [resid](#)

- [resname](#)

- [boxes](#)

8.45.1 Detailed Description

Lee-Ping's general file format conversion class.

The purpose of this class is to read and write chemical file formats in a way that is convenient for research. There are highly general file format converters out there (e.g. catdcd, openbabel) but I find that writing my own class can be very helpful for specific purposes. Here are some things this class can do:

- Convert a .gro file to a .xyz file, or a .pdb file to a .dcd file. Data is stored internally, so any readable file can be converted into any writable file as long as there is sufficient information to write that file.
- Accumulate information from different files. For example, we may read A.gro to get a list of coordinates, add quantum settings from a B.in file, and write A.in (this gives us a file that we can use to run QM calculations)
- Concatenate two trajectories together as long as they're compatible. This is done by creating two [Molecule](#) objects and then simply adding them. Addition means two things: (1) Information fields missing from each class, but present in the other, are added to the sum, and (2) Appendable or per-frame fields (i.e. coordinates) are concatenated together.
- Slice trajectories using reasonable Python language. That is to say, MyMolecule[1:10] returns a new [Molecule](#) object that contains frames 1 through 9 (inclusive and numbered starting from zero.)

Next step: Read in Q-Chem output data using this too!

Special variables: These variables cannot be set manually because there is a special method associated with getting them.

na = The number of atoms. You'll get this if you use MyMol.na or MyMol['na']. na = The number of snapshots. You'll get this if you use MyMol.ns or MyMol['ns'].

Unit system: Angstroms.

Definition at line 691 of file molecule.py.

8.45.2 Constructor & Destructor Documentation

```
def forcebalance.molecule.Molecule.__init__( self, fnm = None, ftype = None, positive_resid = True, build_topology = True, kwargs )
```

To create the [Molecule](#) object, we simply define the table of file reading/writing functions and read in a file if it is provided.

Definition at line 896 of file molecule.py.

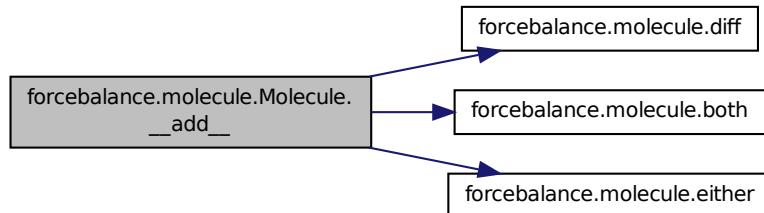
8.45.3 Member Function Documentation

```
def forcebalance.molecule.Molecule.__add__( self, other )
```

Add method for [Molecule](#) objects.

Definition at line 800 of file molecule.py.

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.__delitem__( self, key )
```

Similarly, in order to delete a frame, we simply perform item deletion on framewise variables.

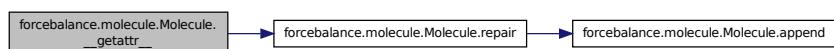
Definition at line 780 of file molecule.py.

```
def forcebalance.molecule.Molecule.__getattr__( self, key )
```

Whenever we try to get a class attribute, it first tries to get the attribute from the Data dictionary.

Definition at line 711 of file molecule.py.

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.__getitem__ ( self, key )
```

The `Molecule` class has list-like behavior, so we can get slices of it.

If we say `MyMolecule[0:10]`, then we'll return a copy of `MyMolecule` with frames 0 through 9.

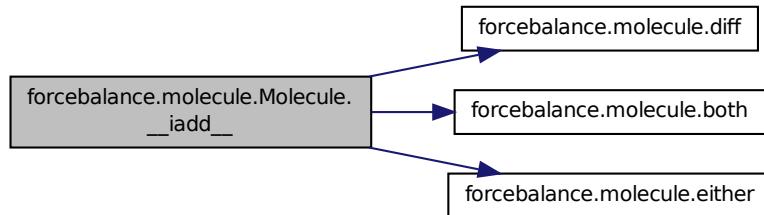
Definition at line 759 of file `molecule.py`.

```
def forcebalance.molecule.Molecule.__iadd__ ( self, other )
```

Add method for `Molecule` objects.

Definition at line 839 of file `molecule.py`.

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.__iter__ ( self )
```

List-like behavior for looping over trajectories.

Note that these values are returned by reference. Note that this is intended to be more efficient than `getitem`, so when we loop over a trajectory, it's best to go "for m in M" instead of "for i in range(len(M)): m = M[i]"

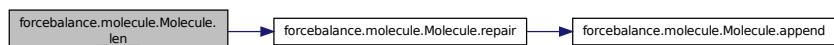
Definition at line 789 of file `molecule.py`.

```
def forcebalance.molecule.Molecule.__len__ ( self )
```

Return the number of frames in the trajectory.

Definition at line 695 of file `molecule.py`.

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.__setattr__ ( self, key, value )
```

Whenever we try to get a class attribute, it first tries to get the attribute from the Data dictionary.

Definition at line 747 of file `molecule.py`.

```
def forcebalance.molecule.Molecule.add_quantum ( self, other )
```

Definition at line 1125 of file `molecule.py`.

```
def forcebalance.molecule.Molecule.add_virtual_site ( self, idx, kwargs )
```

Add a virtual site to the system.

This does NOT set the position of the virtual site; it sits at the origin.

Definition at line 1137 of file `molecule.py`.

```
def forcebalance.molecule.Molecule.align( self, smooth = False, center = True, center_mass = False, select = None ) Align molecules.
```

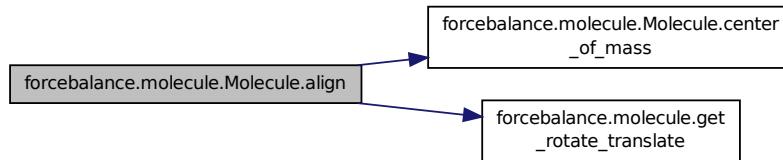
Has the option to create smooth trajectories (align each frame to the previous one) or to align each frame to the first one.

Also has the option to remove the center of mass.

Provide a list of atom indices to align along selected atoms.

Definition at line 1280 of file molecule.py.

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.align_by_moments( self ) Align molecules using the moment of inertia.
```

Departs from MSMBuilder convention of using arithmetic mean for mass.

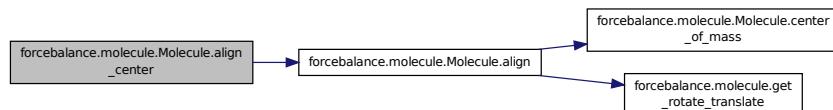
Definition at line 1258 of file molecule.py.

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.align_center( self ) Definition at line 1583 of file molecule.py.
```

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.all_pairwise_rmsd( self ) Find pairwise RMSD (super slow, not like the one in MSMBuilder.)
```

Definition at line 1534 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.append (self, other) Definition at line 889 of file molecule.py.

def forcebalance.molecule.Molecule.atom_select (self, atomslice) Return a copy of the object with certain atoms selected.

Takes an integer, list or array as argument.

Definition at line 1175 of file molecule.py.

def forcebalance.molecule.Molecule.atom_stack (self, other) Return a copy of the object with another molecule object appended.

WARNING: This function may invalidate stuff like QM energies.

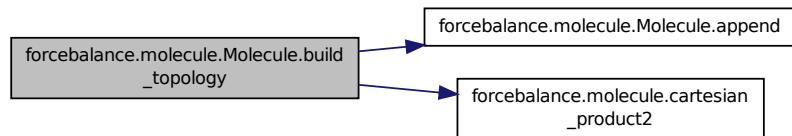
Definition at line 1214 of file molecule.py.

def forcebalance.molecule.Molecule.build_topology (self, sn = None, Fac = 1.2) A bare-bones implementation of the bond graph capability in the nanoreactor code.

Returns a NetworkX graph that depicts the molecular topology, which might be useful for stuff. Provide, optionally, the frame number used to compute the topology.

Definition at line 1310 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.center_of_mass (self) Definition at line 1042 of file molecule.py.

def forcebalance.molecule.Molecule.edit_qcrems (self, in_dict, subcalc = None) Edit Q-Chem rem variables with a dictionary.

Pass a value of None to delete a rem variable.

Definition at line 1110 of file molecule.py.

def forcebalance.molecule.Molecule.find_angles(self) Return a list of 3-tuples corresponding to all of the angles in the system.

Verified for lysine and tryptophan dipeptide when comparing to TINKER's analyze program.

Definition at line 1458 of file molecule.py.

def forcebalance.molecule.Molecule.find_dihedrals(self) Return a list of 4-tuples corresponding to all of the dihedral angles in the system.

Verified for alanine and tryptophan dipeptide when comparing to TINKER's analyze program.

Definition at line 1484 of file molecule.py.

def forcebalance.molecule.Molecule.load_frames(self, fnm) Definition at line 1101 of file molecule.py.

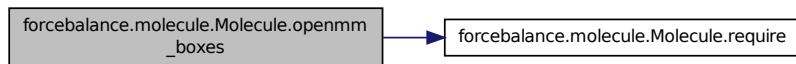
def forcebalance.molecule.Molecule.measure_dihedrals(self, i, j, k, l) Return a series of dihedral angles, given four atom indices numbered from zero.

Definition at line 1507 of file molecule.py.

def forcebalance.molecule.Molecule.openmm_boxes(self) Returns the periodic box vectors in the [Molecule](#) object in a list of OpenMM-compatible boxes, so it is possible to type simulation.context.setPeriodicBoxVectors(Mol.-openmm_boxes()[0]) or something like that.

Definition at line 1609 of file molecule.py.

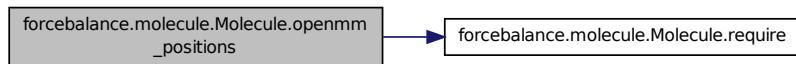
Here is the call graph for this function:



def forcebalance.molecule.Molecule.openmm_positions(self) Returns the Cartesian coordinates in the [Molecule](#) object in a list of OpenMM-compatible positions, so it is possible to type simulation.context.setPositions(Mol.-openmm_positions()[0]) or something like that.

Definition at line 1592 of file molecule.py.

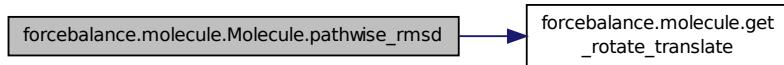
Here is the call graph for this function:



def forcebalance.molecule.Molecule.pathwise_rmsd(self) Find RMSD between frames along path.

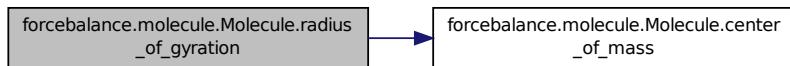
Definition at line 1552 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.radius_of_gyration (self) Definition at line 1046 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.read_arc (self, fnm, kwargs) Read a TINKER .arc file.

Parameters

in	fnm	The input file name
----	-----	---------------------

Returns

xyzs A list for the XYZ coordinates.

boxes A list of periodic boxes (newer .arc files have these)

resid The residue ID numbers. These are not easy to get!

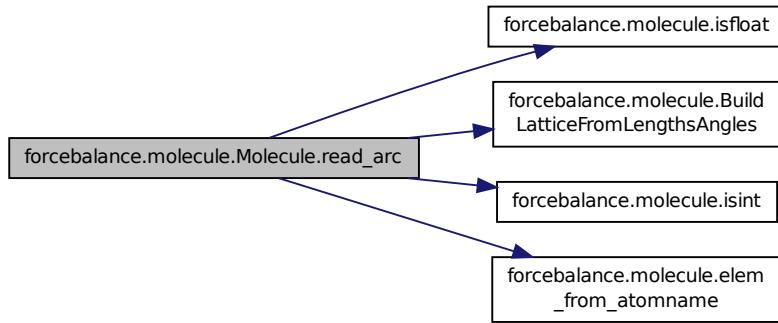
elem A list of chemical elements in the XYZ file

comms A single-element list for the comment.

tinkersuf The suffix that comes after lines in the XYZ coordinates; this is usually topology info

Definition at line 1898 of file molecule.py.

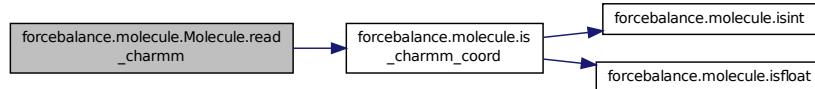
Here is the call graph for this function:



def forcebalance.molecule.Molecule.read_charmm (*self*, *fnm*, *kwargs*) Read a CHARMM .cor (or .crd) file.

Definition at line 2051 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.read_com (*self*, *fnm*, *kwargs*) Parse a Gaussian .com file and return a SINGLE-ELEMENT list of xyz coordinates (no multiple file support)

Parameters

in	<i>fnm</i>	The input file name
----	------------	---------------------

Returns

elem A list of chemical elements in the XYZ file

comms A single-element list for the comment.

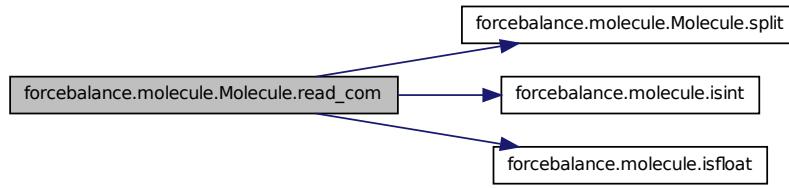
xyzs A single-element list for the XYZ coordinates.

charge The total charge of the system.

mult The spin multiplicity of the system.

Definition at line 1853 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.read_dcd (self, fnm, kwargs) Definition at line 1814 of file molecule.py.

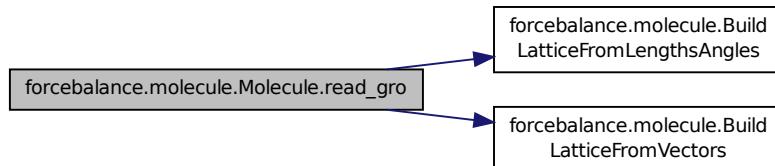
Here is the call graph for this function:



def forcebalance.molecule.Molecule.read_gro (self, fnm, kwargs) Read a GROMACS .gro file.

Definition at line 1971 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.read_mdcrd (self, fnm, kwargs) Parse an AMBER .mdcrd file.

This requires at least the number of atoms. This will FAIL for monatomic trajectories (but who the heck makes those?)

Parameters

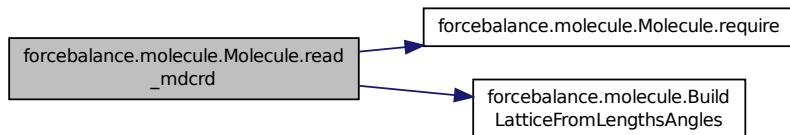
in	<i>fnm</i>	The input file name
----	------------	---------------------

Returns

xyzs A list of XYZ coordinates (number of snapshots times number of atoms)
boxes Boxes (if present.)

Definition at line 1704 of file molecule.py.

Here is the call graph for this function:

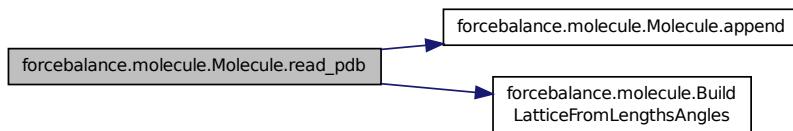


def forcebalance.molecule.Molecule.read_mol2 (self, fnm, kwargs) Definition at line 1765 of file molecule.py.

def forcebalance.molecule.Molecule.read_pdb (self, fnm, kwargs) Loads a PDB and returns a dictionary containing its data.

Definition at line 2237 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.read_qcesp (self, fnm, kwargs) Definition at line 2312 of file molecule.py.

Here is the call graph for this function:



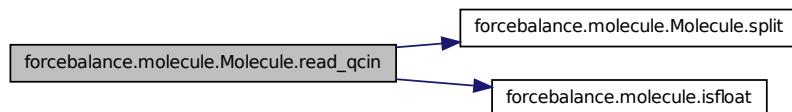
```
def forcebalance.molecule.Molecule.read_qcin( self, fnm, kwargs ) Read a Q-Chem input file.
```

These files can be very complicated, and I can't write a completely general parser for them. It is important to keep our goal in mind:

- 1) The main goal is to convert a trajectory to Q-Chem input files with identical calculation settings.
- 2) When we print the Q-Chem file, we should preserve the line ordering of the 'rem' section, but also be able to add 'rem' options at the end.
- 3) We should accommodate the use case that the Q-Chem file may have follow-up calculations delimited by '@@'.
- 4) We can read in all of the xyz's as a trajectory, but only the Q-Chem settings belonging to the first xyz will be saved.

Definition at line 2120 of file molecule.py.

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.read_qcout( self, fnm, errok = [], kwargs ) Q-Chem output file reader, adapted for our parser.
```

Q-Chem output files are very flexible and there's no way I can account for all of them. Here's what I am able to account for:

A list of:

- Coordinates
- Energies
- Forces

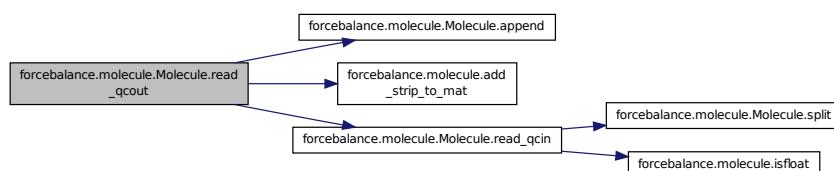
Calling with `errok` will proceed with reading file even if the specified error messages are encountered.

Note that each step in a geometry optimization counts as a frame.

As with all Q-Chem output files, note that successive calculations can have different numbers of atoms.

Definition at line 2344 of file molecule.py.

Here is the call graph for this function:

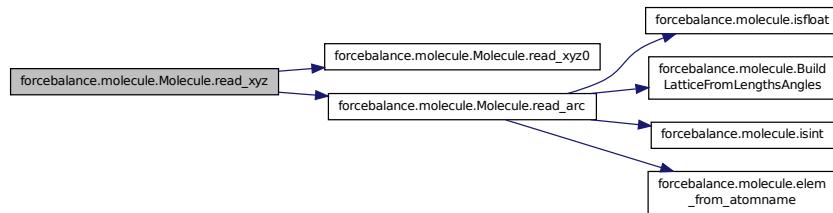


```
def forcebalance.molecule.Molecule.read_qdata( self, fnm, kwargs ) Definition at line 1729 of file molecule.py.
```

```
def forcebalance.molecule.Molecule.read_xyz( self, fnm, kwargs ) .xyz files can be TINKER formatted which  
is why we have the try/except here.
```

Definition at line 1642 of file molecule.py.

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.read_xyz0( self, fnm, kwargs ) Parse a .xyz file which contains several  
xyz coordinates, and return their elements.
```

Parameters

in	fnm	The input file name
----	-----	---------------------

Returns

elem A list of chemical elements in the XYZ file

comms A list of comments.

xyzs A list of XYZ coordinates (number of snapshots times number of atoms)

Definition at line 1657 of file molecule.py.

```
def forcebalance.molecule.Molecule.ref_rmsd( self, i ) Find RMSD to a reference frame.
```

Definition at line 1569 of file molecule.py.

Here is the call graph for this function:



```
def forcebalance.molecule.Molecule.repair( self, key, klast ) Attempt to repair trivial issues that would  
otherwise break the object.
```

Definition at line 874 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.replace_peratom (self, key, orig, want) Replace all of the data for a certain attribute in the system from orig to want.

Definition at line 1154 of file molecule.py.

def forcebalance.molecule.Molecule.replace_peratom_conditional (self, key1, cond, key2, orig, want)

Replace all of the data for a attribute key2 from orig to want, contingent on key1 being equal to cond.

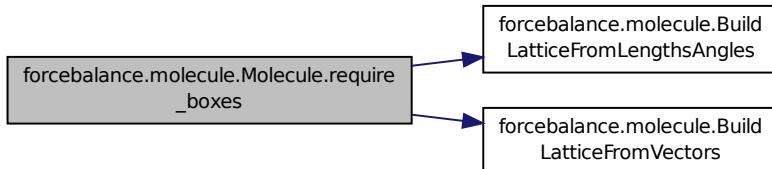
For instance: replace H1 with H2 if resname is SOL.

Definition at line 1165 of file molecule.py.

def forcebalance.molecule.Molecule.require (self, args) Definition at line 987 of file molecule.py.

def forcebalance.molecule.Molecule.require_boxes (self) Definition at line 2956 of file molecule.py.

Here is the call graph for this function:



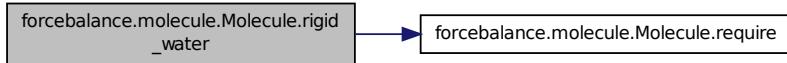
def forcebalance.molecule.Molecule.require_resid (self) Definition at line 2943 of file molecule.py.

def forcebalance.molecule.Molecule.require_resname (self) Definition at line 2951 of file molecule.py.

def forcebalance.molecule.Molecule.rigid_water (self) If one atom is oxygen and the next two are hydrogen, make the water molecule rigid.

Definition at line 1058 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.split (self, fnm = None, ftype = None, method = "chunks", num = None) Split the molecule object into a number of separate files (chunks), either by specifying the number of frames per chunk or the number of chunks.

Only relevant for "trajectories". The type of file may be specified; if they aren't specified then the original file type is used.

The output file names are [name].[numbers].[extension] where [name] can be specified by passing 'fnm' or taken from the object's 'fnm' attribute by default. [numbers] are integers ranging from the lowest to the highest chunk number, prepended by zeros.

If the number of chunks / frames is not specified, then one file is written for each frame.

Returns

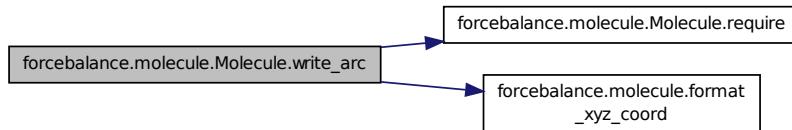
fnms A list of the file names that were written.

Definition at line 1632 of file molecule.py.

def forcebalance.molecule.Molecule.write (self, fnm = None, ftype = None, append = False, select = None, kwargs) Definition at line 1002 of file molecule.py.

def forcebalance.molecule.Molecule.write_arc (self, select, kwargs) Definition at line 2710 of file molecule.py.

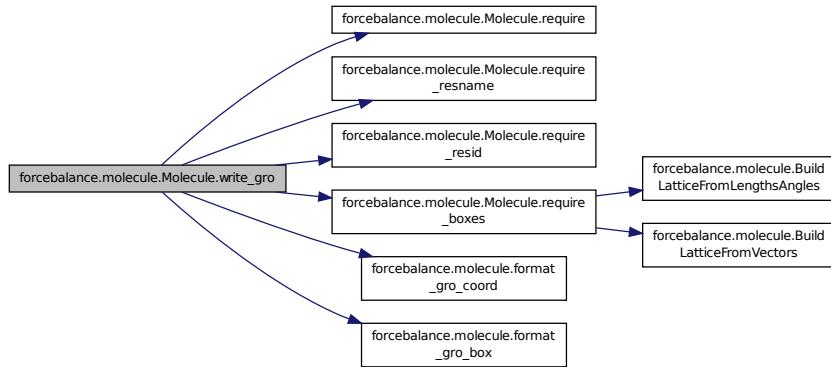
Here is the call graph for this function:



def forcebalance.molecule.Molecule.write_dcd (self, select, kwargs) Definition at line 2760 of file molecule.py.

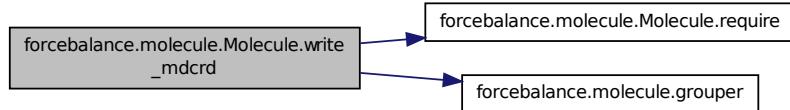
def forcebalance.molecule.Molecule.write_gro (self, select, kwargs) Definition at line 2725 of file molecule.py.

Here is the call graph for this function:



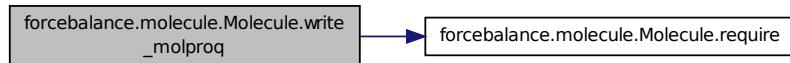
def forcebalance.molecule.Molecule.write_mdcrd (self, select, kwargs) Definition at line 2699 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.write_molproq (self, select, kwargs) Definition at line 2687 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.write_pdb (self, select, kwargs) Save to a PDB.

Copied wholesale from MSMBuilder.

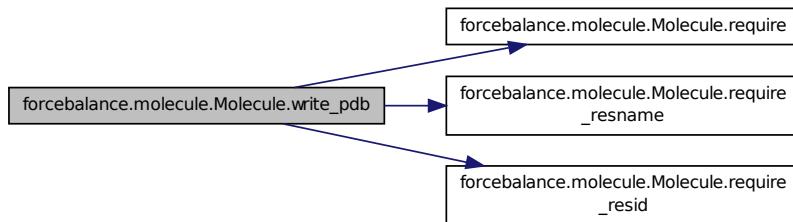
COLUMNS TYPE FIELD DEFINITION 7-11 int serial Atom serial number. 13-16 string name Atom name. 17 string altLoc Alternate location indicator. 18-20 (17-21 KAB) string resName Residue name. 22 string chainID Chain identifier. 23-26 int resSeq Residue sequence number. 27 string iCode Code for insertion of residues. 31-38 float x Orthogonal coordinates for X in Angstroms. 39-46 float y Orthogonal coordinates for Y in Angstroms. 47-54 float z Orthogonal coordinates for Z in Angstroms. 55-60 float occupancy Occupancy. 61-66 float tempFactor Temperature factor. 73-76 string segID Segment identifier, left-justified. 77-78 string element Element symbol, right-justified. 79-80 string charge Charge on the atom.

CRYST1 line, added by Lee-Ping

COLUMNS TYPE FIELD DEFINITION 7-15 float a a (Angstroms). 16-24 float b b (Angstroms). 25-33 float c c (Angstroms). 34-40 float alpha alpha (degrees). 41-47 float beta beta (degrees). 48-54 float gamma gamma (degrees). 56-66 string sGroup Space group. 67-70 int z Z value.

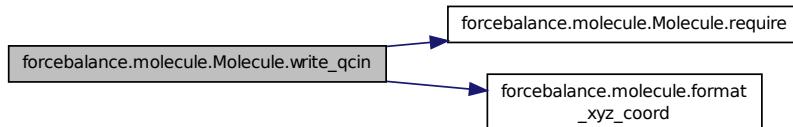
Definition at line 2816 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.write_qcin (self, select, kwargs) Definition at line 2611 of file molecule.py.

Here is the call graph for this function:



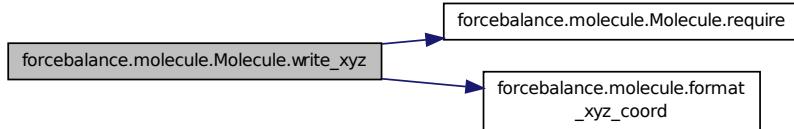
def forcebalance.molecule.Molecule.write_qdata (self, select, kwargs) Text quantum data format. Definition at line 2922 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.Molecule.write_xyz(self, select, kwargs) Definition at line 2676 of file molecule.py.

Here is the call graph for this function:



8.45.4 Member Data Documentation

forcebalance.molecule.Molecule.boxes Definition at line 3004 of file molecule.py.

forcebalance.molecule.Molecule.built_bonds Definition at line 944 of file molecule.py.

forcebalance.molecule.Molecule.comms Read in stuff if we passed in a file name, otherwise return an empty instance.

Try to determine from the file name using the extension. Actually read the file. Set member variables. Create a list of comment lines if we don't already have them from reading the file.

Definition at line 965 of file molecule.py.

forcebalance.molecule.Molecule.Data Definition at line 948 of file molecule.py.

forcebalance.molecule.Molecule.fout Fill in comments.

I needed to add in this line because the DCD writer requires the file name, but the other methods don't.

Definition at line 1013 of file molecule.py.

forcebalance.molecule.Molecule.Funnel A funnel dictionary that takes redundant file types and maps them down to a few.

Definition at line 928 of file molecule.py.

forcebalance.molecule.Molecule.molecules Definition at line 976 of file molecule.py.

forcebalance.molecule.Molecule.positive_resid Creates entries like 'gromacs' : 'gromacs' and 'xyz' : 'xyz' in the Funnel.

Definition at line 943 of file molecule.py.

forcebalance.molecule.Molecule.Read_Tab The table of file readers.

Definition at line 903 of file molecule.py.

forcebalance.molecule.Molecule.resid Definition at line 2947 of file molecule.py.

forcebalance.molecule.Molecule.resname Definition at line 2954 of file molecule.py.

forcebalance.molecule.Molecule.topology Make sure the comment line isn't too long for i in range(len(self.comms)): self.comms[i] = self.comms[i][:100] if len(self.comms[i]) > 100 else self.comms[i]. Attempt to build the topology for small systems.

:)

Definition at line 975 of file molecule.py.

forcebalance.molecule.Molecule.Write_Tab The table of file writers.

Definition at line 917 of file molecule.py.

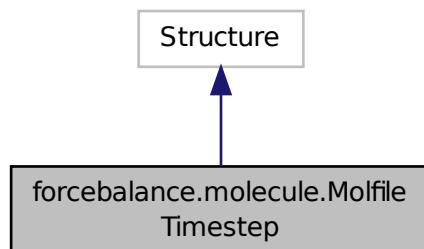
The documentation for this class was generated from the following file:

- [molecule.py](#)

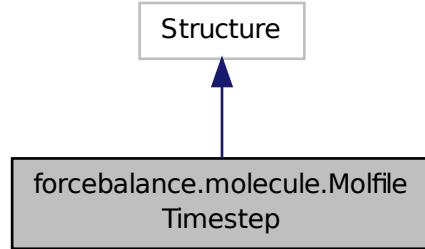
8.46 forcebalance.molecule.MolfileTimestep Class Reference

Wrapper for the timestep C structure used in molfile plugins.

Inheritance diagram for forcebalance.molecule.MolfileTimestep:



Collaboration diagram for forcebalance.molecule.MolfileTimestep:



8.46.1 Detailed Description

Wrapper for the timestep C structure used in molfile plugins.

Definition at line 499 of file molecule.py.

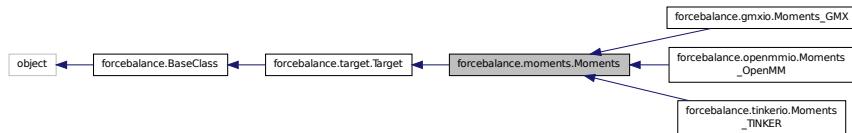
The documentation for this class was generated from the following file:

- [molecule.py](#)

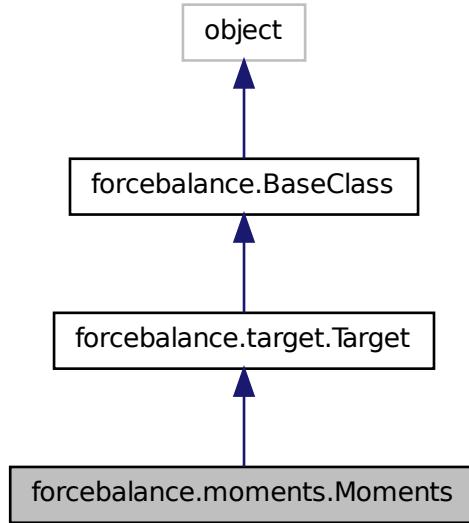
8.47 forcebalance.moments.Moments Class Reference

Subclass of Target for fitting force fields to multipole moments (from experiment or theory).

Inheritance diagram for forcebalance.moments.Moments:



Collaboration diagram for forcebalance.moments.Moments:



Public Member Functions

- def `__init__`
Initialization.
- def `read_reference_data`
Read the reference data from a file.
- def `indicate`
Print qualitative indicator.
- def `unpack_moments`
- def `get`
Evaluate objective function.
- def `get_X`
Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
Computes the objective function contribution and its gradient.
- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.

- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `denoms`
- `mfnm`
The mdata.txt file that contains the moments.
- `ref_moments`
Dictionary of reference multipole moments.
- `engine`
Read in the reference data.
- `na`
Number of atoms.
- `ref_eigvals`
- `ref_eigvecs`
- `calc_moments`
- `objective`
- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`
Relative directory of target.
- `tempdir`
- `rundir`
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- `FF`
Need the forcefield (here for now)

- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**
Whether to write indicate.log at every iteration (true for all but remote.)
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

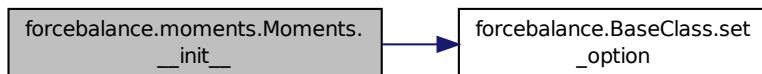
8.47.1 Detailed Description

Subclass of Target for fitting force fields to multipole moments (from experiment or theory).
Currently Tinker is supported.
Definition at line 30 of file moments.py.

8.47.2 Constructor & Destructor Documentation

def forcebalance.moments.Moments.__init__(self, options, tgt_opts, forcefield) Initialization.

Definition at line 35 of file moments.py.
Here is the call graph for this function:



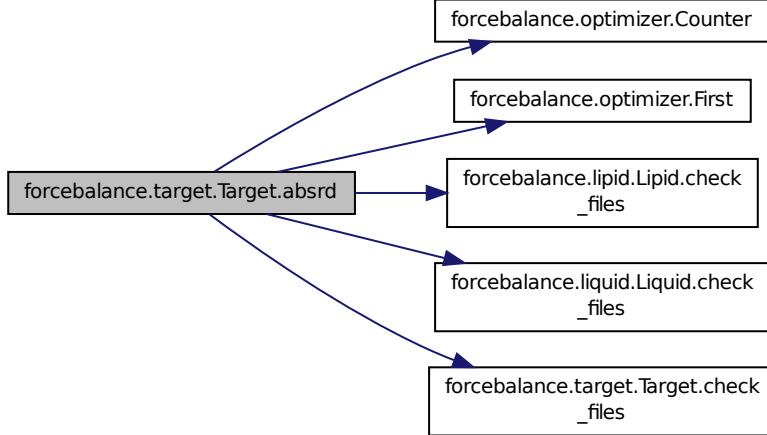
8.47.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__(self, key, value) [inherited] Definition at line 28 of file __init__.py.

def forcebalance.target.Target.absrd(self, inum = None) [inherited] Supply the correct directory specified by user's "read" option.

Definition at line 393 of file target.py.

Here is the call graph for this function:



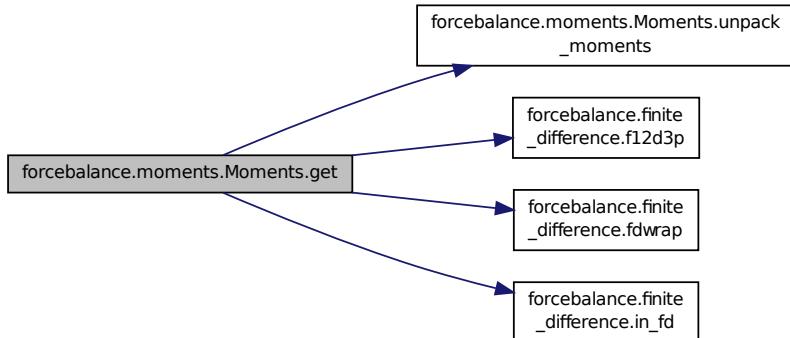
def forcebalance.target.Target.check_files(self, there) [inherited] Check this directory for the presence of readable files when the 'read' option is set.

Definition at line 364 of file target.py.

def forcebalance.moments.Moments.get(self, mvals, AGrad = False, AHess = False) Evaluate objective function.

Definition at line 171 of file moments.py.

Here is the call graph for this function:



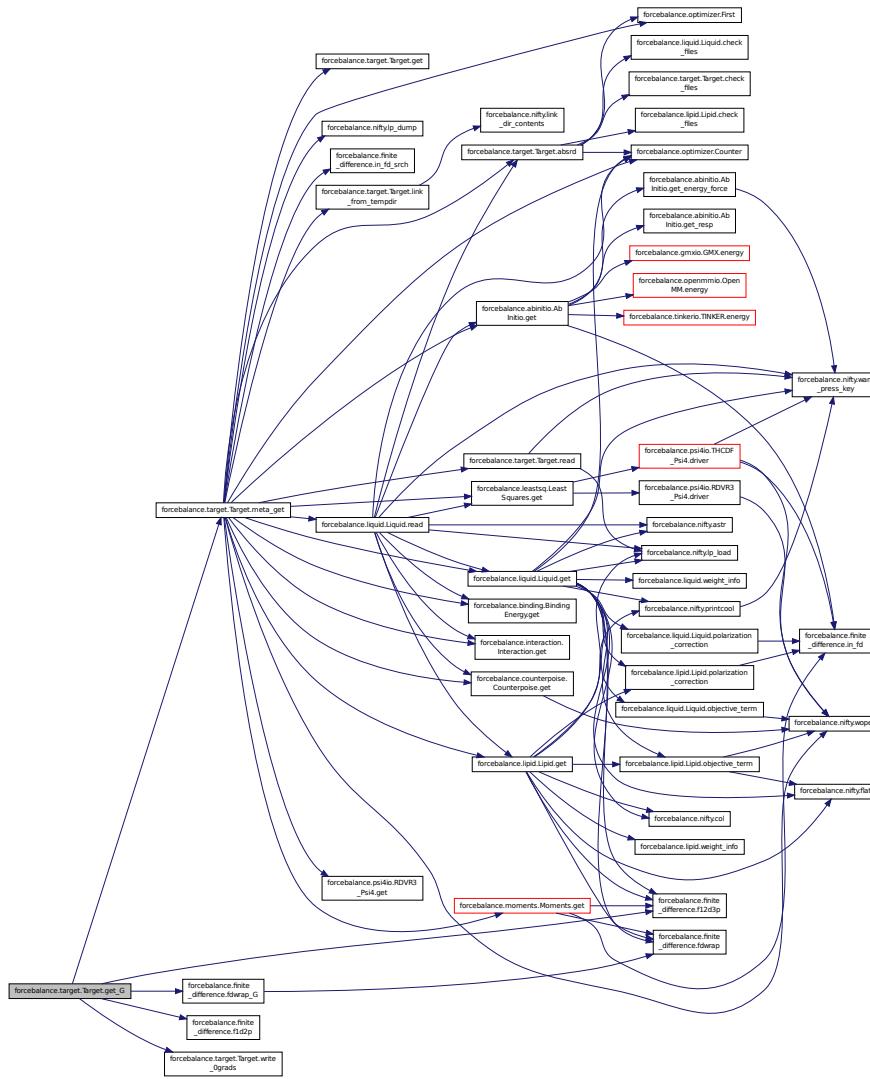
def forcebalance.target.Target.get_G(self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



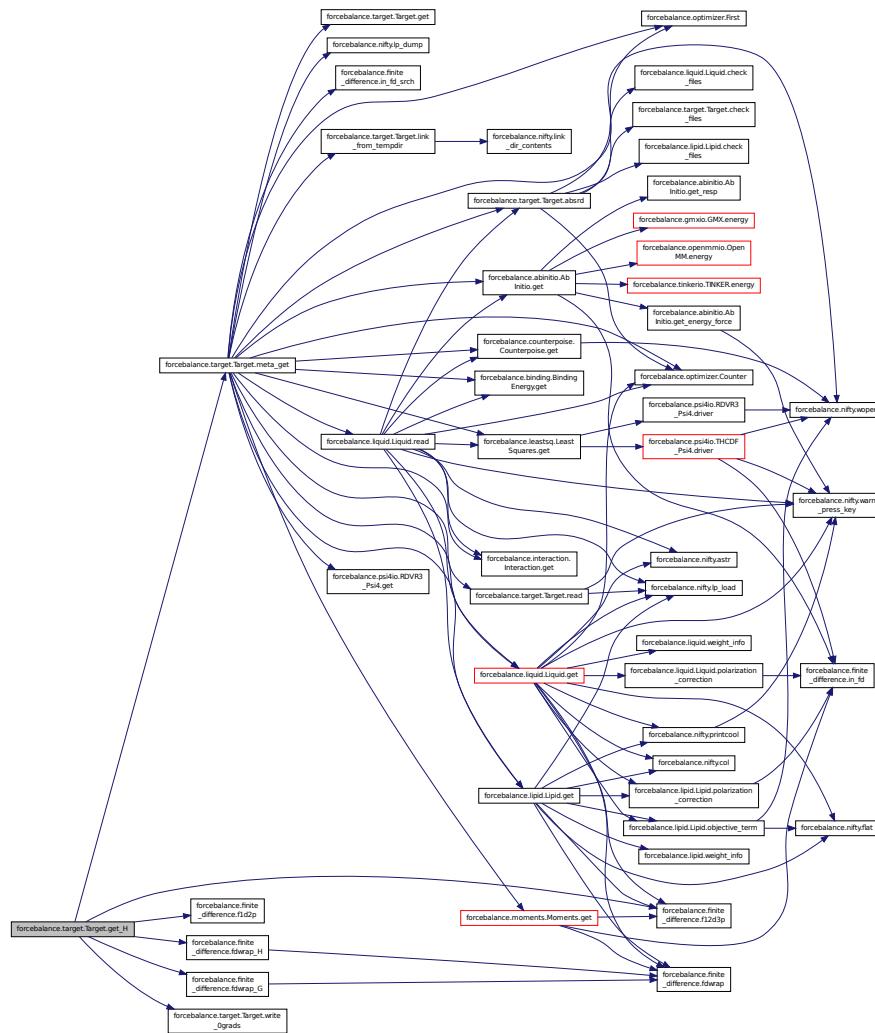
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

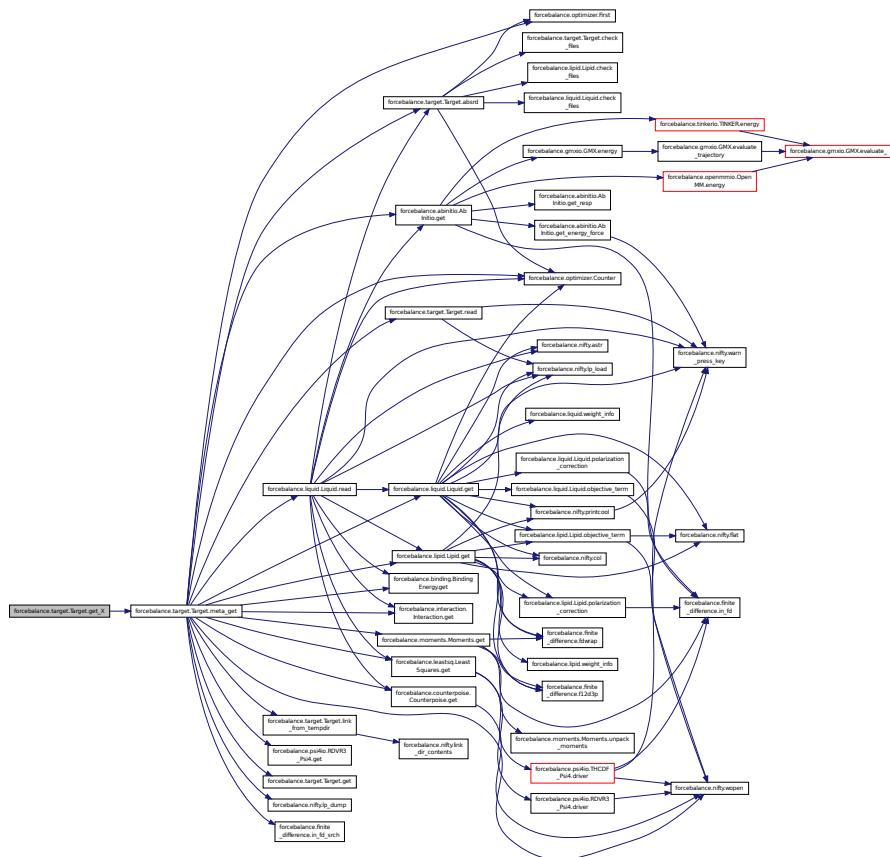
Here is the call graph for this function:



def forcebalance.target.Target.get_X(self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

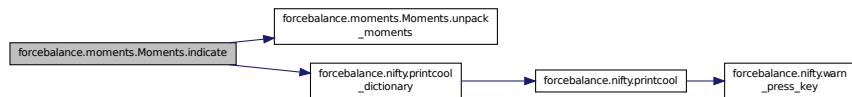
Here is the call graph for this function:



def forcebalance.moments.Moments.indicate (self) Print qualitative indicator.

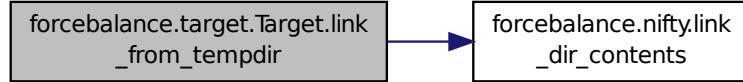
Definition at line 139 of file moments.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

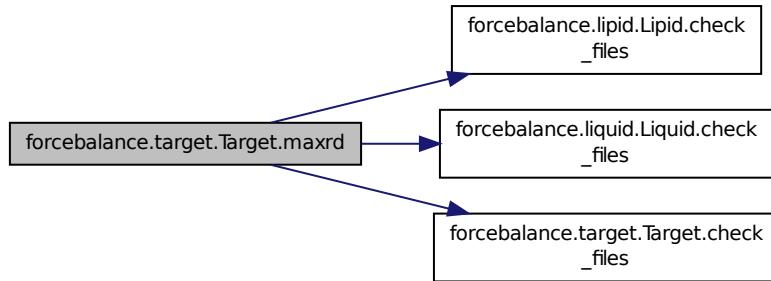
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

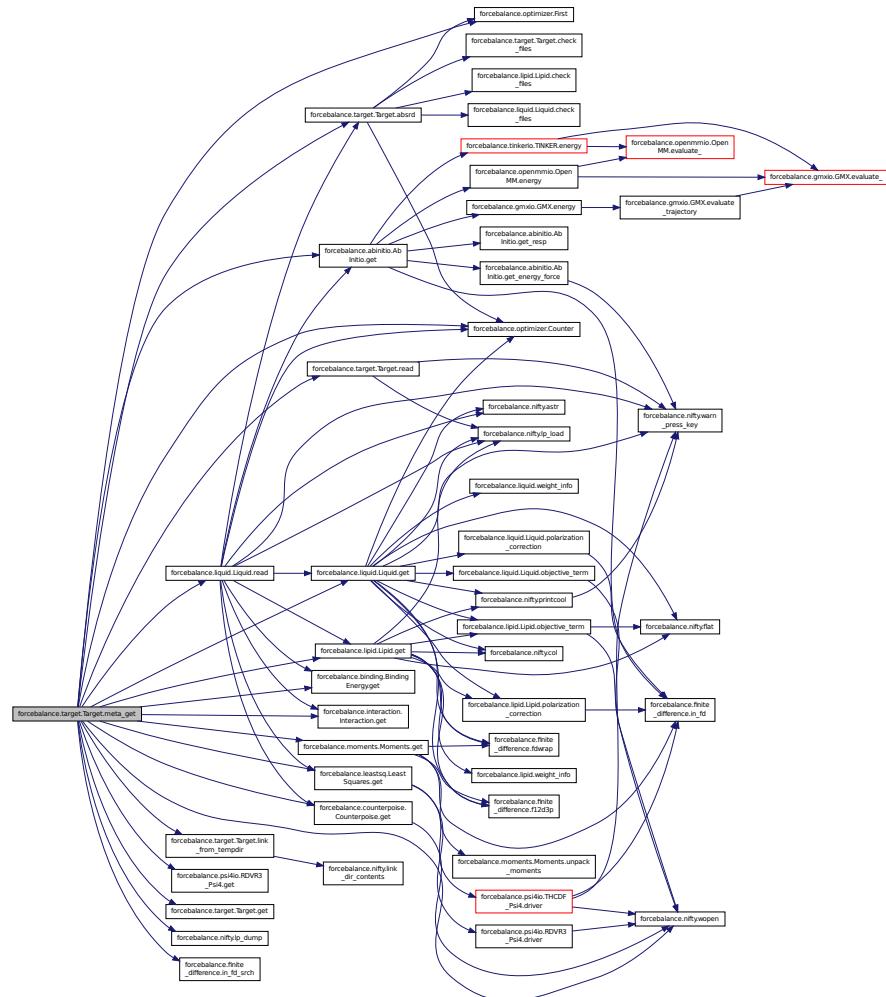


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

Here is the call graph for this function:

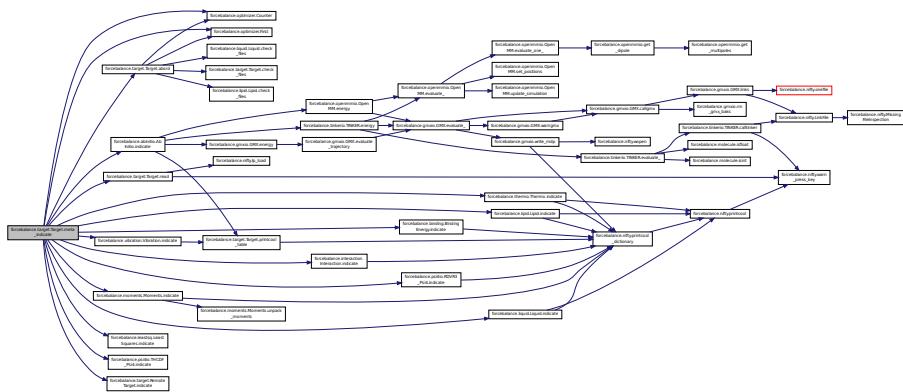


def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.

Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

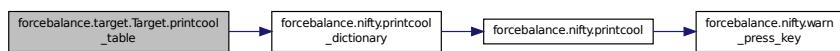
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

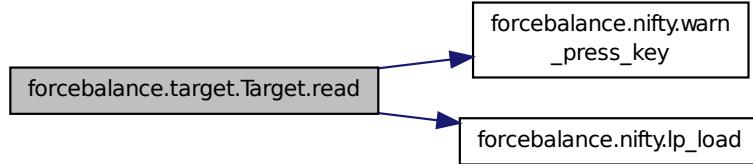
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.moments.Moments.read_reference_data (self) Read the reference data from a file.

Definition at line 70 of file moments.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

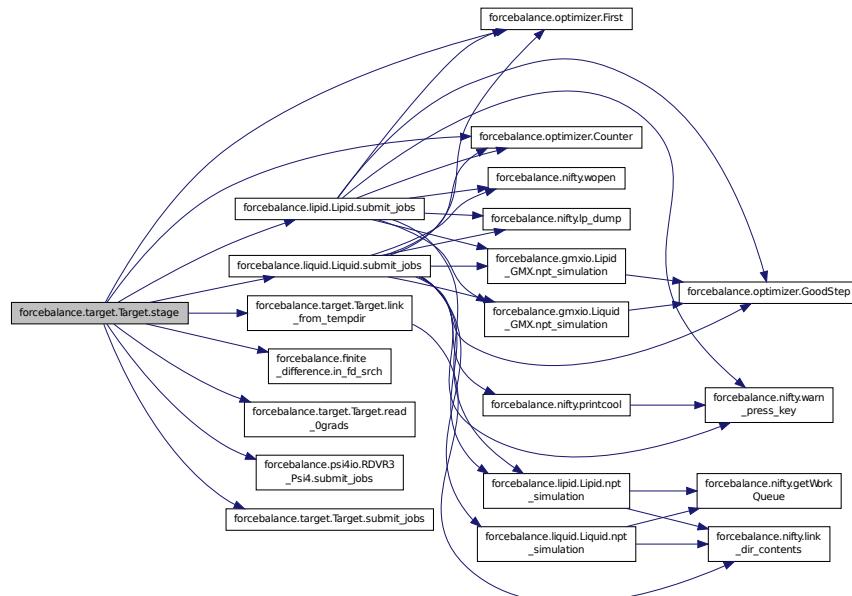
def forcebalance.BaseClass.set_option (self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



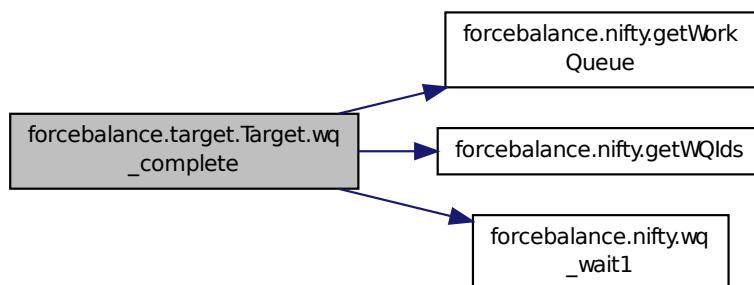
```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.moments.Moments.unpack_moments ( self, moment_dict ) Definition at line 165 of file moments.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.47.4 Member Data Documentation

forcebalance.moments.Moments.calc_moments Definition at line 198 of file moments.py.

forcebalance.moments.Moments.denoms Definition at line 48 of file moments.py.

forcebalance.moments.Moments.engine Read in the reference data.

Build keyword dictionaries to pass to engine. Create engine object.

Definition at line 66 of file moments.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.moments.Moments.mfnm The mdata.txt file that contains the moments.

Definition at line 57 of file moments.py.

forcebalance.moments.Moments.na Number of atoms.

Definition at line 72 of file moments.py.

forcebalance.moments.Moments.objective Definition at line 199 of file moments.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [**inherited**] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.moments.Moments.ref_eigvals Definition at line 73 of file moments.py.

forcebalance.moments.Moments.ref_eigvecs Definition at line 74 of file moments.py.

forcebalance.moments.Moments.ref_moments Dictionary of reference multipole moments.

Definition at line 59 of file moments.py.

forcebalance.target.Target.rundir [**inherited**] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number. The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [**inherited**] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [**inherited**] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [**inherited**] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

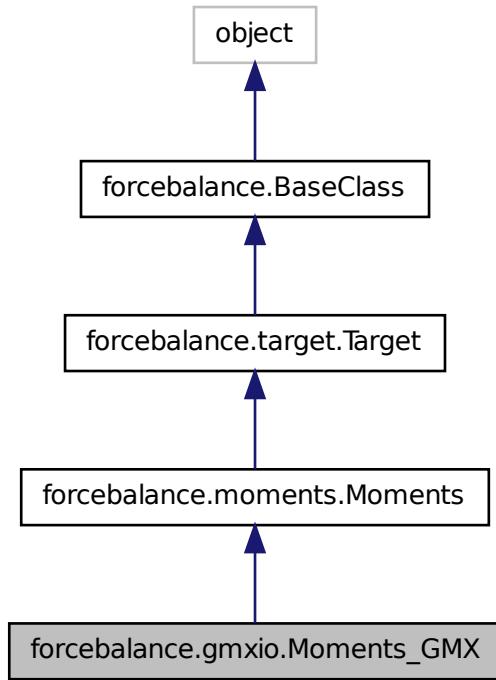
The documentation for this class was generated from the following file:

- [moments.py](#)

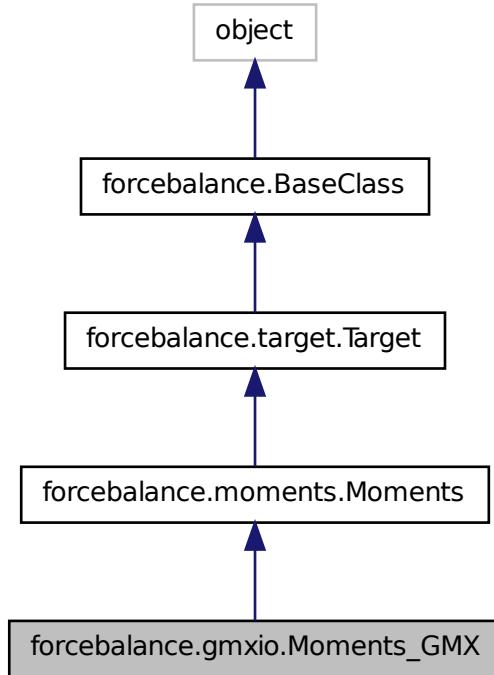
8.48 forcebalance.gmxio.Moments_GMX Class Reference

Multipole moment matching using GROMACS.

Inheritance diagram for forcebalance.gmxio.Moments_GMX:



Collaboration diagram for forcebalance.gmxio.Moments_GMX:



Public Member Functions

- def `__init__`
- def `read_reference_data`

Read the reference data from a file.
- def `indicate`

Print qualitative indicator.
- def `unpack_moments`
- def `get`

Evaluate objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.

- def `link_from_tempdir`
 Back up the temporary directory if desired, delete it and then create a new one.
- def `refresh_temp_directory`
 Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
 Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
 Supply the correct directory specified by user's "read" option.
- def `maxrd`
 Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
 Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
 Wrapper around the get function.
- def `submit_jobs`
- def `stage`
 Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
 This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
 Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
 Default file names for coordinates and key file.
- `denoms`
- `mfnm`
 The mdata.txt file that contains the moments.
- `ref_moments`
 Dictionary of reference multipole moments.
- `engine`
 Read in the reference data.
- `na`
 Number of atoms.
- `ref_eigvals`
- `ref_eigvecs`
- `calc_moments`
- `objective`
- `rd`
 Root directory of the whole project.
- `pgrad`
 Iteration where we turn on zero-gradient skipping.
- `tempbase`
 Relative directory of target.

- `tempdir`
`self.tempdir = os.path.join('temp',self.name)` The directory in which the simulation is running - this can be updated.
- `FF`
`Need the forcefield (here for now)`
- `xct`
`Counts how often the objective function was computed.`
- `gct`
`Counts how often the gradient was computed.`
- `hct`
`Counts how often the Hessian was computed.`
- `read_indicate`
`Whether to read indicate.log from file when restarting an aborted run.`
- `write_indicate`
`Whether to write indicate.log at every iteration (true for all but remote.)`
- `read_objective`
`Whether to read objective.p from file when restarting an aborted run.`
- `write_objective`
`Whether to write objective.p at every iteration (true for all but remote.)`
- `verbose_options`
- `PrintOptionDict`

8.48.1 Detailed Description

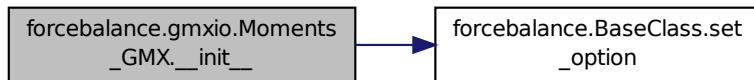
Multipole moment matching using GROMACS.

Definition at line 1481 of file gmxio.py.

8.48.2 Constructor & Destructor Documentation

`def forcebalance.gmxio.Moments_GMX.__init__ (self, options, tgt_opts, forcefield)` Definition at line 1482 of file gmxio.py.

Here is the call graph for this function:



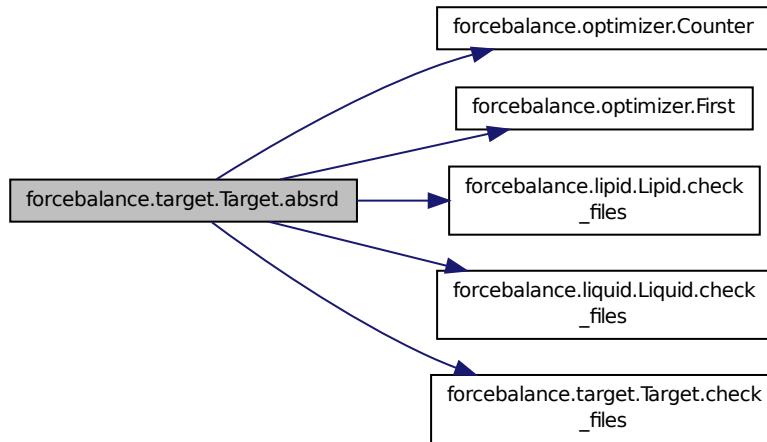
8.48.3 Member Function Documentation

`def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited]` Definition at line 28 of file __init__.py.

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory  
specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



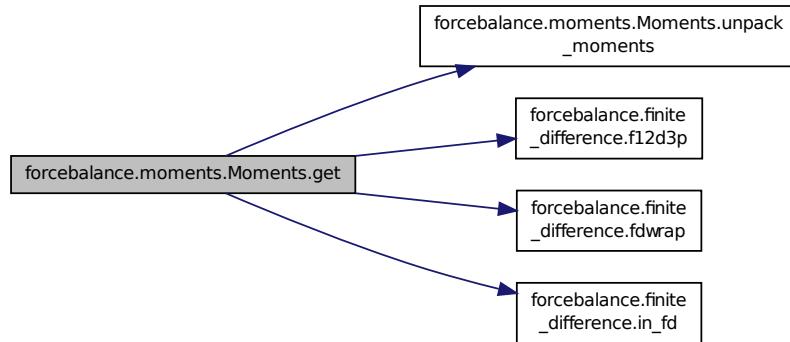
```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence  
of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.moments.Moments.get ( self, mvals, AGrad=False, AHess=False ) [inherited]  
Evaluate objective function.
```

Definition at line 171 of file moments.py.

Here is the call graph for this function:



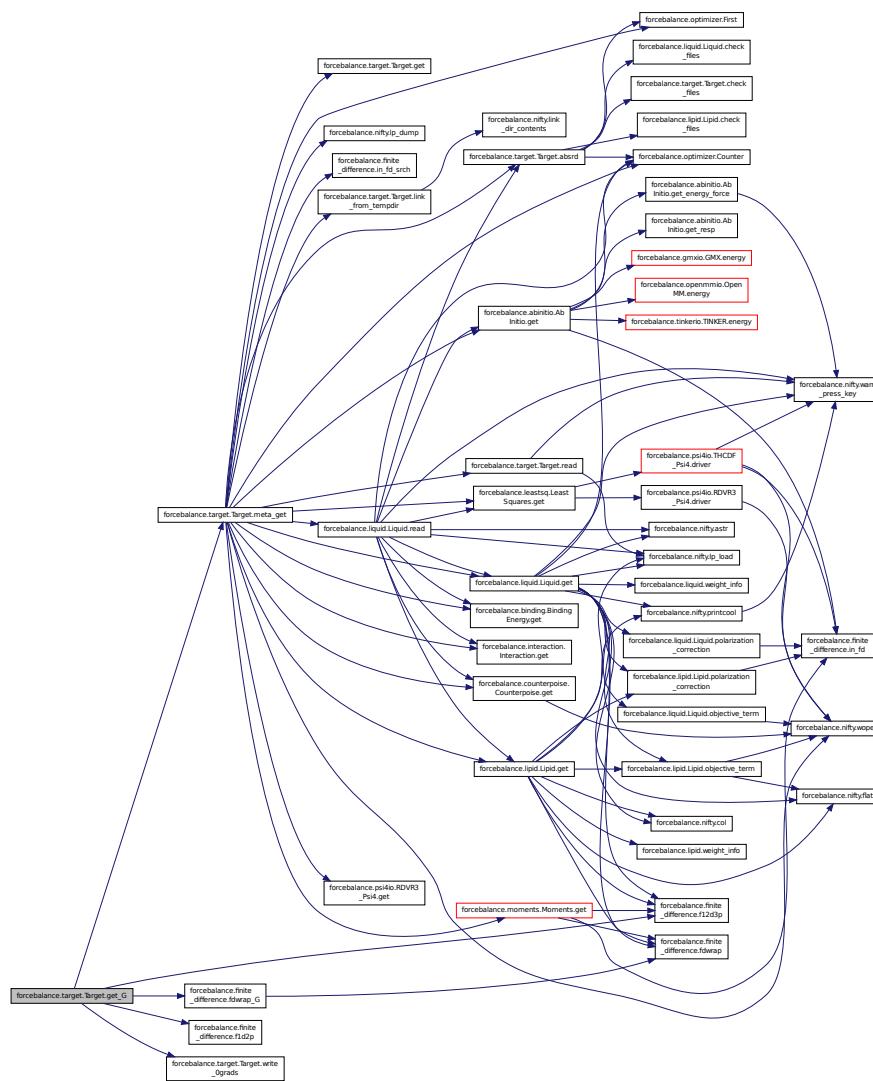
```
def forcebalance.target.Target.get_G ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.get_H ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient / Hessian.
```

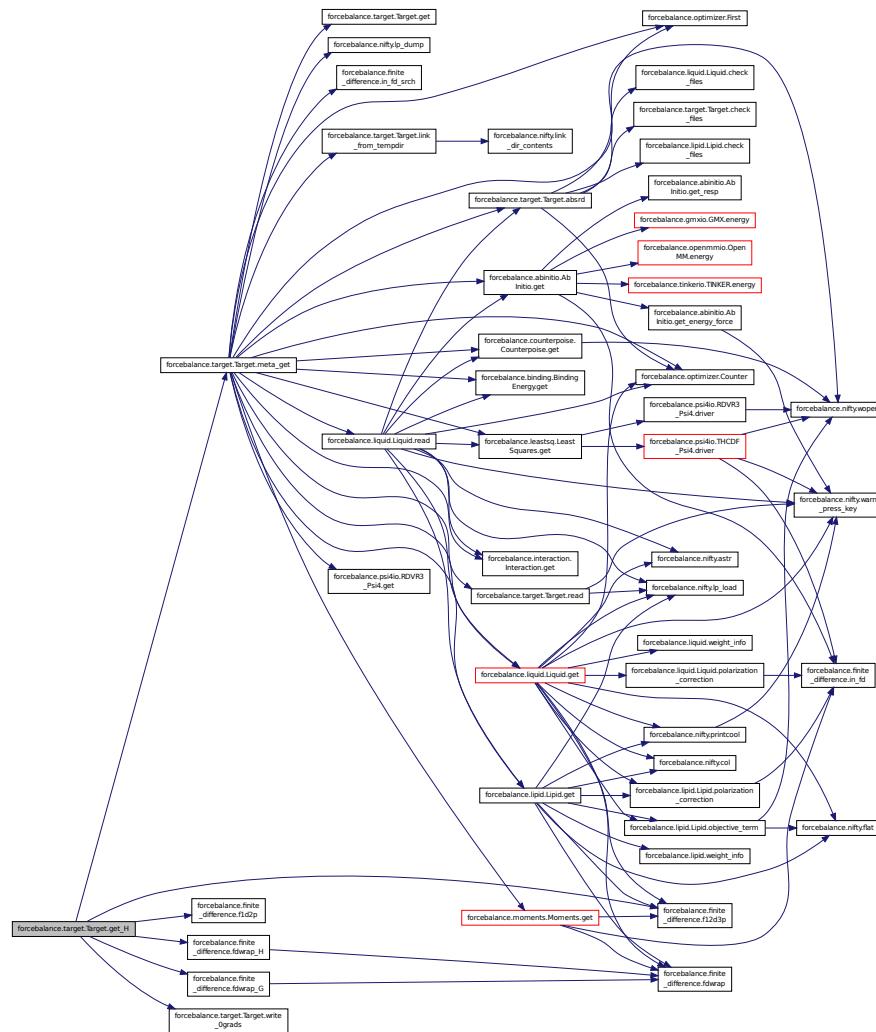
First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through

the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

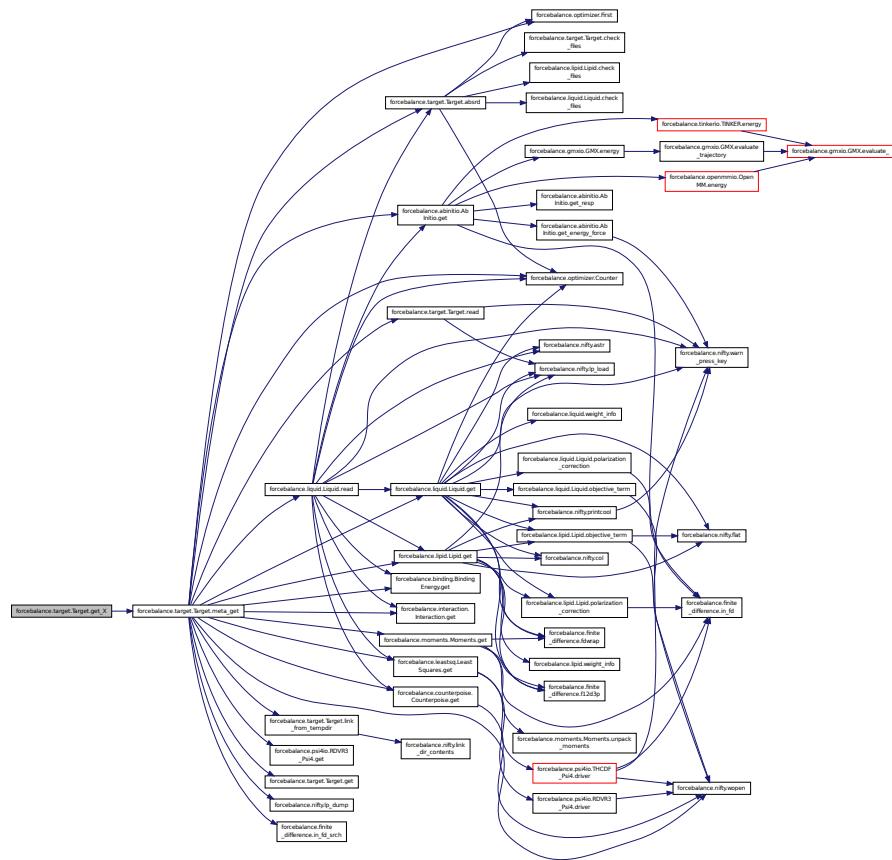
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

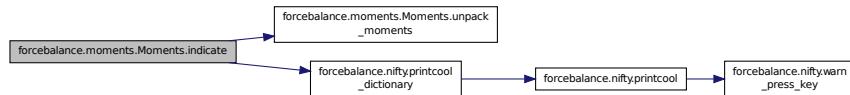
Here is the call graph for this function:



def forcebalance.moments.Moments.indicate (self) [inherited] Print qualitative indicator.

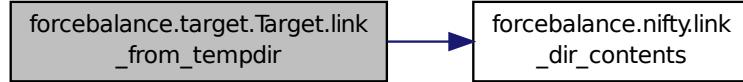
Definition at line 139 of file moments.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

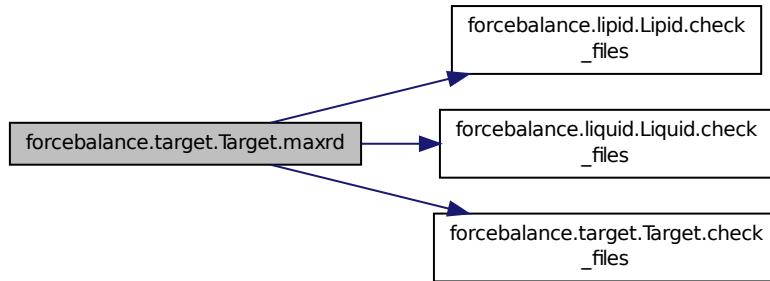
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

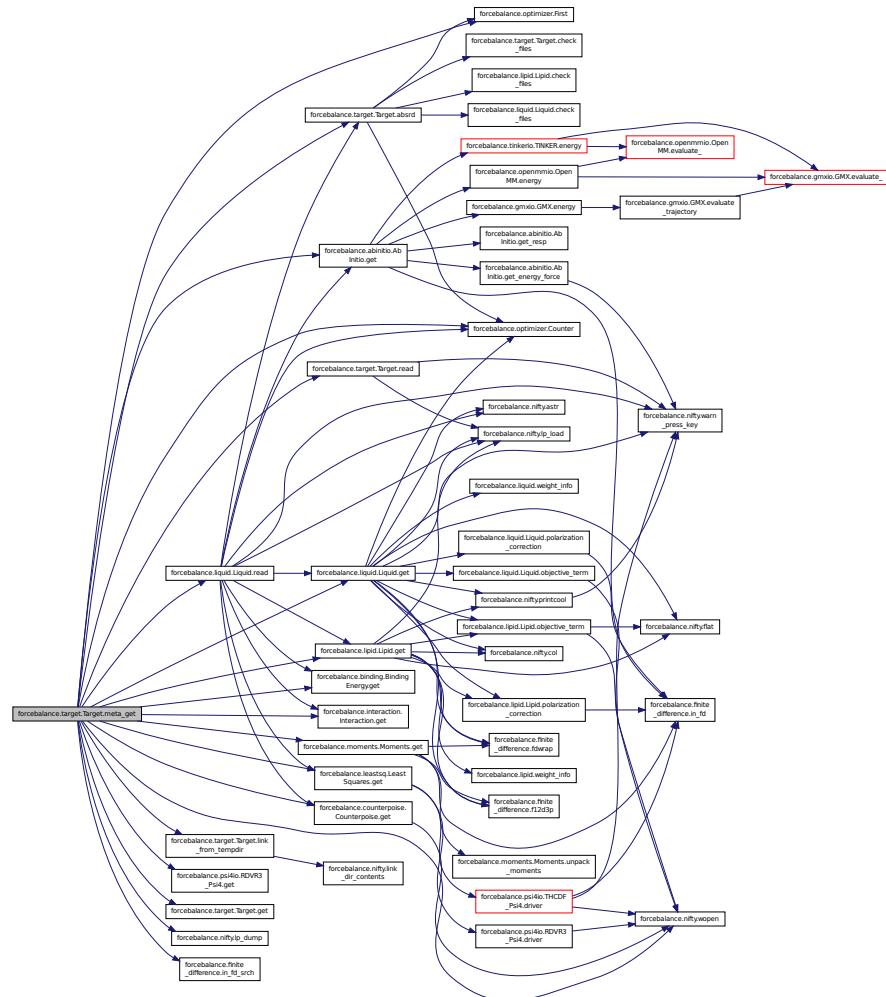


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

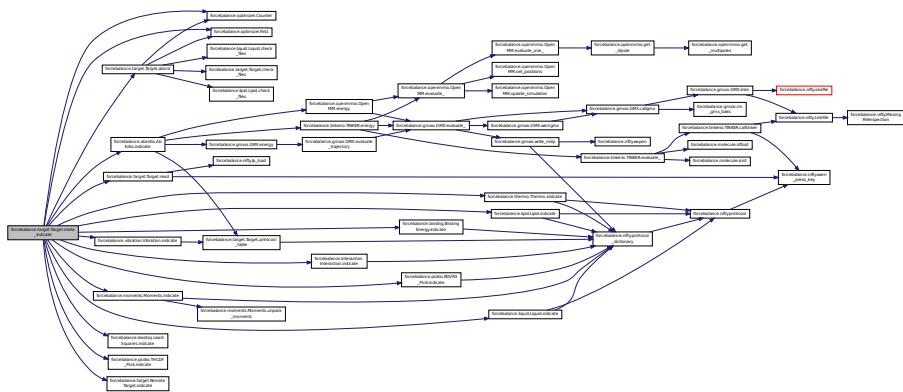
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict ([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

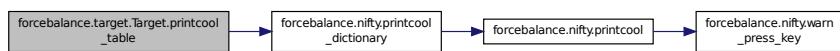
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

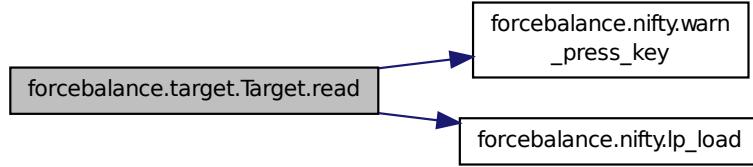
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.moments.Moments.read_reference_data (self) [inherited] Read the reference data from a file.

Definition at line 70 of file moments.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

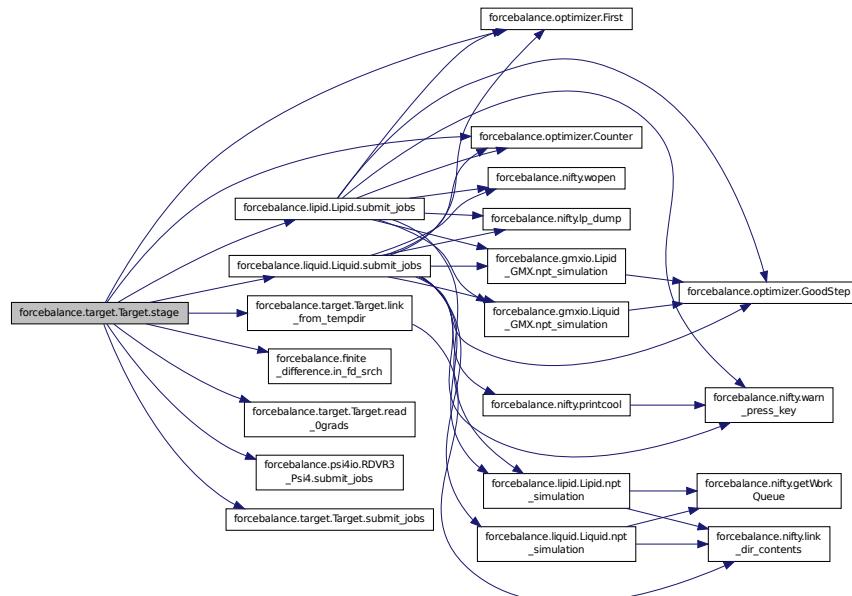
def forcebalance.BaseClass.set_option (self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



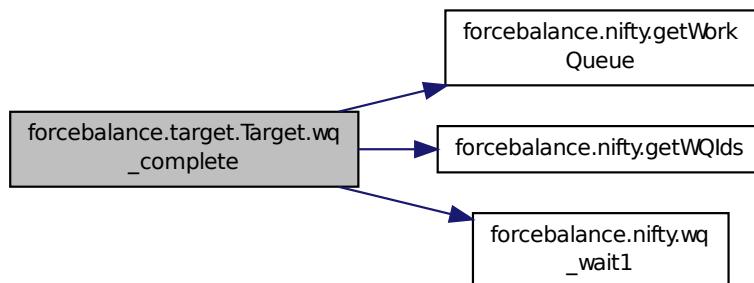
```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.moments.Moments.unpack_moments ( self, moment_dict ) [inherited] Definition at
line 165 of file moments.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work
Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.48.4 Member Data Documentation

forcebalance.moments.Moments.calc_moments [inherited] Definition at line 198 of file moments.py.

forcebalance.moments.Moments.denoms [inherited] Definition at line 48 of file moments.py.

forcebalance.moments.Moments.engine [inherited] Read in the reference data.

Build keyword dictionaries to pass to engine. Create engine object.

Definition at line 66 of file moments.py.

forcebalance.gmxio.Moments_GMX.engine Default file names for coordinates and key file.

Definition at line 1487 of file gmxio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.moments.Moments.mfnm [inherited] The mdata.txt file that contains the moments.

Definition at line 57 of file moments.py.

forcebalance.moments.Moments.na [inherited] Number of atoms.

Definition at line 72 of file moments.py.

forcebalance.moments.Moments.objective [inherited] Definition at line 199 of file moments.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.moments.Moments.ref_eigvals [inherited] Definition at line 73 of file moments.py.

forcebalance.moments.Moments.ref_eigvecs [inherited] Definition at line 74 of file moments.py.

forcebalance.moments.Moments.ref_moments [inherited] Dictionary of reference multipole moments.

Definition at line 59 of file moments.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number
The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

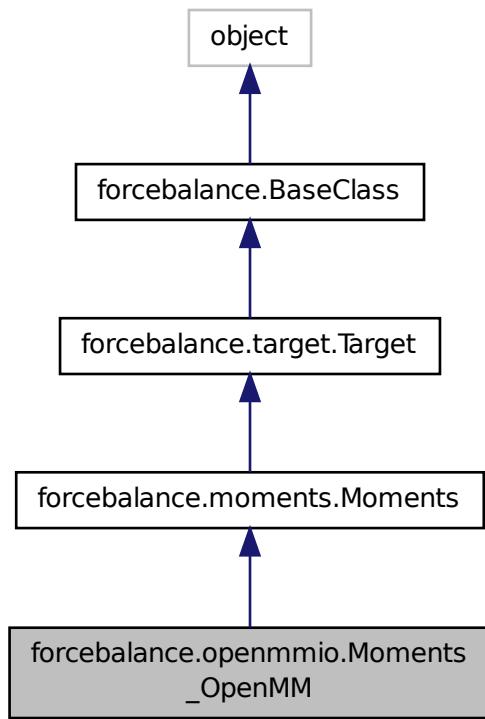
The documentation for this class was generated from the following file:

- [gmxio.py](#)

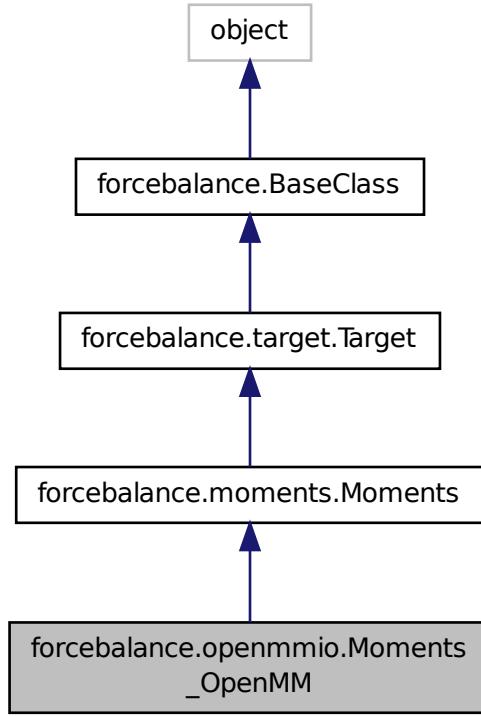
8.49 forcebalance.openmmio.Moments_OpenMM Class Reference

Multipole moment matching using [OpenMM](#).

Inheritance diagram for forcebalance.openmmio.Moments_OpenMM:



Collaboration diagram for forcebalance.openmmio.Moments_OpenMM:



Public Member Functions

- def `_init_`
- def `read_reference_data`

Read the reference data from a file.
- def `indicate`

Print qualitative indicator.
- def `unpack_moments`
- def `get`

Evaluate objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

- def `link_from_tempdir`
Computes the objective function contribution and its gradient / Hessian.
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool.table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
Default file names for coordinates and key file.
- `denoms`
- `mfnm`
The mdata.txt file that contains the moments.
- `ref_moments`
Dictionary of reference multipole moments.
- `engine`
Read in the reference data.
- `na`
Number of atoms.
- `ref_eigvals`
- `ref_eigvecs`
- `calc_moments`
- `objective`
- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`

- Relative directory of target.*
- `tempdir`
`self.tempdir = os.path.join('temp',self.name)` *The directory in which the simulation is running - this can be updated.*
 - `FF`
Need the forcefield (here for now)
 - `xct`
Counts how often the objective function was computed.
 - `gct`
Counts how often the gradient was computed.
 - `hct`
Counts how often the Hessian was computed.
 - `read_indicate`
Whether to read indicate.log from file when restarting an aborted run.
 - `write_indicate`
Whether to write indicate.log at every iteration (true for all but remote.)
 - `read_objective`
Whether to read objective.p from file when restarting an aborted run.
 - `write_objective`
Whether to write objective.p at every iteration (true for all but remote.)
 - `verbose_options`
 - `PrintOptionDict`

8.49.1 Detailed Description

Multipole moment matching using [OpenMM](#).

Definition at line 1202 of file openmmio.py.

8.49.2 Constructor & Destructor Documentation

def forcebalance.openmmio.Moments_OpenMM.__init__ (`self`, `options`, `tgt_opts`, `forcefield`) Definition at line 1203 of file openmmio.py.

Here is the call graph for this function:



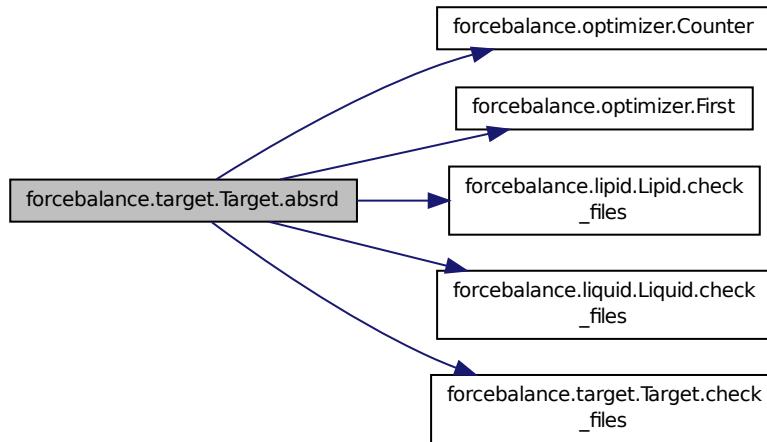
8.49.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (`self`, `key`, `value`) [inherited] Definition at line 28 of file __init__.py.

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory  
specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



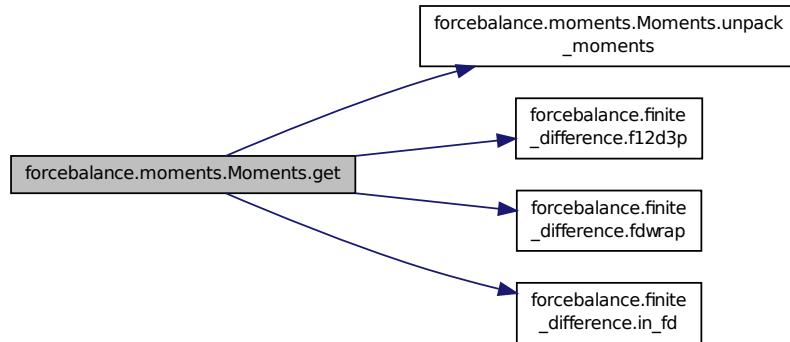
```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence  
of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.moments.Moments.get ( self, mvals, AGrad=False, AHess=False ) [inherited]  
Evaluate objective function.
```

Definition at line 171 of file moments.py.

Here is the call graph for this function:



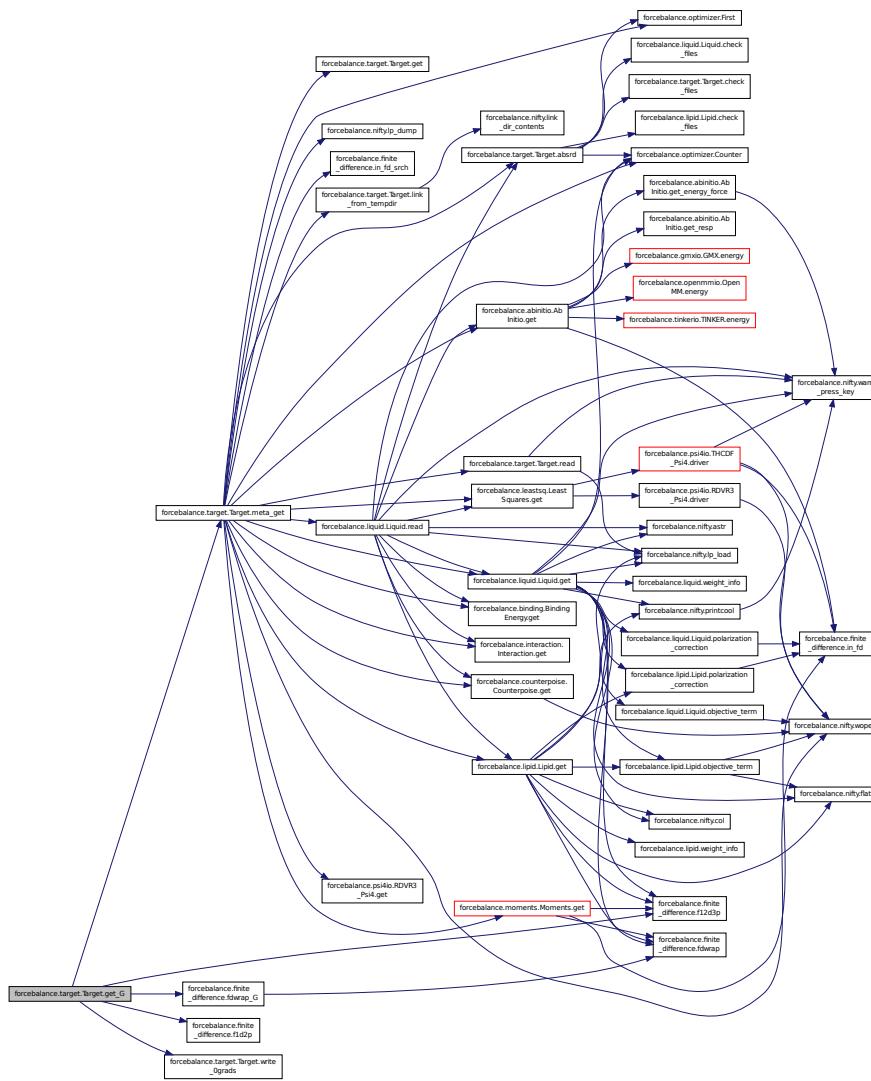
```
def forcebalance.target.Target.get_G ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.get_H ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient / Hessian.
```

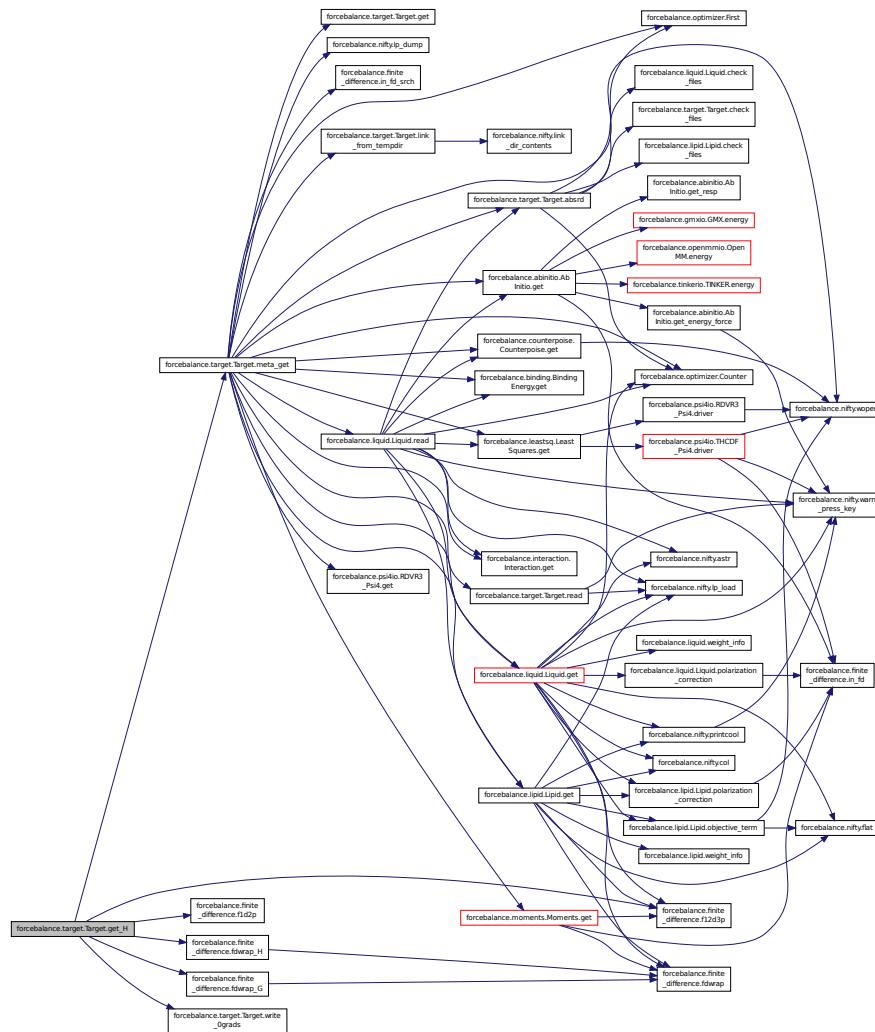
First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through

the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

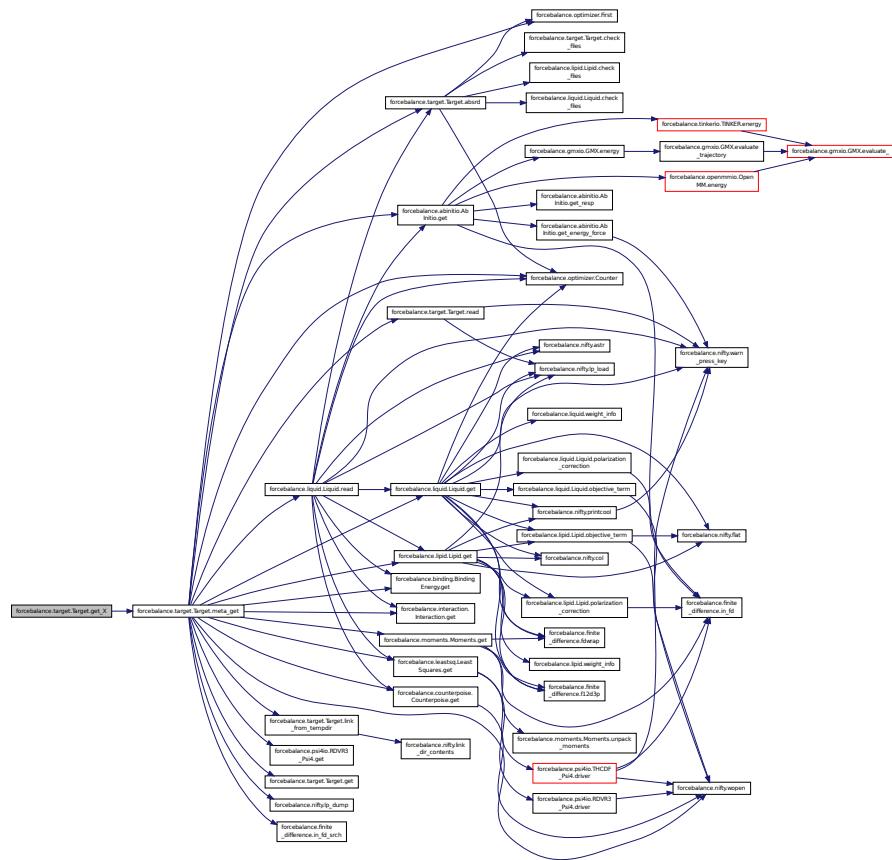
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

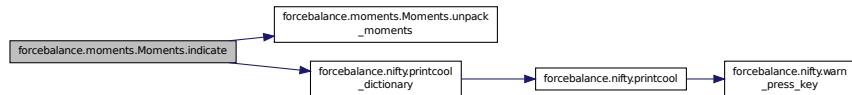
Here is the call graph for this function:



def forcebalance.moments.Moments.indicate (self) [inherited] Print qualitative indicator.

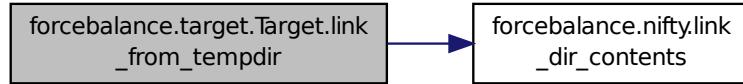
Definition at line 139 of file moments.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

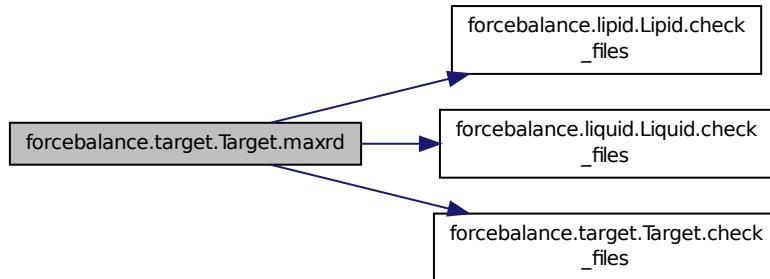
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

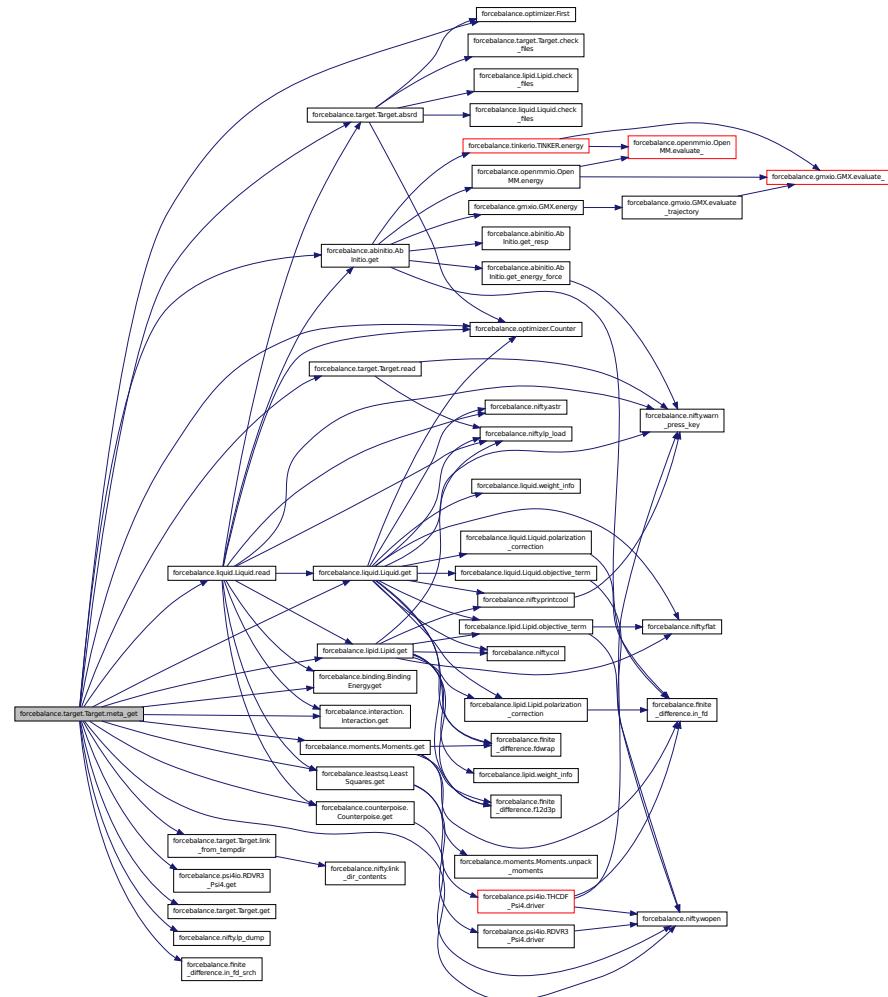


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

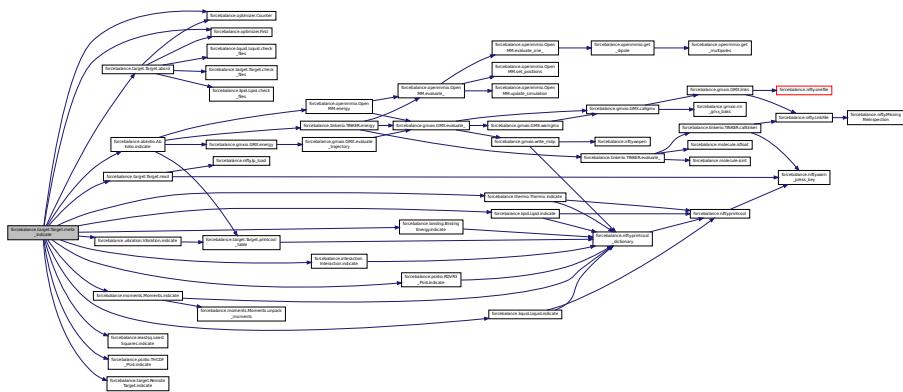
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

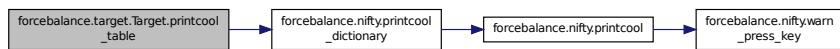
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

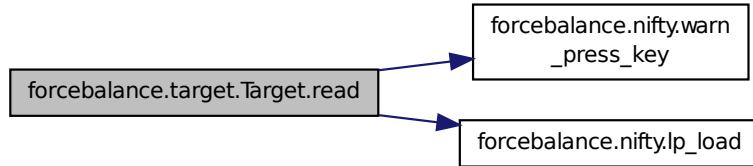
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.moments.Moments.read_reference_data (self) [inherited] Read the reference data from a file.

Definition at line 70 of file moments.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

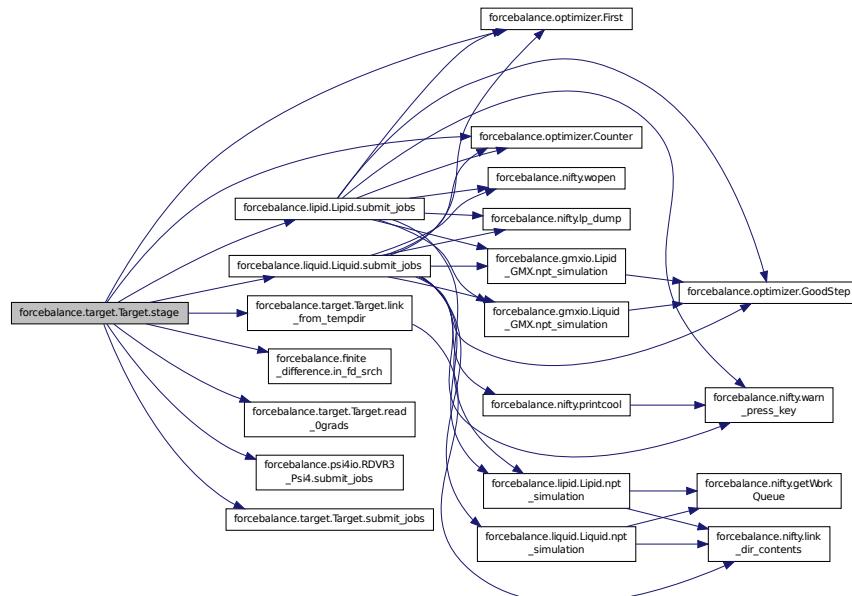
def forcebalance.BaseClass.set_option (self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



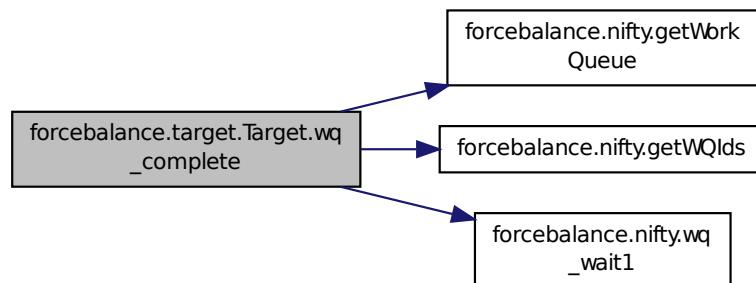
```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.moments.Moments.unpack_moments ( self, moment_dict ) [inherited] Definition at line 165 of file moments.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.49.4 Member Data Documentation

forcebalance.moments.Moments.calc_moments [inherited] Definition at line 198 of file moments.py.

forcebalance.moments.Moments.denoms [inherited] Definition at line 48 of file moments.py.

forcebalance.moments.Moments.engine [inherited] Read in the reference data.

Build keyword dictionaries to pass to engine. Create engine object.

Definition at line 66 of file moments.py.

forcebalance.openmmio.Moments_OpenMM.engine Default file names for coordinates and key file.

Definition at line 1208 of file openmmio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.moments.Moments.mfnm [inherited] The mdata.txt file that contains the moments.

Definition at line 57 of file moments.py.

forcebalance.moments.Moments.na [inherited] Number of atoms.

Definition at line 72 of file moments.py.

forcebalance.moments.Moments.objective [inherited] Definition at line 199 of file moments.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.moments.Moments.ref_eigvals [inherited] Definition at line 73 of file moments.py.

forcebalance.moments.Moments.ref_eigvecs [inherited] Definition at line 74 of file moments.py.

forcebalance.moments.Moments.ref_moments [inherited] Dictionary of reference multipole moments.

Definition at line 59 of file moments.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number
The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

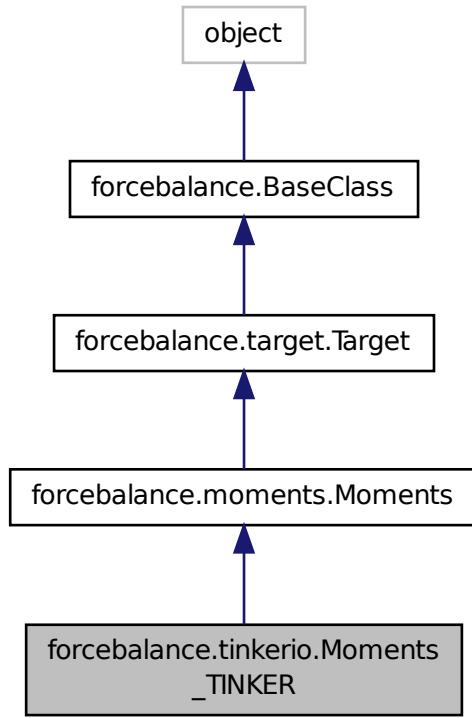
The documentation for this class was generated from the following file:

- [openmmio.py](#)

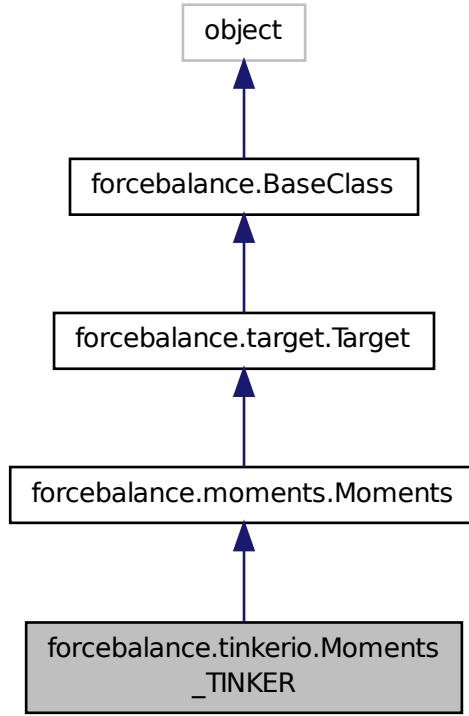
8.50 forcebalance.tinkerio.Moments_TINKER Class Reference

Subclass of Target for multipole moment matching using TINKER.

Inheritance diagram for forcebalance.tinkerio.Moments_TINKER:



Collaboration diagram for forcebalance.tinkerio.Moments_TINKER:



Public Member Functions

- def `__init__`
- def `read_reference_data`

Read the reference data from a file.
- def `indicate`

Print qualitative indicator.
- def `unpack_moments`
- def `get`

Evaluate objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

- def `link_from_tempdir`
Computes the objective function contribution and its gradient / Hessian.
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool.table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
Default file names for coordinates and key file.
- `denoms`
- `mfnm`
The mdata.txt file that contains the moments.
- `ref_moments`
Dictionary of reference multipole moments.
- `engine`
Read in the reference data.
- `na`
Number of atoms.
- `ref_eigvals`
- `ref_eigvecs`
- `calc_moments`
- `objective`
- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`

- Relative directory of target.*
- **tempdir**
 - **rundir**

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
 - **FF**

Need the forcefield (here for now)
 - **xct**

Counts how often the objective function was computed.
 - **gct**

Counts how often the gradient was computed.
 - **hct**

Counts how often the Hessian was computed.
 - **read_indicate**

Whether to read indicate.log from file when restarting an aborted run.
 - **write_indicate**

Whether to write indicate.log at every iteration (true for all but remote.)
 - **read_objective**

Whether to read objective.p from file when restarting an aborted run.
 - **write_objective**

Whether to write objective.p at every iteration (true for all but remote.)
 - **verbose_options**
 - **PrintOptionDict**

8.50.1 Detailed Description

Subclass of Target for multipole moment matching using TINKER.
Definition at line 1097 of file tinkerio.py.

8.50.2 Constructor & Destructor Documentation

def forcebalance.tinkerio.Moments.TINKER.__init__ (self, options, tgt_opts, forcefield) Definition at line 1098 of file tinkerio.py.

Here is the call graph for this function:



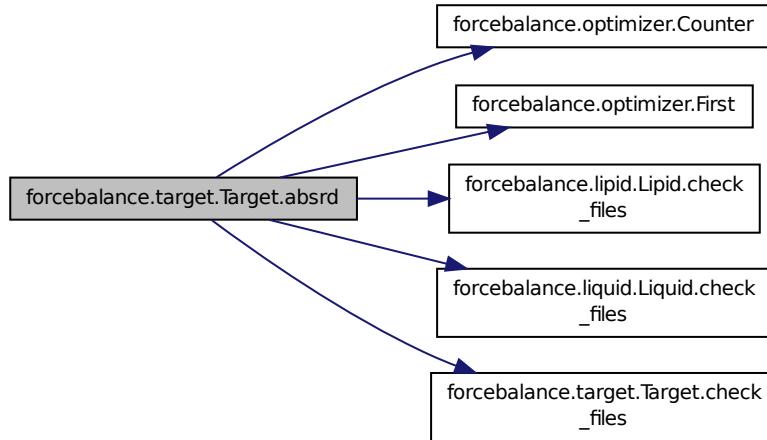
8.50.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited] Definition at line 28 of file __init__.py.

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory  
specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



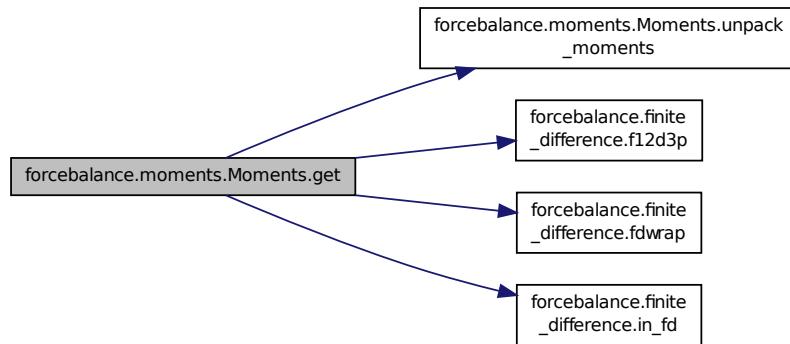
```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence  
of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.moments.Moments.get ( self, mvals, AGrad=False, AHess=False ) [inherited]  
Evaluate objective function.
```

Definition at line 171 of file moments.py.

Here is the call graph for this function:



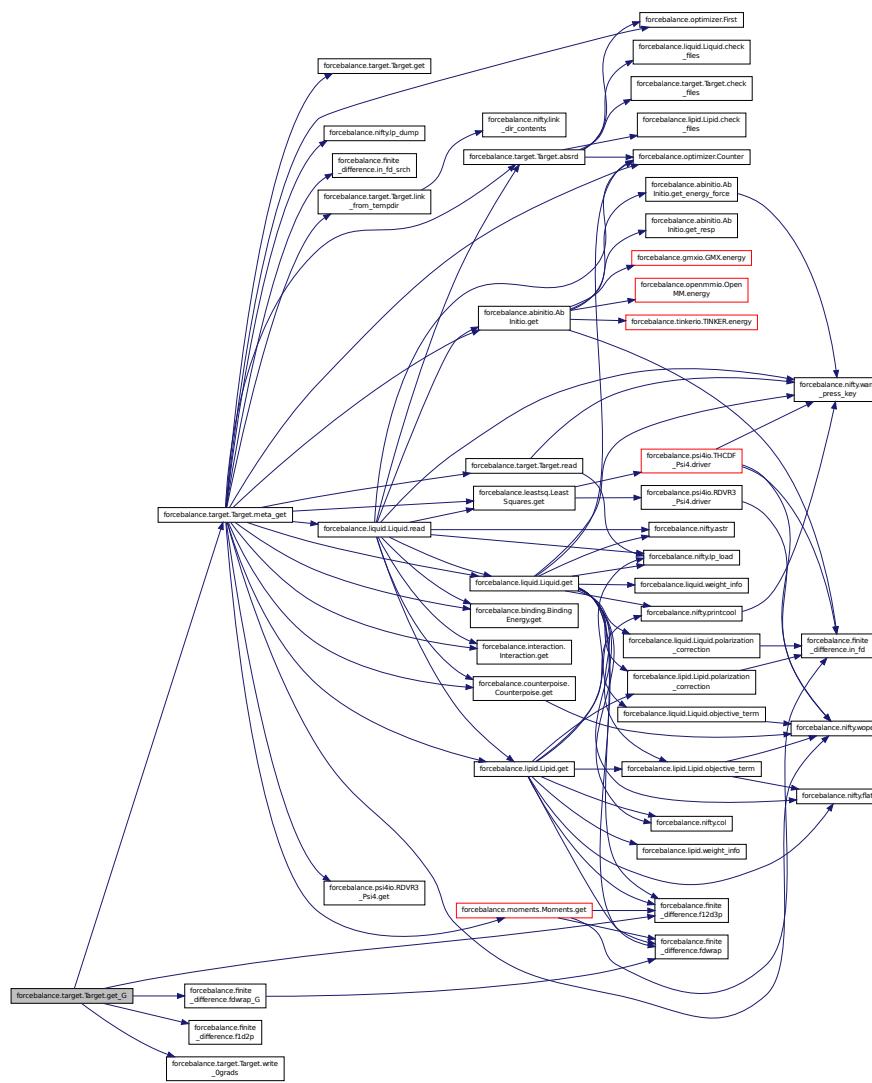
```
def forcebalance.target.Target.get_G ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.get_H ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient / Hessian.
```

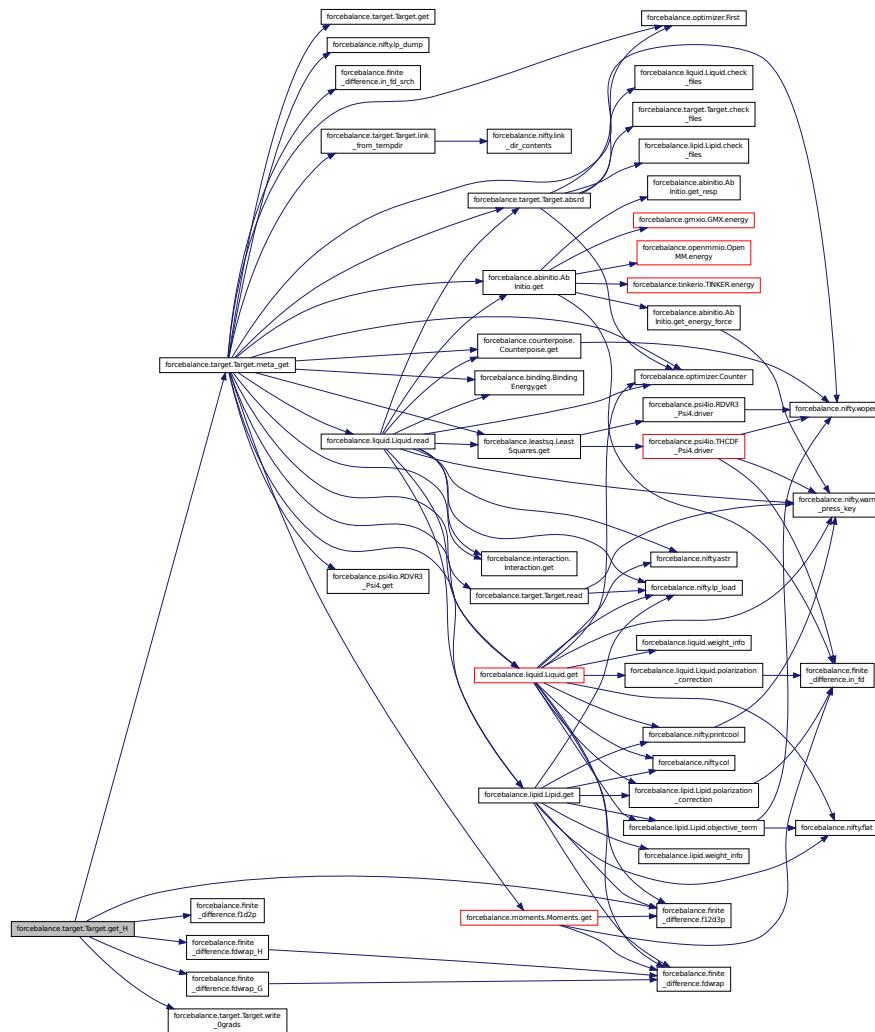
First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through

the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

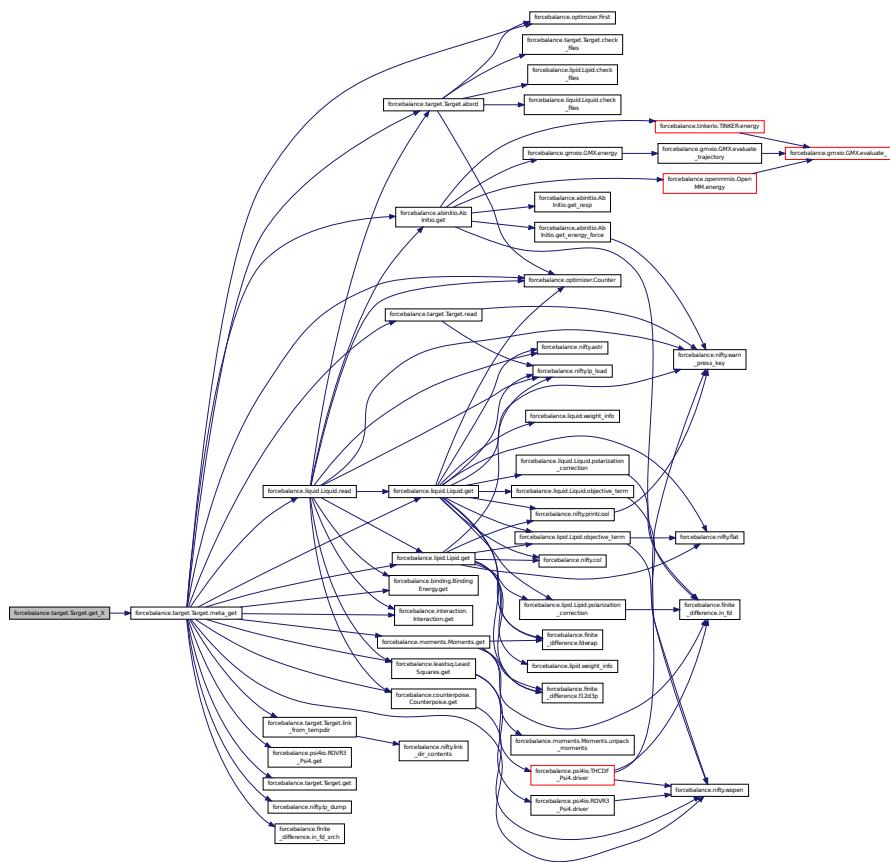
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

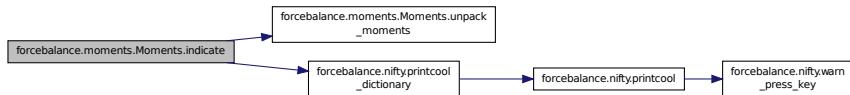
Here is the call graph for this function:



def forcebalance.moments.Moments.indicate(self) [inherited] Print qualitative indicator.

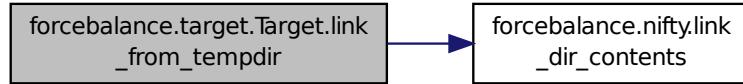
Definition at line 139 of file moments.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

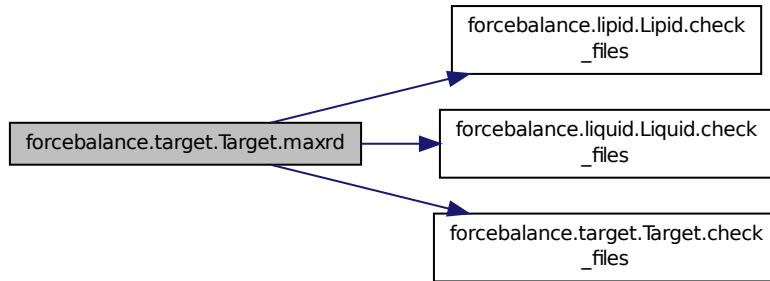
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

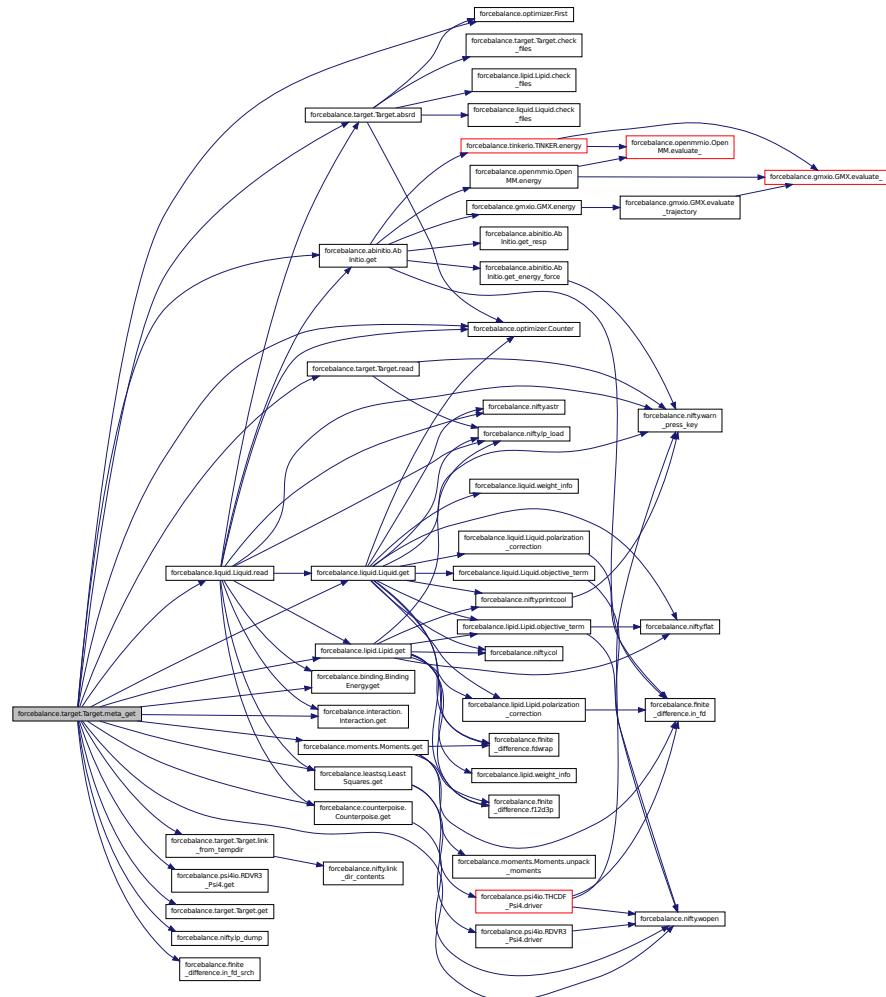


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

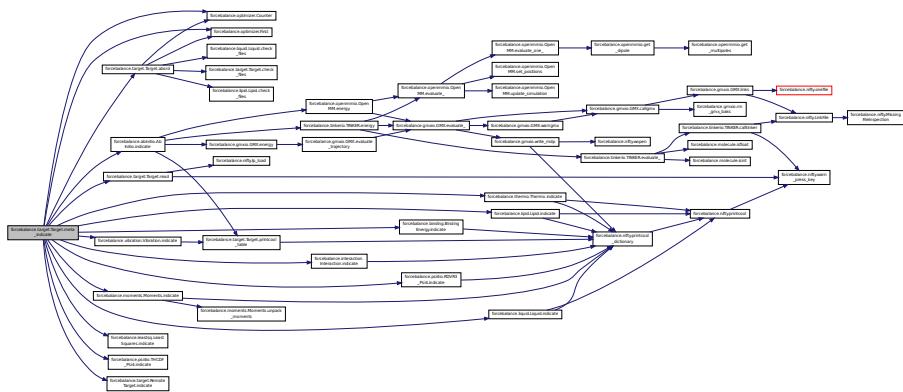
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

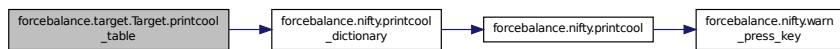
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

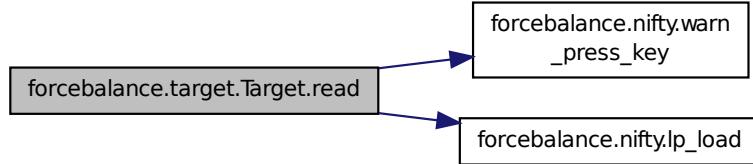
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.moments.Moments.read_reference_data (self) [inherited] Read the reference data from a file.

Definition at line 70 of file moments.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

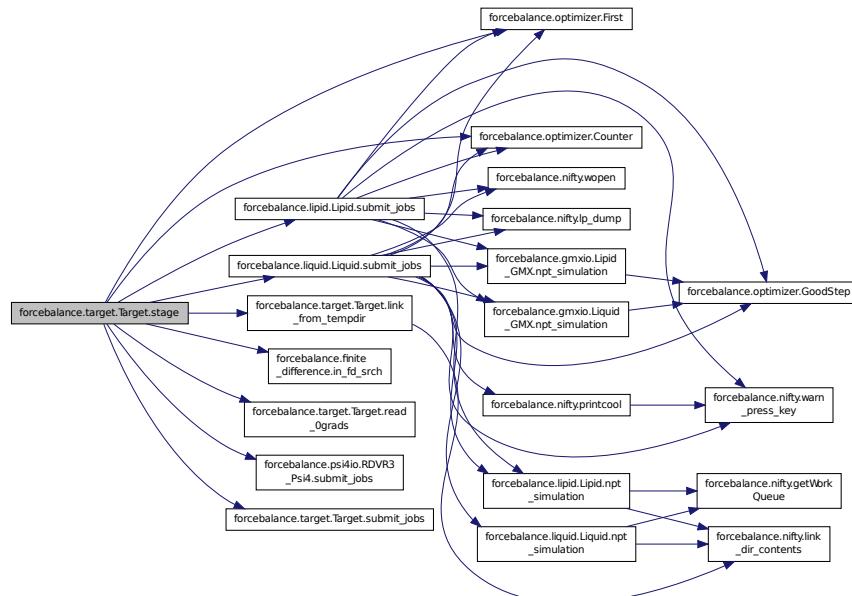
def forcebalance.BaseClass.set_option (self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



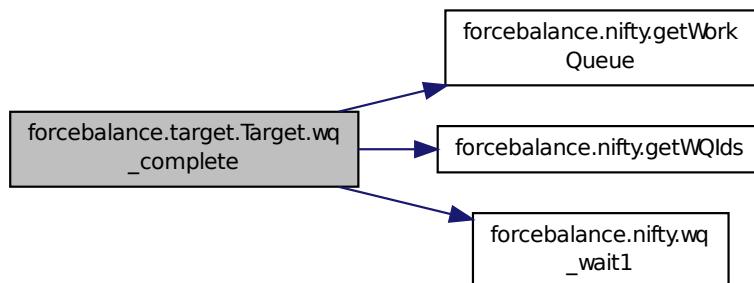
```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.moments.Moments.unpack_moments ( self, moment_dict ) [inherited] Definition at
line 165 of file moments.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work
Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.50.4 Member Data Documentation

forcebalance.moments.Moments.calc_moments [inherited] Definition at line 198 of file moments.py.

forcebalance.moments.Moments.denoms [inherited] Definition at line 48 of file moments.py.

forcebalance.moments.Moments.engine [inherited] Read in the reference data.

Build keyword dictionaries to pass to engine. Create engine object.

Definition at line 66 of file moments.py.

forcebalance.tinkerio.Moments.TINKER.engine_ Default file names for coordinates and key file.

Definition at line 1102 of file tinkerio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.moments.Moments.mfnm [inherited] The mdata.txt file that contains the moments.

Definition at line 57 of file moments.py.

forcebalance.moments.Moments.na [inherited] Number of atoms.

Definition at line 72 of file moments.py.

forcebalance.moments.Moments.objective [inherited] Definition at line 199 of file moments.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.moments.Moments.ref_eigvals [inherited] Definition at line 73 of file moments.py.

forcebalance.moments.Moments.ref_eigvecs [inherited] Definition at line 74 of file moments.py.

forcebalance.moments.Moments.ref_moments [inherited] Dictionary of reference multipole moments.

Definition at line 59 of file moments.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number
The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

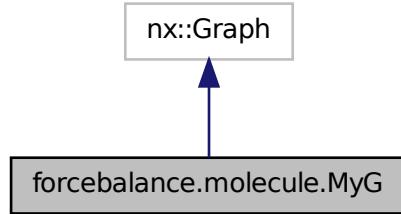
Definition at line 162 of file target.py.

The documentation for this class was generated from the following file:

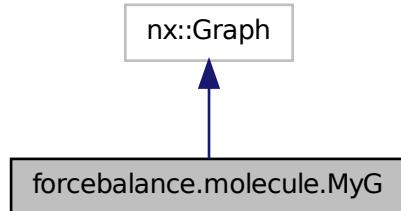
- [tinkerio.py](#)

8.51 forcebalance.molecule.MyG Class Reference

Inheritance diagram for forcebalance.molecule.MyG:



Collaboration diagram for forcebalance.molecule.MyG:



Public Member Functions

- def `_init_`
- def `_eq_`
- def `_hash_`

The hash function is something we can use to discard two things that are obviously not equal.

- def `L`

Return a list of the sorted atom numbers in this graph.

- def `AStr`

Return a string of atoms, which serves as a rudimentary 'fingerprint' : '99,100,103,151'.

- def `e`

Return an array of the elements.

- def `ef`

Create an Empirical Formula.

- def `x`

Get a list of the coordinates.

Public Attributes

- Alive

8.51.1 Detailed Description

Definition at line 324 of file molecule.py.

8.51.2 Constructor & Destructor Documentation

def forcebalance.molecule.MyG.__init__ (self) Definition at line 325 of file molecule.py.

8.51.3 Member Function Documentation

def forcebalance.molecule.MyG.__eq__ (self, other) Definition at line 328 of file molecule.py.

def forcebalance.molecule.MyG.__hash__ (self) The hash function is something we can use to discard two things that are obviously not equal.

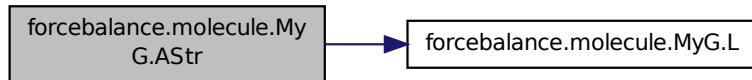
Here we neglect the hash.

Definition at line 337 of file molecule.py.

def forcebalance.molecule.MyG.AStr (self) Return a string of atoms, which serves as a rudimentary 'fingerprint' : '99,100,103,151' .

Definition at line 345 of file molecule.py.

Here is the call graph for this function:

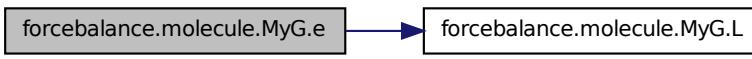


def forcebalance.molecule.MyG.e (self) Return an array of the elements.

For instance ['H' 'C' 'C' 'H'].

Definition at line 349 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.MyG.ef (self) Create an Empirical Formula.

Definition at line 354 of file molecule.py.

Here is the call graph for this function:



def forcebalance.molecule.MyG.L (self) Return a list of the sorted atom numbers in this graph.

Definition at line 341 of file molecule.py.

def forcebalance.molecule.MyG.x (self) Get a list of the coordinates.

Definition at line 359 of file molecule.py.

Here is the call graph for this function:



8.51.4 Member Data Documentation

forcebalance.molecule.MyG.Alive Definition at line 327 of file molecule.py.

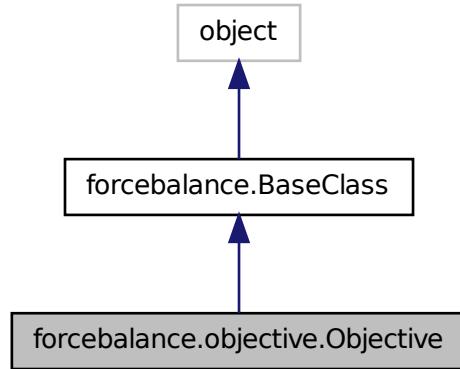
The documentation for this class was generated from the following file:

- [molecule.py](#)

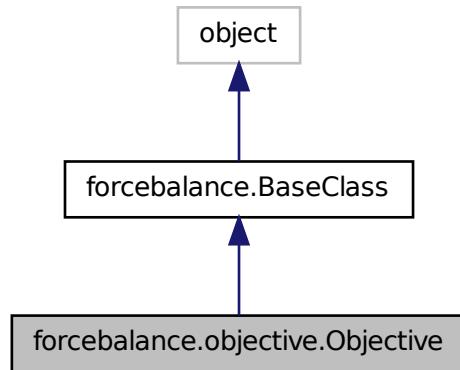
8.52 forcebalance.objective.Objective Class Reference

[Objective](#) function.

Inheritance diagram for forcebalance.objective.Objective:



Collaboration diagram for forcebalance.objective.Objective:



Public Member Functions

- def `_init_`
- def `Target_Terms`
- def `Indicate`
 Print objective function contributions.
- def `Full`
- def `__setattr__`
- def `set_option`

Public Attributes

- [Targets](#)
Work Queue Port (The specific target itself may or may not actually use this.)
- [FF](#)
The force field (it seems to be everywhere)
- [Penalty](#)
Initialize the penalty function.
- [WTot](#)
Obtain the denominator.
- [ObjDict](#)
- [ObjDict.Last](#)
- [verbose_options](#)
- [PrintOptionDict](#)

8.52.1 Detailed Description

[Objective](#) function.

The objective function is a combination of contributions from the different fitting targets. Basically, it loops through the targets, gets their contributions to the objective function and then sums all of them (although more elaborate schemes are conceivable). The return value is the same data type as calling the target itself: a dictionary containing the objective function, the gradient and the Hessian.

The penalty function is also computed here; it keeps the parameters from straying too far from their initial values.

Parameters

in	<i>mvals</i>	The mathematical parameters that enter into computing the objective function
in	<i>Order</i>	The requested order of differentiation

Definition at line 115 of file objective.py.

8.52.2 Constructor & Destructor Documentation

def forcebalance.objective.Objective.__init__ (*self*, *options*, *tgt_opts*, *forcefield*) Definition at line 116 of file objective.py.

Here is the call graph for this function:

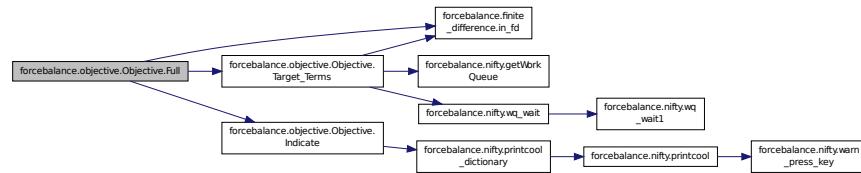


8.52.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (*self*, *key*, *value*) [inherited] Definition at line 28 of file __init__.py.

```
def forcebalance.objective.Objective.Full ( self, mvals, Order = 0, verbose = False ) Definition at line 261  
of file objective.py.
```

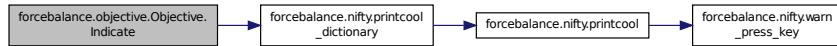
Here is the call graph for this function:



```
def forcebalance.objective.Objective.Indicate ( self ) Print objective function contributions.
```

Definition at line 223 of file objective.py.

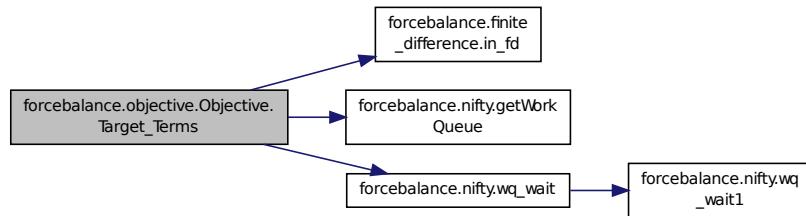
Here is the call graph for this function:



```
def forcebalance.BaseClass.set_option ( self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

```
def forcebalance.objective.Objective.Target_Terms ( self, mvals, Order = 0, verbose = False ) Definition at line 163 of file objective.py.
```

Here is the call graph for this function:



8.52.4 Member Data Documentation

forcebalance.objective.Objective.FF The force field (it seems to be everywhere)
Definition at line 142 of file objective.py.

forcebalance.objective.Objective.ObjDict Definition at line 152 of file objective.py.

forcebalance.objective.Objective.ObjDict_Last Definition at line 153 of file objective.py.

forcebalance.objective.Objective.Penalty Initialize the penalty function.

Definition at line 144 of file objective.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.objective.Objective.Targets Work Queue Port (The specific target itself may or may not actually use this.)

Asynchronous objective function evaluation (i.e. execute Work Queue and local objective concurrently.) The list of fitting targets

Definition at line 131 of file objective.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.objective.Objective.WTot Obtain the denominator.

Definition at line 149 of file objective.py.

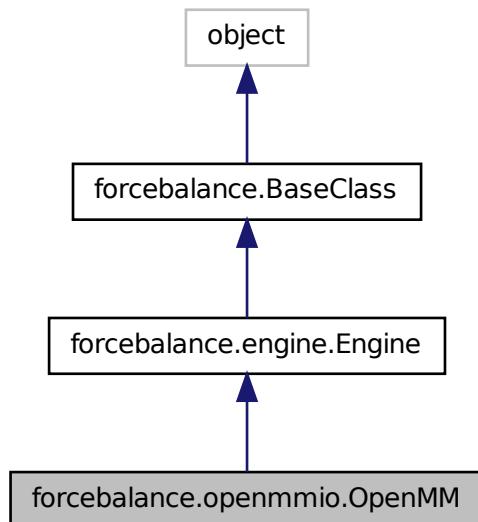
The documentation for this class was generated from the following file:

- [objective.py](#)

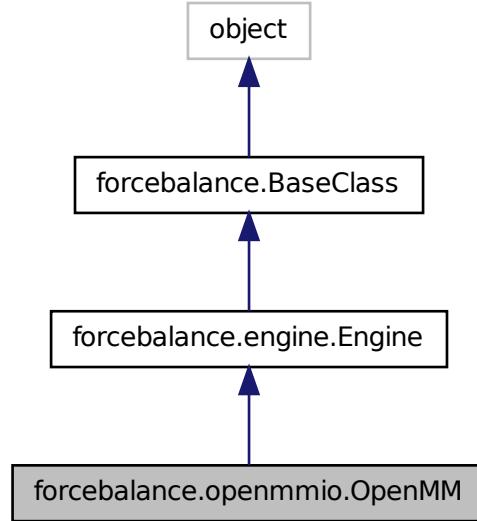
8.53 forcebalance.openmmio.OpenMM Class Reference

Derived from Engine object for carrying out general purpose [OpenMM](#) calculations.

Inheritance diagram for forcebalance.openmmio.OpenMM:



Collaboration diagram for forcebalance.openmmio.OpenMM:



Public Member Functions

- def [`_init_`](#)
- def [`setopts`](#)

Called by `init` ; Set OpenMM-specific options.
- def [`readsrc`](#)

Called by `init` ; read files from the source directory.
- def [`prepare`](#)

Prepare the calculation.
- def [`create_simulation`](#)

Create simulation object.
- def [`update_simulation`](#)

Create the simulation object, or update the force field parameters in the existing simulation object.
- def [`set_positions`](#)

Set the positions and periodic box vectors to one of the stored coordinates.
- def [`compute_volume`](#)

Compute the total volume of an `OpenMM` system.
- def [`compute_mass`](#)

Compute the total mass of an `OpenMM` system.
- def [`evaluate_one`](#)
- def [`evaluate_`](#)

Utility function for computing energy, and (optionally) forces and dipoles using `OpenMM`.
- def [`energy_one`](#)
- def [`energy_force_one`](#)

- def `energy`
- def `energy_force`

Loop through the snapshots and compute the energies and forces using OpenMM.
- def `energy_dipole`

Loop through the snapshots and compute the energies and forces using OpenMM.
- def `normal_modes`
- def `optimize`

Optimize the geometry and align the optimized geometry to the starting geometry, and return the RMSD.
- def `multipole_moments`

Return the multipole moments of the i-th snapshot in Debye and Buckingham units.
- def `energy_rmsd`

Calculate energy of the 1st structure (optionally minimize and return the minimized energy and RMSD).
- def `interaction_energy`

Calculate the interaction energy for two fragments.
- def `molecular_dynamics`

Method for running a molecular dynamics simulation.
- def `setopts`
- def `prepare`
- def `__setattr__`
- def `set_option`

Public Attributes

- `valkwds`
- `platname`

Target settings override.
- `precision`
- `platform`

Set the simulation platform.
- `simkargs`
- `mol`
- `pdb`

Create the OpenMM PDB object.
- `ffxml`

Create the OpenMM ForceField object.
- `forcefield`
- `mmopts`

OpenMM options for setting up the System.
- `AMOEBA`

Are we using AMOEBA?
- `pbc`

Set system options from ForceBalance force field options.
- `xyz_omm`

Generate OpenMM-compatible positions.
- `AtomMask`

Build a topology and atom lists.
- `AtomLists`
- `tdiv`

Determine the integrator.

- [simulation](#)
If no temperature control, default to the Verlet integrator.

- [mod](#)
- [system](#)
- [vsinfo](#)
- [nbcharges](#)
- [vsprm](#)
- [name](#)
- [A](#)
- [B](#)
- [mass](#)
- [ndof](#)
- [verbose](#)
- [target](#)

Engines can get properties from the Target that creates them.

- [root](#)
- [srcdir](#)
- [tempdir](#)
- [FF](#)
- [verbose_options](#)
- [PrintOptionDict](#)

8.53.1 Detailed Description

Derived from Engine object for carrying out general purpose [OpenMM](#) calculations.

Definition at line 467 of file openmmio.py.

8.53.2 Constructor & Destructor Documentation

def forcebalance.openmmio.OpenMM.__init__(self, name = "openmm", kwargs) Definition at line 470 of file openmmio.py.

8.53.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__(self, key, value) [inherited] Definition at line 28 of file __init__.py.

def forcebalance.openmmio.OpenMM.compute_mass(self, system) Compute the total mass of an [OpenMM](#) system.

Definition at line 773 of file openmmio.py.

def forcebalance.openmmio.OpenMM.compute_volume(self, box_vectors) Compute the total volume of an [OpenMM](#) system.

Definition at line 764 of file openmmio.py.

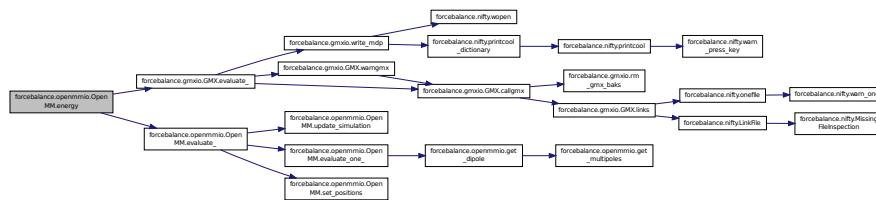
def forcebalance.openmmio.OpenMM.create_simulation(self, timestep = 1.0, faststep = 0.25, temperature = None, pressure = None, anisotropic = False, mts = False, collision = 1.0, nbarostat = 25, rmpd_beads = 0, kwargs) Create simulation object.

Note that this also takes in some options pertinent to system setup, including the type of MD integrator and type of pressure control.

Definition at line 644 of file openmmio.py.

def forcebalance.openmmio.OpenMM.energy (self) Definition at line 835 of file openmmio.py.

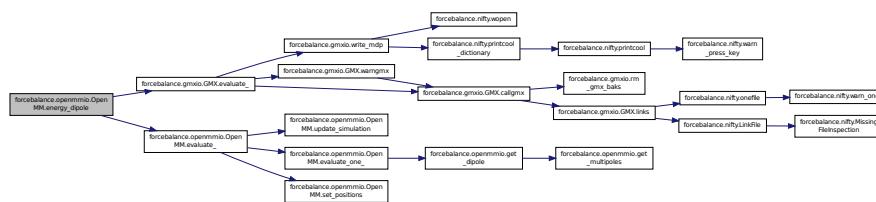
Here is the call graph for this function:



def forcebalance.openmmio.OpenMM.energy_dipole (self) Loop through the snapshots and compute the energies and forces using OpenMM.

Definition at line 848 of file openmmio.py.

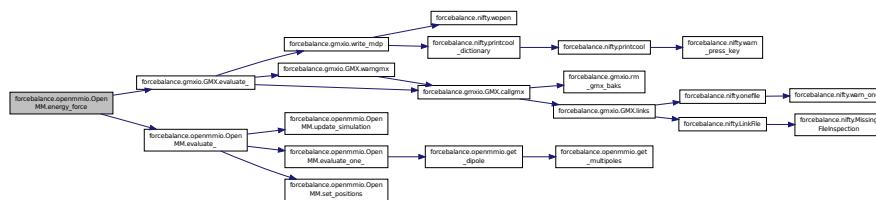
Here is the call graph for this function:



def forcebalance.openmmio.OpenMM.energy_force (self) Loop through the snapshots and compute the energies and forces using OpenMM.

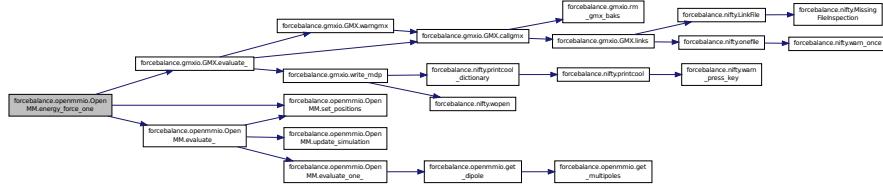
Definition at line 840 of file openmmio.py.

Here is the call graph for this function:



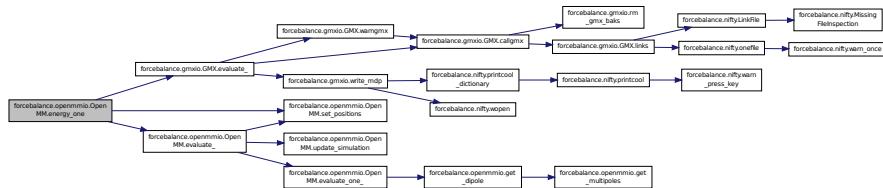
def forcebalance.openmmio.OpenMM.energy_force_one (self) Definition at line 830 of file openmmio.py.

Here is the call graph for this function:



def forcebalance.openmmio.OpenMM.energy_one (self, shot) Definition at line 826 of file openmmio.py.

Here is the call graph for this function:

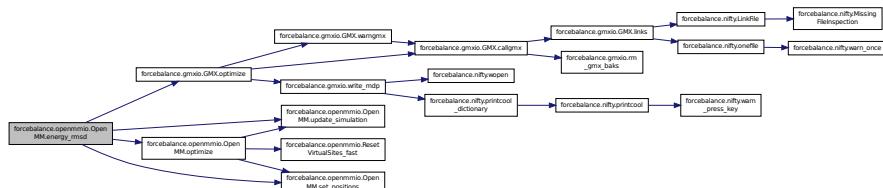


def forcebalance.openmmio.OpenMM.energy_rmsd (self, shot = 0, optimize = True) Calculate energy of the 1st structure (optionally minimize and return the minimized energy and RMSD).

In kcal/mol.

Definition at line 909 of file openmmio.py.

Here is the call graph for this function:



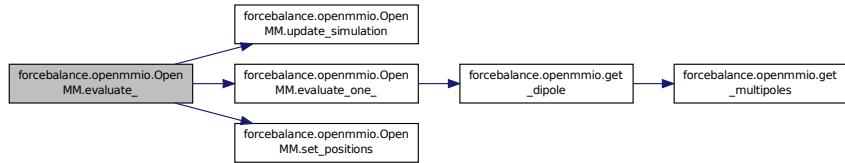
def forcebalance.openmmio.OpenMM.evaluate_ (self, force = False, dipole = False, traj = False) Utility function for computing energy, and (optionally) forces and dipoles using OpenMM.

Inputs: force: Switch for calculating the force. dipole: Switch for calculating the dipole. traj: Trajectory (listing of coordinate and box 2-tuples). If provide, will loop over these snapshots. Otherwise will do a single point evaluation at the current geometry.

Outputs: Result: Dictionary containing energies, forces and/or dipoles.

Definition at line 804 of file openmmio.py.

Here is the call graph for this function:



def forcebalance.openmmio.OpenMM.evaluate_one_(self, force = False, dipole = False) Definition at line 779 of file openmmio.py.

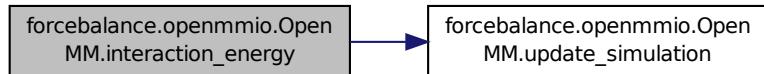
Here is the call graph for this function:



def forcebalance.openmmio.OpenMM.interaction_energy(self, fraga, fragb) Calculate the interaction energy for two fragments.

Definition at line 930 of file openmmio.py.

Here is the call graph for this function:



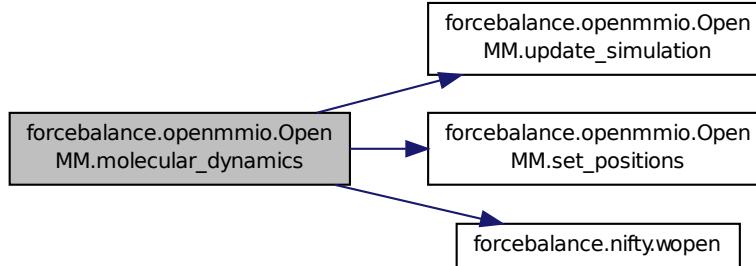
def forcebalance.openmmio.OpenMM.molecular_dynamics(self, nsteps, timestep, temperature = None, pressure = None, nequil = 0, nsave = 1000, minimize = True, anisotropic = False, save_traj = False, verbose = False, kwargs) Method for running a molecular dynamics simulation.

Required arguments: nsteps = (int) Number of total time steps timestep = (float) Time step in FEMTOSECOND-S temperature = (float) Temperature control (Kelvin) pressure = (float) Pressure control (atmospheres) nequil = (int) Number of additional time steps at the beginning for equilibration nsave = (int) Step interval for saving and printing data minimize = (bool) Perform an energy minimization prior to dynamics

Returns simulation data: Rhos = (array) Density in kilogram m^-3 Potentials = (array) Potential energies Kinetics = (array) Kinetic energies Volumes = (array) Box volumes Dips = (3xN array) Dipole moments EComps = (dict) Energy components

Definition at line 980 of file openmmio.py.

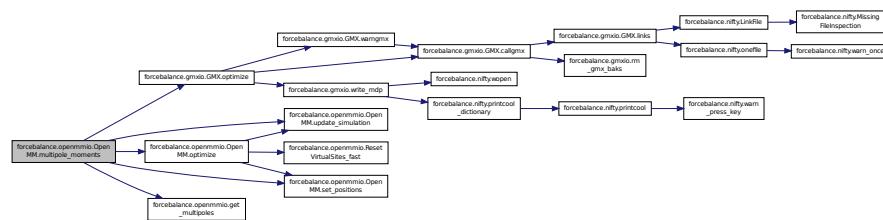
Here is the call graph for this function:



def forcebalance.openmmio.OpenMM.multipole_moments (self, shot = 0, optimize = True, polarizability = False) Return the multipole moments of the i-th snapshot in Debye and Buckingham units.

Definition at line 887 of file openmmio.py.

Here is the call graph for this function:

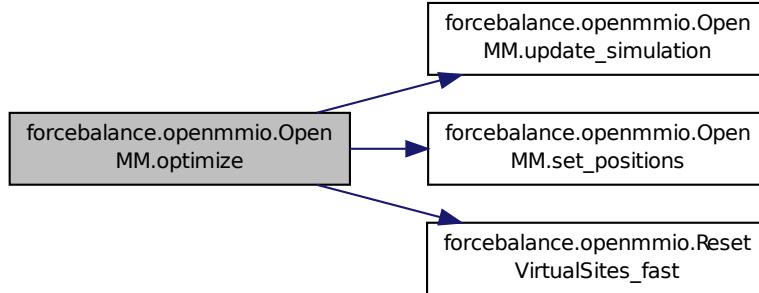


def forcebalance.openmmio.OpenMM.normal_modes (self, shot = 0, optimize = True) Definition at line 852 of file openmmio.py.

def forcebalance.openmmio.OpenMM.optimize(self, shot = 0, crit = 1e-4) Optimize the geometry and align the optimized geometry to the starting geometry, and return the RMSD.

Definition at line 857 of file openmmio.py.

Here is the call graph for this function:



def forcebalance.engine.Engine.prepare(self, kwargs) [inherited] Definition at line 95 of file engine.py.

def forcebalance.openmmio.OpenMM.prepare(self, pbc = False, mmopts = {}, kwargs) Prepare the calculation.

Note that we don't create the Simulation object yet, because that may depend on MD integrator parameters, thermostat, barostat etc.

Definition at line 545 of file openmmio.py.

def forcebalance.openmmio.OpenMM.readsrc(self, kwargs) Called by `init` ; read files from the source directory.

Provide a molecule object or a coordinate file. Add an optional PDB file for residues, atom names etc.

Definition at line 517 of file openmmio.py.

def forcebalance.BaseClass.set_option(self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.openmmio.OpenMM.set_positions(self, shot = 0, traj = None) Set the positions and periodic box vectors to one of the stored coordinates.

*** NOTE: If you run a MD simulation, then the coordinates are overwritten by the MD trajectory. ***

Definition at line 743 of file openmmio.py.

def forcebalance.engine.Engine.setopts(self, kwargs) [inherited] Definition at line 89 of file engine.py.

def forcebalance.openmmio.OpenMM.setopts(self, platname = "CUDA", precision = "single", kwargs) Called by `init` ; Set OpenMM-specific options.

Definition at line 476 of file openmmio.py.

def forcebalance.openmmio.OpenMM.update_simulation(self, kwargs) Create the simulation object, or update the force field parameters in the existing simulation object.

This should be run when we write a new force field XML file.

Definition at line 705 of file openmmio.py.

8.53.4 Member Data Documentation

forcebalance.openmmio.OpenMM.A Definition at line 941 of file openmmio.py.

forcebalance.openmmio.OpenMM.AMOEBA Are we using AMOEBA?

Definition at line 571 of file openmmio.py.

forcebalance.openmmio.OpenMM.AtomLists Definition at line 632 of file openmmio.py.

forcebalance.openmmio.OpenMM.AtomMask Build a topology and atom lists.

Definition at line 631 of file openmmio.py.

forcebalance.openmmio.OpenMM.B Definition at line 943 of file openmmio.py.

forcebalance.engine.Engine.FF [inherited] Definition at line 65 of file engine.py.

forcebalance.openmmio.OpenMM.ffxml Create the [OpenMM](#) ForceField object.

Definition at line 556 of file openmmio.py.

forcebalance.openmmio.OpenMM.forcefield Definition at line 557 of file openmmio.py.

forcebalance.openmmio.OpenMM.mass Definition at line 1016 of file openmmio.py.

forcebalance.openmmio.OpenMM.mmopts [OpenMM](#) options for setting up the System.

Definition at line 568 of file openmmio.py.

forcebalance.openmmio.OpenMM.mod Definition at line 710 of file openmmio.py.

forcebalance.openmmio.OpenMM.mol Definition at line 528 of file openmmio.py.

forcebalance.openmmio.OpenMM.name Definition at line 935 of file openmmio.py.

forcebalance.openmmio.OpenMM.nbcharges Definition at line 715 of file openmmio.py.

forcebalance.openmmio.OpenMM.ndof Definition at line 1019 of file openmmio.py.

forcebalance.openmmio.OpenMM.pbc Set system options from ForceBalance force field options.

Set system options from periodic boundary conditions.

Definition at line 587 of file openmmio.py.

forcebalance.openmmio.OpenMM.pdb Create the [OpenMM](#) PDB object.

Definition at line 550 of file openmmio.py.

forcebalance.openmmio.OpenMM.platform Set the simulation platform.

Definition at line 497 of file openmmio.py.

forcebalance.openmmio.OpenMM.platname Target settings override.

Set the device to the environment variable or zero otherwise.

Definition at line 481 of file openmmio.py.

forcebalance.openmmio.OpenMM.precision Definition at line 482 of file openmmio.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.engine.Engine.root [inherited] Definition at line 56 of file engine.py.

forcebalance.openmmio.OpenMM.simkwargs Definition at line 511 of file openmmio.py.

forcebalance.openmmio.OpenMM.simulation If no temperature control, default to the Verlet integrator.

Add the barostat. Set up for energy component analysis. If virtual particles are used with AMOEBA... Finally create the simulation object.

Definition at line 691 of file openmmio.py.

forcebalance.engine.Engine.srcdir [inherited] Definition at line 57 of file engine.py.

forcebalance.openmmio.OpenMM.system Definition at line 713 of file openmmio.py.

forcebalance.engine.Engine.target [inherited] Engines can get properties from the Target that creates them.

Definition at line 55 of file engine.py.

forcebalance.openmmio.OpenMM.tdiv Determine the integrator.

If temperature control is turned on, then run Langevin dynamics.

Definition at line 648 of file openmmio.py.

forcebalance.engine.Engine.tempdir [inherited] Definition at line 58 of file engine.py.

forcebalance.openmmio.OpenMM.valkwd Definition at line 471 of file openmmio.py.

forcebalance.engine.Engine.verbose [inherited] Definition at line 50 of file engine.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.openmmio.OpenMM.vsinfo Definition at line 714 of file openmmio.py.

forcebalance.openmmio.OpenMM.vsprm Definition at line 728 of file openmmio.py.

forcebalance.openmmio.OpenMM.xyz_omms Generate OpenMM-compatible positions.

Definition at line 605 of file openmmio.py.

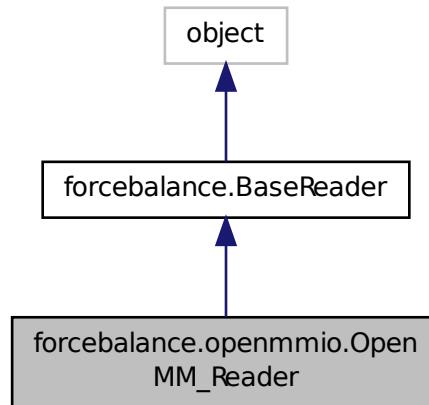
The documentation for this class was generated from the following file:

- [openmmio.py](#)

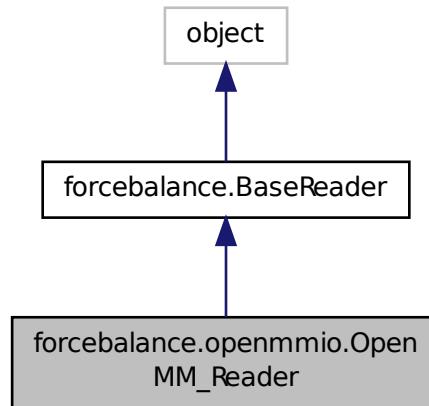
8.54 forcebalance.openmmio.OpenMM_Reader Class Reference

Class for parsing [OpenMM](#) force field files.

Inheritance diagram for forcebalance.openmmio.OpenMM_Reader:



Collaboration diagram for forcebalance.openmmio.OpenMM_Reader:



Public Member Functions

- def [__init__](#)
- def [build.pid](#)

Build the parameter identifier (see link for an example)

- def [Split](#)
- def [Whites](#)
- def [feed](#)
- def [build_pid](#)

Returns the parameter type (e.g.

Public Attributes

- [pdict](#)
Initialize the superclass.
- [In](#)
- [itype](#)
- [suffix](#)
- [adict](#)
The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.
- [molatom](#)
The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.
- [Molecules](#)
- [AtomTypes](#)

8.54.1 Detailed Description

Class for parsing [OpenMM](#) force field files.

Definition at line 440 of file openmmio.py.

8.54.2 Constructor & Destructor Documentation

def forcebalance.openmmio.OpenMM_Reader.__init__ (self, fnm) Definition at line 441 of file openmmio.py.

8.54.3 Member Function Documentation

def forcebalance.BaseReader.build_pid (self, pfd) [inherited] Returns the parameter type (e.g. K in BONDSK) based on the current interaction type.

Both the 'pdict' dictionary (see [gmxio.pdict](#)) and the interaction type 'state' (here, BONDS) are needed to get the parameter type.

If, however, 'pdict' does not contain the ptype value, a suitable substitute is simply the field number.

Note that if the interaction type state is not set, then it defaults to the file name, so a generic parameter ID is 'filename.line.num.field.num'

Definition at line 124 of file __init__.py.

def forcebalance.openmmio.OpenMM_Reader.build_pid (self, element, parameter) Build the parameter identifier (see [link](#) for an example)

Todo Add a link here

Definition at line 450 of file openmmio.py.

def forcebalance.BaseReader.feed (self, line) [inherited] Definition at line 105 of file __init__.py.

def forcebalance.BaseReader.Split (self, line) [inherited] Definition at line 99 of file __init__.py.

def forcebalance.BaseReader.Whites (self, line) [inherited] Definition at line 102 of file __init__.py.

8.54.4 Member Data Documentation

forcebalance.BaseReader.adict [inherited] The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

Definition at line 89 of file __init__.py.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file __init__.py.

forcebalance.BaseReader.itype [inherited] Definition at line 85 of file __init__.py.

forcebalance.BaseReader.In [inherited] Definition at line 84 of file __init__.py.

forcebalance.BaseReader.molatom [inherited] The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

self.moleculerdict = OrderedDict() The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.

Definition at line 94 of file __init__.py.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file __init__.py.

forcebalance.openmmio.OpenMM_Reader.pdict Initialize the superclass.

:) The parameter dictionary (defined in this file)

Definition at line 445 of file openmmio.py.

forcebalance.BaseReader.suffix [inherited] Definition at line 86 of file __init__.py.

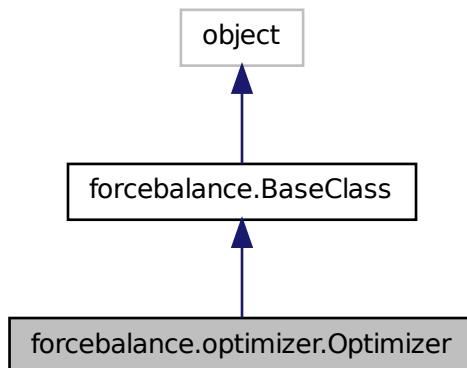
The documentation for this class was generated from the following file:

- [openmmio.py](#)

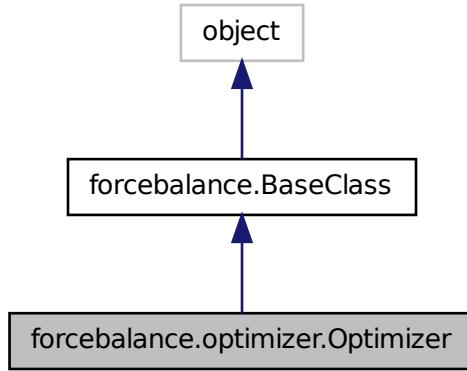
8.55 forcebalance.optimizer.Optimizer Class Reference

[Optimizer](#) class.

Inheritance diagram for forcebalance.optimizer.Optimizer:



Collaboration diagram for forcebalance.optimizer.Optimizer:



Public Member Functions

- def [`_init_`](#)
Create an [Optimizer](#) object.
- def [`recover`](#)
- def [`save_mvals_to_input`](#)
Write a new input file (`s_save.in`) containing the current mathematical parameters.
- def [`Run`](#)
Call the appropriate optimizer.
- def [`adjh`](#)
- def [`MainOptimizer`](#)
The main ForceBalance adaptive trust-radius pseudo-Newton optimizer.
- def [`step`](#)
Computes the next step in the parameter space.
- def [`NewtonRaphson`](#)
Optimize the force field parameters using the Newton-Raphson method .
- def [`BFGS`](#)
Optimize the force field parameters using the BFGS method; currently the recommended choice .
- def [`ScipyOptimizer`](#)
Driver for SciPy optimizations.
- def [`GeneticAlgorithm`](#)
Genetic algorithm, under development.
- def [`Simplex`](#)
Use SciPy's built-in simplex algorithm to optimize the parameters.
- def [`Powell`](#)
Use SciPy's built-in Powell direction-set algorithm to optimize the parameters.
- def [`Anneal`](#)
Use SciPy's built-in simulated annealing algorithm to optimize the parameters.

- def **ConjugateGradient**
Use SciPy's built-in conjugate gradient algorithm to optimize the parameters.
- def **Scipy_BFGS**
Use SciPy's built-in BFGS algorithm to optimize the parameters.
- def **BasinHopping**
Use SciPy's built-in basin hopping algorithm to optimize the parameters.
- def **TruncatedNewton**
Use SciPy's built-in truncated Newton (fmin_tnc) algorithm to optimize the parameters.
- def **NewtonCG**
Use SciPy's built-in Newton-CG (fmin_ncg) algorithm to optimize the parameters.
- def **Scan_Values**
Scan through parameter values.
- def **ScanMVals**
Scan through the mathematical parameter space.
- def **ScanPVals**
Scan through the physical parameter space.
- def **SinglePoint**
A single-point objective function computation.
- def **Gradient**
A single-point gradient computation.
- def **Hessian**
A single-point Hessian computation.
- def **FDCheckG**
Finite-difference checker for the objective function gradient.
- def **FDCheckH**
Finite-difference checker for the objective function Hessian.
- def **readchk**
Read the checkpoint file for the main optimizer.
- def **writechk**
Write the checkpoint file for the main optimizer.
- def **__setattr__**
- def **set_option**

Public Attributes

- **OptTab**
A list of all the things we can ask the optimizer to do.
- **mvals_bak**
The root directory.
- **failmsg**
Print a special message on failure.
- **Objective**
The objective function (needs to pass in when I instantiate)
- **bhyp**
Whether the penalty function is hyperbolic.
- **FF**
The force field itself.
- **uncert**

Target types which introduce uncertainty into the objective function.

- `bakdir`
- `resdir`
- `excision`

The indices to be excluded from the Hessian update.

- `np`

Number of parameters.

- `mvals0`

The original parameter values.

- `h`
- `chk`
- `H`
- `dx`
- `Val`
- `Grad`
- `Hess`
- `Penalty`
- `prev_bad`
- `xk_prev`
- `x_prev`
- `x_best`
- `verbose_options`
- `PrintOptionDict`

8.55.1 Detailed Description

`Optimizer` class.

Contains several methods for numerical optimization.

For various reasons, the optimizer depends on the force field and fitting targets (i.e. we cannot treat it as a fully independent numerical optimizer). The dependency is rather weak which suggests that I can remove it someday.

Definition at line 51 of file optimizer.py.

8.55.2 Constructor & Destructor Documentation

`def forcebalance.optimizer.Optimizer.__init__ (self, options, Objective, FF)` Create an `Optimizer` object.

The optimizer depends on both the FF and the fitting targets so there is a chain of dependencies: FF → FitSim → `Optimizer`, and FF → `Optimizer`

Here's what we do:

- Take options from the parser
- Pass in the objective function, force field, all fitting targets

Definition at line 64 of file optimizer.py.

8.55.3 Member Function Documentation

`def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited]` Definition at line 28 of file __init__.py.

`def forcebalance.optimizer.Optimizer.adjh (self, trust)` Definition at line 334 of file optimizer.py.

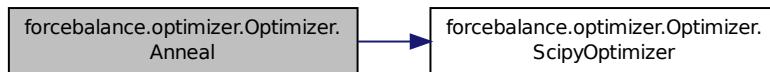
```
def forcebalance.optimizer.Optimizer.Anneal ( self ) Use SciPy's built-in simulated annealing algorithm to optimize the parameters.
```

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 1098 of file optimizer.py.

Here is the call graph for this function:



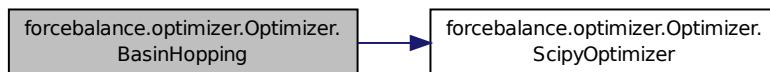
```
def forcebalance.optimizer.Optimizer.BasinHopping ( self ) Use SciPy's built-in basin hopping algorithm to optimize the parameters.
```

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 1113 of file optimizer.py.

Here is the call graph for this function:



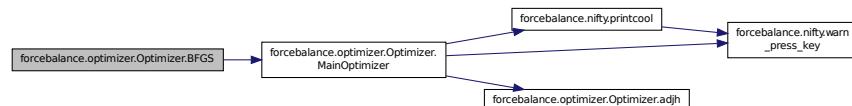
```
def forcebalance.optimizer.Optimizer.BFGS ( self ) Optimize the force field parameters using the BFGS method; currently the recommended choice () .
```

See Also

[MainOptimizer](#))

Definition at line 846 of file optimizer.py.

Here is the call graph for this function:



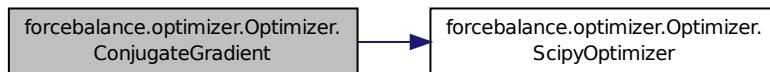
```
def forcebalance.optimizer.Optimizer.ConjugateGradient ( self ) Use SciPy's built-in conjugate gradient algorithm to optimize the parameters.
```

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 1103 of file optimizer.py.

Here is the call graph for this function:

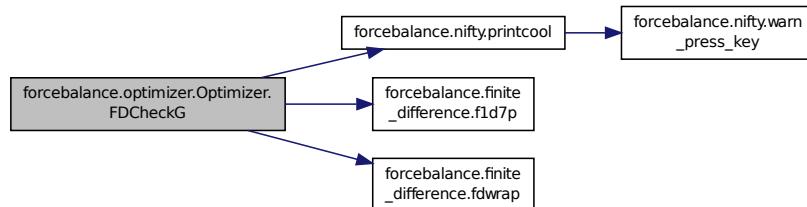


```
def forcebalance.optimizer.Optimizer.FDCheckG ( self ) Finite-difference checker for the objective function gradient.
```

For each element in the gradient, use a five-point finite difference stencil to compute a finite-difference derivative, and compare it to the analytic result.

Definition at line 1222 of file optimizer.py.

Here is the call graph for this function:



```
def forcebalance.optimizer.Optimizer.FDCheckH ( self ) Finite-difference checker for the objective function Hessian.
```

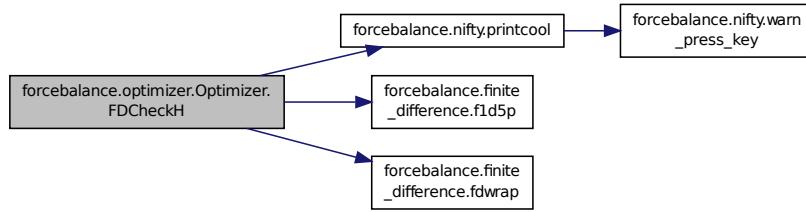
For each element in the Hessian, use a five-point stencil in both parameter indices to compute a finite-difference derivative, and compare it to the analytic result.

This is meant to be a foolproof checker, so it is pretty slow. We could write a faster checker if we assumed we had accurate first derivatives, but it's better to not make that assumption.

The second derivative is computed by double-wrapping the objective function via the 'wrap2' function.

Definition at line 1254 of file optimizer.py.

Here is the call graph for this function:



def forcebalance.optimizer.Optimizer.GeneticAlgorithm (self) Genetic algorithm, under development.
It currently works but a genetic algorithm is more like a concept; i.e. there is no single way to implement it.

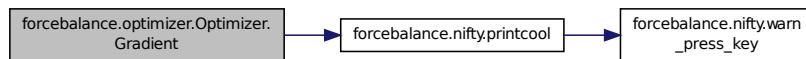
Todo Massive parallelization hasn't been implemented yet

Definition at line 995 of file optimizer.py.

def forcebalance.optimizer.Optimizer.Gradient (self) A single-point gradient computation.

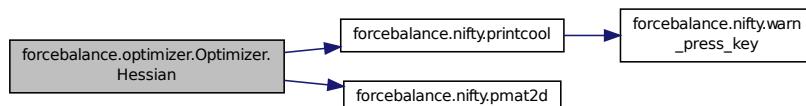
Definition at line 1197 of file optimizer.py.

Here is the call graph for this function:



def forcebalance.optimizer.Optimizer.Hessian (self) A single-point Hessian computation.
Definition at line 1205 of file optimizer.py.

Here is the call graph for this function:



def forcebalance.optimizer.Optimizer.MainOptimizer (self, b_BFGS = 0) The main ForceBalance adaptive trust-radius pseudo-Newton optimizer.
Tried and true in many situations. :)

Usually this function is called with the BFGS or NewtonRaphson method. The NewtonRaphson method is consistently the best method I have, because I always provide at least an approximate Hessian to the objective function. The BFGS method works well, but if gradients are cheap the SciPy_BFGS method also works nicely.

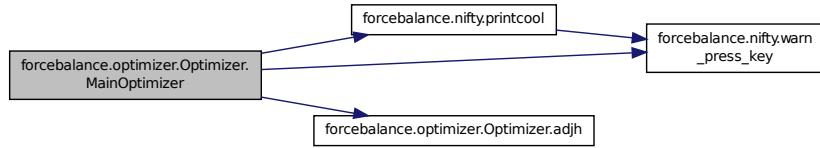
The method adaptively changes the step size. If the step is sufficiently good (i.e. the objective function goes down by a large fraction of the predicted decrease), then the step size is increased; if the step is bad, then it rejects the step and tries again.

The optimization is terminated after either a function value or step size tolerance is reached.

```
@param[in] b_BFGS Switch to use BFGS (True) or Newton-Raphson (False)
```

Definition at line 368 of file optimizer.py.

Here is the call graph for this function:



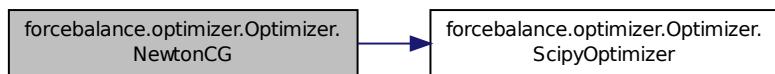
def forcebalance.optimizer.Optimizer.NewtonCG (self) Use SciPy's built-in Newton-CG (fmin_ncg) algorithm to optimize the parameters.

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 1123 of file optimizer.py.

Here is the call graph for this function:



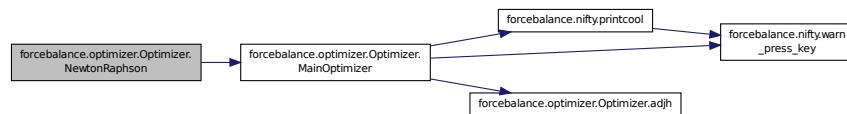
def forcebalance.optimizer.Optimizer.NewtonRaphson (self) Optimize the force field parameters using the Newton-Raphson method (.

See Also

[MainOptimizer](#))

Definition at line 841 of file optimizer.py.

Here is the call graph for this function:



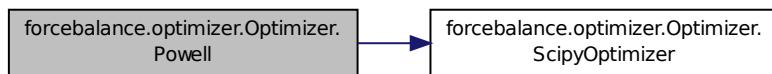
def forcebalance.optimizer.Optimizer.Powell (self) Use SciPy's built-in Powell direction-set algorithm to optimize the parameters.

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 1093 of file optimizer.py.

Here is the call graph for this function:

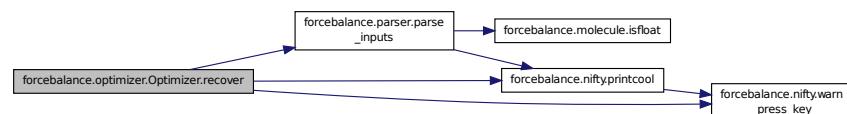


def forcebalance.optimizer.Optimizer.readchk (self) Read the checkpoint file for the main optimizer.

Definition at line 1282 of file optimizer.py.

def forcebalance.optimizer.Optimizer.recover (self) Definition at line 206 of file optimizer.py.

Here is the call graph for this function:

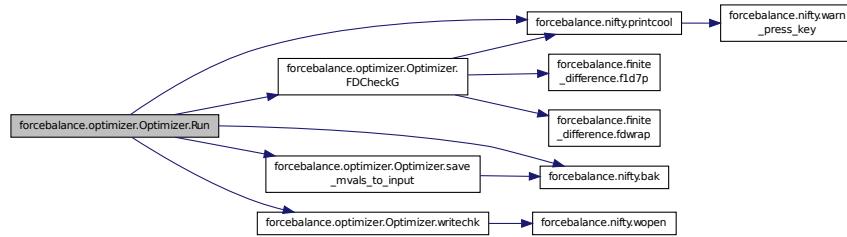


def forcebalance.optimizer.Optimizer.Run (self) Call the appropriate optimizer.

This is the method we might want to call from an executable.

Definition at line 284 of file optimizer.py.

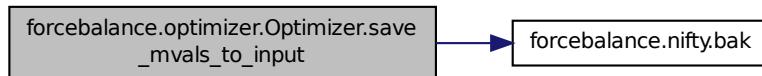
Here is the call graph for this function:



def forcebalance.optimizer.Optimizer.save_mvals_to_input (self, mvals) Write a new input file (s_save.in) containing the current mathematical parameters.

Definition at line 243 of file optimizer.py.

Here is the call graph for this function:



def forcebalance.optimizer.Optimizer.Scan_Values (self, MathPhys = 1) Scan through parameter values.

This option is activated using the inputs:

```
1 scan[mp]vals
2 scan_vals low:hi:nsteps
3 scan_idxnum (number) -or-
4 scan_idxname (name)
```

This method goes to the specified parameter indices and scans through the supplied values, evaluating the objective function at every step.

I hope this method will be useful for people who just want to look at changing one or two parameters and seeing how it affects the force field performance.

Todo Maybe a multidimensional grid can be done.

Parameters

in	MathPhys	Switch to use mathematical (True) or physical (False) parameters.
----	----------	---

Definition at line 1149 of file optimizer.py.

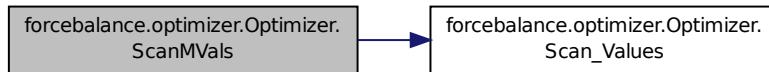
```
def forcebalance.optimizer.Optimizer.ScanMVals ( self ) Scan through the mathematical parameter space.
```

See Also

[Optimizer::ScanValues](#)

Definition at line 1181 of file optimizer.py.

Here is the call graph for this function:



```
def forcebalance.optimizer.Optimizer.ScanPVals ( self ) Scan through the physical parameter space.
```

See Also

[Optimizer::ScanValues](#)

Definition at line 1186 of file optimizer.py.

Here is the call graph for this function:



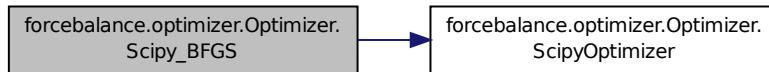
```
def forcebalance.optimizer.Optimizer.Scipy_BFGS ( self ) Use SciPy's built-in BFGS algorithm to optimize the\nparameters.
```

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 1108 of file optimizer.py.

Here is the call graph for this function:



```
def forcebalance.optimizer.Optimizer.ScipyOptimizer ( self, Algorithm = "None" ) Driver for SciPy optimizations.
```

Using any of the SciPy optimizers requires that SciPy is installed. This method first defines several wrappers around the objective function that the SciPy optimizers can use. Then it calls the algorithm itself.

Parameters

in	Algorithm	The optimization algorithm to use, for example 'powell', 'simplex' or 'anneal'
----	-----------	--

Definition at line 859 of file optimizer.py.

```
def forcebalance.BaseClass.set_option ( self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

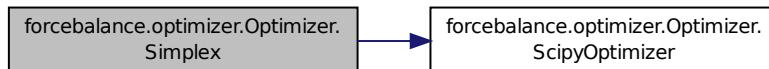
```
def forcebalance.optimizer.Optimizer.Simplex ( self ) Use SciPy's built-in simplex algorithm to optimize the parameters.
```

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 1088 of file optimizer.py.

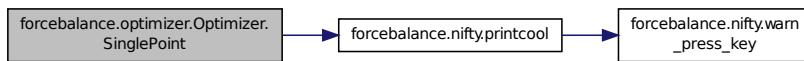
Here is the call graph for this function:



```
def forcebalance.optimizer.Optimizer.SinglePoint ( self ) A single-point objective function computation.
```

Definition at line 1191 of file optimizer.py.

Here is the call graph for this function:



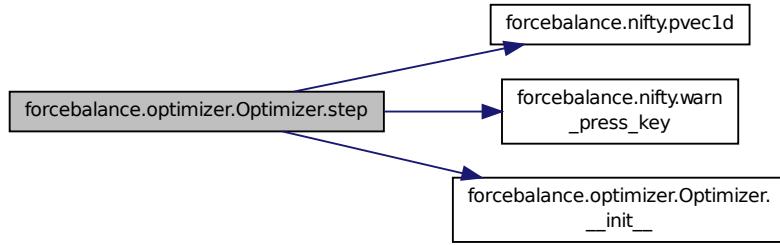
```
def forcebalance.optimizer.Optimizer.step ( self, xk, data, trust ) Computes the next step in the parameter space.
```

There are lots of tricks here that I will document later.

```
@param[in] G The gradient  
@param[in] H The Hessian  
@param[in] trust The trust radius
```

Definition at line 659 of file optimizer.py.

Here is the call graph for this function:



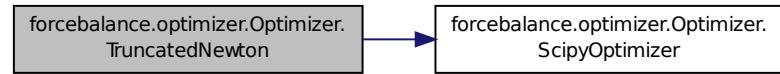
def forcebalance.optimizer.Optimizer.TruncatedNewton (*self*) Use SciPy's built-in truncated Newton (`fmin_tnc`) algorithm to optimize the parameters.

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 1118 of file optimizer.py.

Here is the call graph for this function:



def forcebalance.optimizer.Optimizer.writechk (*self*) Write the checkpoint file for the main optimizer.

Definition at line 1294 of file optimizer.py.

Here is the call graph for this function:



8.55.4 Member Data Documentation

forcebalance.optimizer.Optimizer.bakdir Definition at line 178 of file optimizer.py.

forcebalance.optimizer.Optimizer.bhyp Whether the penalty function is hyperbolic.

Definition at line 172 of file optimizer.py.

forcebalance.optimizer.Optimizer.chk Definition at line 491 of file optimizer.py.

forcebalance.optimizer.Optimizer.dx Definition at line 688 of file optimizer.py.

forcebalance.optimizer.Optimizer.excision The indices to be excluded from the Hessian update.
Definition at line 185 of file optimizer.py.

forcebalance.optimizer.Optimizer.failmsg Print a special message on failure.
Definition at line 164 of file optimizer.py.

forcebalance.optimizer.Optimizer.FF The force field itself.
Definition at line 174 of file optimizer.py.

forcebalance.optimizer.Optimizer.Grad Definition at line 690 of file optimizer.py.

forcebalance.optimizer.Optimizer.h Definition at line 339 of file optimizer.py.

forcebalance.optimizer.Optimizer.H Definition at line 687 of file optimizer.py.

forcebalance.optimizer.Optimizer.Hess Definition at line 691 of file optimizer.py.

forcebalance.optimizer.Optimizer.mvals0 The original parameter values.
Check derivatives by finite difference after the optimization is over (for good measure)
Don't print a "result" force field if it's the same as the input.
Determine the save file name.
Parse the save file for mvals, if exist.
Definition at line 192 of file optimizer.py.

forcebalance.optimizer.Optimizer.mvals_bak The root directory.

Determine the output file name.
The job type Initial step size trust radius Minimum trust radius (for noisy objective functions) Lower bound on Hessian eigenvalue (below this, we add in steepest descent) Lower bound on step size (will fail below this) Guess value for Brent Step size for numerical finite difference When the trust radius get smaller, the finite difference step might need to get smaller. Number of steps to average over Function value convergence threshold Step size convergence threshold Gradient convergence threshold Allow convergence on low quality steps Maximum number of optimization steps For scan[mp]vals: The parameter index to scan over For scan[mp]vals: The parameter name to scan over, it just looks up an index For scan[mp]vals: The values that are fed into the scanner Name of the checkpoint file that we're reading in Name of the checkpoint file that we're writing out Whether to write the checkpoint file at every step Adaptive trust radius adjustment factor Adaptive trust radius adjustment damping Whether to print gradient during each step of the optimization Whether to print Hessian during each step of the optimization Whether to print parameters during each step of the optimization Error tolerance (if objective function rises by less than this, then the optimizer will forge ahead!) Search tolerance (The Hessian diagonal search will stop if the change is below this threshold) Whether to make backup files Name of the original input file Number of convergence criteria that must be met Only backup the "mvals" input file once per calculation.

Clone the input file to the output,
Definition at line 162 of file optimizer.py.

forcebalance.optimizer.Optimizer.np Number of parameters.
Definition at line 188 of file optimizer.py.

forcebalance.optimizer.Optimizer.Objective The objective function (needs to pass in when I instantiate)
Definition at line 170 of file optimizer.py.

forcebalance.optimizer.Optimizer.OptTab A list of all the things we can ask the optimizer to do.
Definition at line 68 of file optimizer.py.

forcebalance.optimizer.Optimizer.Penalty Definition at line 692 of file optimizer.py.

forcebalance.optimizer.Optimizer.prev_bad Definition at line 862 of file optimizer.py.

forcebalance.BaseClass.PrintOptionDict [**inherited**] Definition at line 44 of file __init__.py.

forcebalance.optimizer.Optimizer.resdir Definition at line 179 of file optimizer.py.

forcebalance.optimizer.Optimizer.uncert Target types which introduce uncertainty into the objective function.
Will re-evaluate the objective function when an optimization step is rejected
Definition at line 177 of file optimizer.py.

forcebalance.optimizer.Optimizer.Val Definition at line 689 of file optimizer.py.

forcebalance.BaseClass.verbose_options [**inherited**] Definition at line 40 of file __init__.py.

forcebalance.optimizer.Optimizer.x_best Definition at line 865 of file optimizer.py.

forcebalance.optimizer.Optimizer.x_prev Definition at line 864 of file optimizer.py.

forcebalance.optimizer.Optimizer.xk_prev Definition at line 863 of file optimizer.py.
The documentation for this class was generated from the following file:

- [optimizer.py](#)

8.56 forcebalance.objective.Penalty Class Reference

[Penalty](#) functions for regularizing the force field optimizer.

Public Member Functions

- def [__init__](#)
- def [compute](#)
- def [L2_norm](#)

Harmonic L2-norm constraints.
- def [HYP](#)

Hyperbolic constraints.
- def [FUSE](#)
- def [FUSE_BARRIER](#)
- def [FUSE_L0](#)

Public Attributes

- [fadd](#)
- [fmul](#)
- [a](#)
- [b](#)
- [FF](#)
- [ptyp](#)
- [Pen_Tab](#)
- [spacings](#)

Find exponential spacings.

Static Public Attributes

- [dictionary Pen_Names](#)

8.56.1 Detailed Description

[Penalty](#) functions for regularizing the force field optimizer.

The purpose for this module is to improve the behavior of our optimizer; essentially, our problem is fraught with 'linear dependencies', a.k.a. directions in the parameter space that the objective function does not respond to. This would happen if a parameter is just plain useless, or if there are two or more parameters that describe the same thing.

To accomplish these objectives, a penalty function is added to the objective function. Generally, the more the parameters change (i.e. the greater the norm of the parameter vector), the greater the penalty. Note that this is added on after all of the other contributions have been computed. This only matters if the penalty 'multiplies' the objective function: $\text{Obj} + \text{Obj} * \text{Penalty}$, but we also have the option of an additive penalty: $\text{Obj} + \text{Penalty}$.

Statistically, this is called regularization. If the penalty function is the norm squared of the parameter vector, it is called ridge regression. There is also the option of using simply the norm, and this is called lasso, but I think it presents problems for the optimizer that I need to work out.

Note that the penalty functions can be considered as part of a 'maximum likelihood' framework in which we assume a PRIOR PROBABILITY of the force field parameters around their initial values. The penalty function is related to the prior by an exponential. Ridge regression corresponds to a Gaussian prior and lasso corresponds to an exponential prior. There is also 'elastic net regression' which interpolates between Gaussian and exponential using a tuning parameter.

Our priors are adjustable too - there is one parameter, which is the width of the distribution. We can even use a noninformative prior for the distribution widths (hyperprior!). These are all important things to consider later.

Importantly, note that here there is no code that treats the distribution width. That is because the distribution width is wrapped up in the rescaling factors, which is essentially a coordinate transformation on the parameter space. More documentation on this will follow, perhaps in the 'rsmake' method.

Definition at line 318 of file `objective.py`.

8.56.2 Constructor & Destructor Documentation

```
def forcebalance.objective.Penalty.__init__( self, User_Option, ForceField, Factor_Add = 0.0, Factor_Mult = 0.0, Factor_B = 0.1, Alpha = 1.0 ) Definition at line 324 of file objective.py.
```

8.56.3 Member Function Documentation

```
def forcebalance.objective.Penalty.compute( self, mvals, Objective ) Definition at line 350 of file objective.py.
```

```
def forcebalance.objective.Penalty.FUSE ( self, mvals )
```

Definition at line 410 of file objective.py.
Here is the call graph for this function:



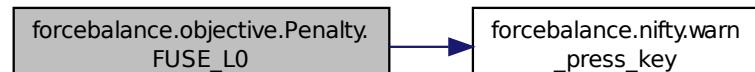
```
def forcebalance.objective.Penalty.FUSE_BARRIER ( self, mvals )
```

Definition at line 451 of file objective.py.
Here is the call graph for this function:



```
def forcebalance.objective.Penalty.FUSE_L0 ( self, mvals )
```

Definition at line 493 of file objective.py.
Here is the call graph for this function:



```
def forcebalance.objective.Penalty.HYP ( self, mvals )
```

Hyperbolic constraints.
Depending on the 'b' parameter, the smaller it is, the closer we are to an L1-norm constraint. If we use these, we expect a properly-behaving optimizer to make several of the parameters very nearly zero (which would be cool).

Parameters

in	mvals	The parameter vector
----	-------	----------------------

Returns

DC0 The hyperbolic penalty

DC1 The gradient

DC2 The Hessian

Definition at line 402 of file objective.py.

```
def forcebalance.objective.Penalty.L2_norm( self, mvals ) Harmonic L2-norm constraints.
```

These are the ones that I use the most often to regularize my optimization.

Parameters

in	mvals	The parameter vector
----	-------	----------------------

Returns

DC0 The norm squared of the vector

DC1 The gradient of DC0

DC2 The Hessian (just a constant)

Definition at line 382 of file objective.py.

8.56.4 Member Data Documentation

forcebalance.objective.Penalty.a Definition at line 327 of file objective.py.

forcebalance.objective.Penalty.b Definition at line 328 of file objective.py.

forcebalance.objective.Penalty.fadd Definition at line 325 of file objective.py.

forcebalance.objective.Penalty.FF Definition at line 329 of file objective.py.

forcebalance.objective.Penalty.fmul Definition at line 326 of file objective.py.

dictionary forcebalance.objective.Penalty.Pen_Names [static] Initial value:

```
1 = {'HYP' : 1, 'HYPER' : 1, 'HYPERBOLIC' : 1, 'L1' : 1, 'HYPERBOLA' : 1,
2           'PARA' : 2, 'PARABOLA' : 2, 'PARABOLIC' : 2, 'L2' : 2, 'QUADRATIC' : 2,
3           'FUSE' : 3, 'FUSION' : 3, 'FUSE_L0' : 4, 'FUSION_L0' : 4, 'FUSION-L0' : 4,
4           'FUSE-BARRIER' : 5, 'FUSE-BARRIER' : 5, 'FUSE_BARRIER' : 5, 'FUSION_BARRIER' : 5}
```

Definition at line 319 of file objective.py.

forcebalance.objective.Penalty.Pen_Tab Definition at line 331 of file objective.py.

forcebalance.objective.Penalty.ptyp Definition at line 330 of file objective.py.

forcebalance.objective.Penalty.spacings Find exponential spacings.

Definition at line 347 of file objective.py.

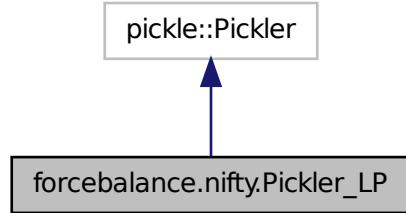
The documentation for this class was generated from the following file:

- [objective.py](#)

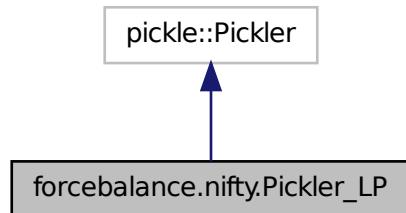
8.57 forcebalance.nifty.Pickler_LP Class Reference

A subclass of the python Pickler that implements pickling of _ElementTree types.

Inheritance diagram for forcebalance.nifty.Pickler_LP:



Collaboration diagram for forcebalance.nifty.Pickler_LP:



Public Member Functions

- def [__init__](#)

8.57.1 Detailed Description

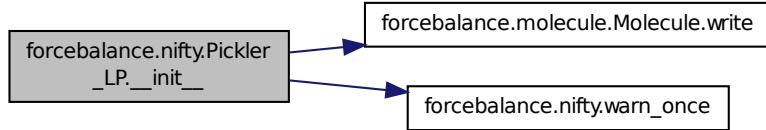
A subclass of the python Pickler that implements pickling of _ElementTree types.

Definition at line 563 of file nifty.py.

8.57.2 Constructor & Destructor Documentation

def forcebalance.nifty.Pickler_LP.__init__(self, file, protocol = None) Definition at line 564 of file nifty.py.

Here is the call graph for this function:

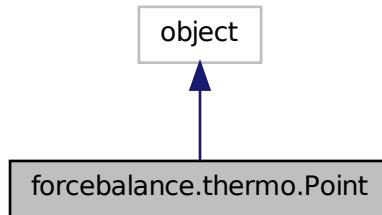


The documentation for this class was generated from the following file:

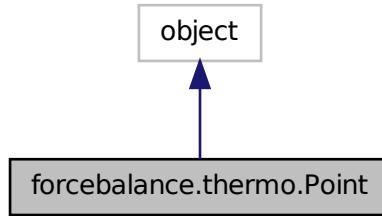
- [nifty.py](#)

8.58 forcebalance.thermo.Point Class Reference

Inheritance diagram for forcebalance.thermo.Point:



Collaboration diagram for forcebalance.thermo.Point:



Public Member Functions

- def [__init__](#)
- def [__str__](#)

Public Attributes

- [idnr](#)
- [ref](#)
- [temperature](#)
- [pressure](#)
- [data](#)

8.58.1 Detailed Description

Definition at line 426 of file thermo.py.

8.58.2 Constructor & Destructor Documentation

```
def forcebalance.thermo.Point.__init__ ( self, idnr, label = None, refs = None, weights = None, names = None, units = None, temperature = None, pressure = None, data = None )
```

Definition at line 428 of file thermo.py.

8.58.3 Member Function Documentation

```
def forcebalance.thermo.Point.__str__ ( self )
```

Definition at line 439 of file thermo.py.

8.58.4 Member Data Documentation

forcebalance.thermo.Point.data Definition at line 437 of file thermo.py.

forcebalance.thermo.Point.idnr Definition at line 429 of file thermo.py.

forcebalance.thermo.Point.pressure Definition at line 436 of file thermo.py.

forcebalance.thermo.Point.ref Definition at line 430 of file thermo.py.

forcebalance.thermo.Point.temperature Definition at line 435 of file thermo.py.

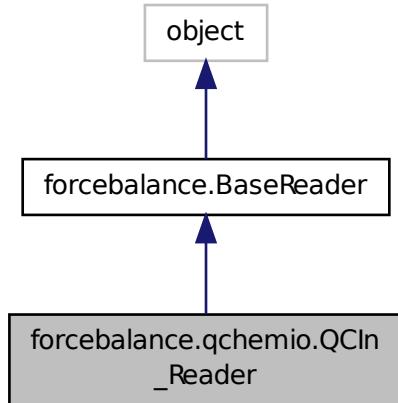
The documentation for this class was generated from the following file:

- [thermo.py](#)

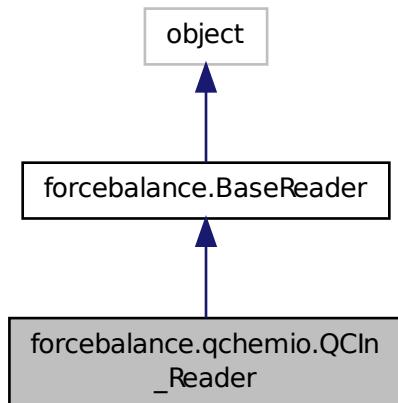
8.59 forcebalance.qchemio.QCIn_ Reader Class Reference

Finite state machine for parsing Q-Chem input files.

Inheritance diagram for forcebalance.qchemio.QCIn_Reader:



Collaboration diagram for forcebalance.qchemio.QCIn_Reader:



Public Member Functions

- def `_init_`
- def `feed`
Feed in a line.
- def `Split`
- def `Whites`

- def [build.pid](#)

Returns the parameter type (e.g.

Public Attributes

- [atom](#)
- [snum](#)
- [cnum](#)
- [shell](#)
- [pdict](#)
- [sec](#)
- [itype](#)
- [suffix](#)
- [In](#)
- [adict](#)

The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

- [molatom](#)

The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

- [Molecules](#)
- [AtomTypes](#)

8.59.1 Detailed Description

Finite state machine for parsing Q-Chem input files.

Definition at line 31 of file qchemio.py.

8.59.2 Constructor & Destructor Documentation

def forcebalance.qchemio.QCIn_Reader.__init__ (self, fnm) Definition at line 33 of file qchemio.py.

8.59.3 Member Function Documentation

def forcebalance.BaseReader.build_pid (self, pfd) [inherited] Returns the parameter type (e.g. K in BONDSK) based on the current interaction type.

Both the 'pdict' dictionary (see [gmxio.pdict](#)) and the interaction type 'state' (here, BONDS) are needed to get the parameter type.

If, however, 'pdict' does not contain the ptype value, a suitable substitute is simply the field number.

Note that if the interaction type state is not set, then it defaults to the file name, so a generic parameter ID is 'filename.line.num.field.num'

Definition at line 124 of file __init__.py.

def forcebalance.qchemio.QCIn_Reader.feed (self, line) Feed in a line.

Parameters

in	line	The line of data
----	------	------------------

Definition at line 48 of file qchemio.py.

def forcebalance.BaseReader.Split (self, line) [inherited] Definition at line 99 of file __init__.py.

def forcebalance.BaseReader.Whites (self, line) [inherited] Definition at line 102 of file __init__.py.

8.59.4 Member Data Documentation

forcebalance.BaseReader.adict [inherited] The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

Definition at line 89 of file `__init__.py`.

forcebalance.qchemio.QCIn_Reader.atom Definition at line 36 of file `qchemio.py`.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file `__init__.py`.

forcebalance.qchemio.QCIn_Reader.cnum Definition at line 38 of file `qchemio.py`.

forcebalance.qchemio.QCIn_Reader.itype Definition at line 67 of file `qchemio.py`.

forcebalance.BaseReader.In [inherited] Definition at line 84 of file `__init__.py`.

forcebalance.BaseReader.molatom [inherited] The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

`self.moleculedict = OrderedDict()` The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.

Definition at line 94 of file `__init__.py`.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file `__init__.py`.

forcebalance.qchemio.QCIn_Reader.pdict Definition at line 40 of file `qchemio.py`.

forcebalance.qchemio.QCIn_Reader.sec Definition at line 58 of file `qchemio.py`.

forcebalance.qchemio.QCIn_Reader.shell Definition at line 39 of file `qchemio.py`.

forcebalance.qchemio.QCIn_Reader.snum Definition at line 37 of file `qchemio.py`.

forcebalance.qchemio.QCIn_Reader.suffix Definition at line 72 of file `qchemio.py`.

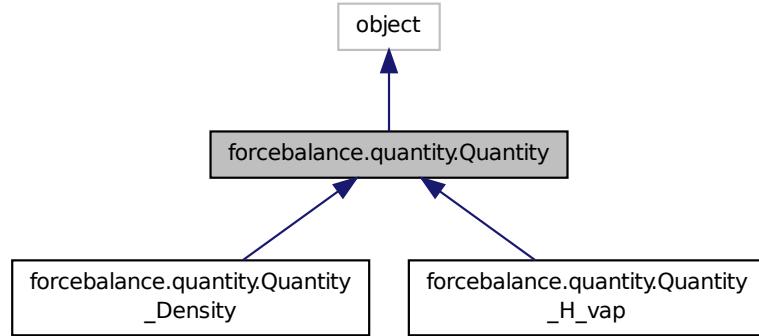
The documentation for this class was generated from the following file:

- [qchemio.py](#)

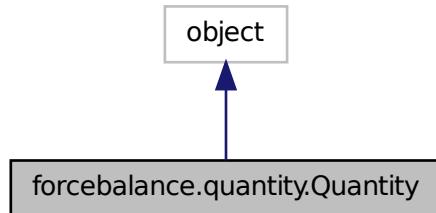
8.60 forcebalance.quantity.Quantity Class Reference

Base class for thermodynamical quantity used for fitting.

Inheritance diagram for forcebalance.quantity.Quantity:



Collaboration diagram for forcebalance.quantity.Quantity:



Public Member Functions

- def `__init__`
- def `__str__`
- def `extract`

Calculate and extract the quantity from MD results.

Public Attributes

- `name`
- `engname`
- `temperature`
- `pressure`

8.60.1 Detailed Description

Base class for thermodynamical quantity used for fitting.

This can be any experimental data that can be calculated as an ensemble average from a simulation.

Data attributes name : string Identifier for the quantity that is specified in quantities in Target options. engname : string Use this engine to extract the quantity from the simulation results. At present, only gromacs is supported. temperature : float Calculate the quantity at this temperature (in K). pressure : float Calculate the quantity at this pressure (in bar).

Definition at line 88 of file quantity.py.

8.60.2 Constructor & Destructor Documentation

```
def forcebalance.quantity.Quantity.__init__ ( self, engname, temperature, pressure, name = None )
```

Definition at line 89 of file quantity.py.

8.60.3 Member Function Documentation

```
def forcebalance.quantity.Quantity.__str__ ( self )
```

Definition at line 95 of file quantity.py.

Returns result : (float, float, np.array) The returned tuple is (Q, Qerr, Qgrad), where Q is the calculated quantity, Qerr is the calculated standard deviation of the quantity, and Qgrad is a M-array with the calculated gradients for the quantity, with M being the number of force field parameters that are being fitted.

How this is done depends on the quantity and the engine so this must be implemented in the subclass.

Parameters engines : list A list of Engine objects that are required to calculate the quantity. FF : FF Force field object. mvals : list Mathematical parameter values. h : float Finite difference step size. AGrad : Boolean Switch that turns derivatives on or off; if off, return all zeros.

Returns result : (float, float, np.array) The returned tuple is (Q, Qerr, Qgrad), where Q is the calculated quantity, Qerr is the calculated standard deviation of the quantity, and Qgrad is a M-array with the calculated gradients for the quantity, with M being the number of force field parameters that are being fitted.

Definition at line 126 of file quantity.py.

8.60.4 Member Data Documentation

forcebalance.quantity.Quantity.engname Definition at line 91 of file quantity.py.

forcebalance.quantity.Quantity.name Definition at line 90 of file quantity.py.

forcebalance.quantity.Quantity.pressure Definition at line 93 of file quantity.py.

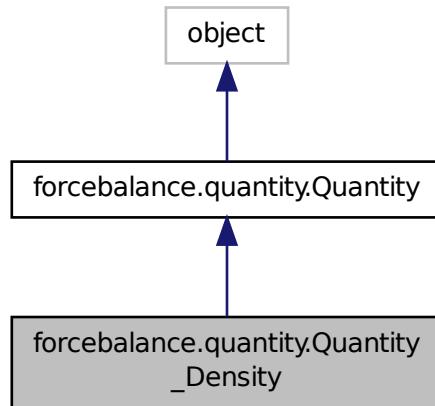
forcebalance.quantity.Quantity.temperature Definition at line 92 of file quantity.py.

The documentation for this class was generated from the following file:

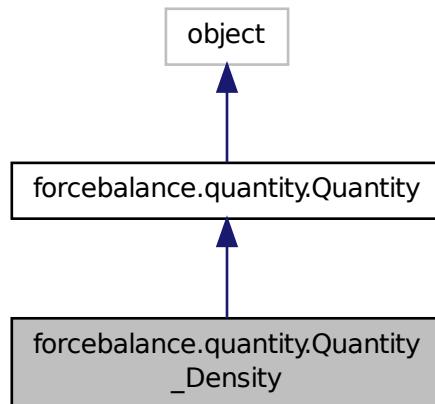
- [quantity.py](#)

8.61 forcebalance.quantity.Quantity_Density Class Reference

Inheritance diagram for forcebalance.quantity.Quantity_Density:



Collaboration diagram for forcebalance.quantity.Quantity_Density:



Public Member Functions

- def `__init__`
Density.
- def `extract`
- def `__str__`

- def [extract](#)

Calculate and extract the quantity from MD results.

Public Attributes

- [name](#)
- [engname](#)
- [temperature](#)
- [pressure](#)

8.61.1 Detailed Description

Definition at line 130 of file `quantity.py`.

8.61.2 Constructor & Destructor Documentation

```
def forcebalance.quantity.Quantity_Density.__init__( self, engname, temperature, pressure, name = None ) Density.
```

Definition at line 133 of file `quantity.py`.

8.61.3 Member Function Documentation

```
def forcebalance.quantity.Quantity.__str__( self ) [inherited] Definition at line 95 of file quantity.py.
```

```
def forcebalance.quantity.Quantity.extract( self, engines, FF, mvals, h, AGrad = True ) [inherited]
```

Calculate and extract the quantity from MD results.

How this is done depends on the quantity and the engine so this must be implemented in the subclass.

Parameters engines : list A list of Engine objects that are required to calculate the quantity. FF : FF Force field object. mvals : list Mathematical parameter values. h : float Finite difference step size. AGrad : Boolean Switch that turns derivatives on or off; if off, return all zeros.

Returns result : (float, float, np.array) The returned tuple is (Q, Qerr, Qgrad), where Q is the calculated quantity, Qerr is the calculated standard deviation of the quantity, and Qgrad is a M-array with the calculated gradients for the quantity, with M being the number of force field parameters that are being fitted.

Definition at line 126 of file `quantity.py`.

```
def forcebalance.quantity.Quantity_Density.extract( self, engines, FF, mvals, h, pgrad, AGrad = True )
```

Definition at line 138 of file `quantity.py`.

8.61.4 Member Data Documentation

forcebalance.quantity.Quantity_Density.engname Definition at line 151 of file `quantity.py`.

forcebalance.quantity.Quantity_Density.name Definition at line 136 of file `quantity.py`.

forcebalance.quantity.Quantity.pressure [inherited] Definition at line 93 of file `quantity.py`.

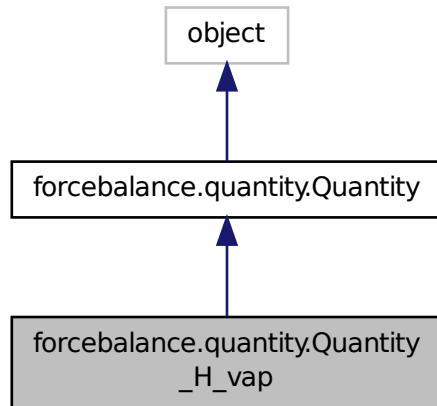
forcebalance.quantity.Quantity.temperature [inherited] Definition at line 92 of file `quantity.py`.

The documentation for this class was generated from the following file:

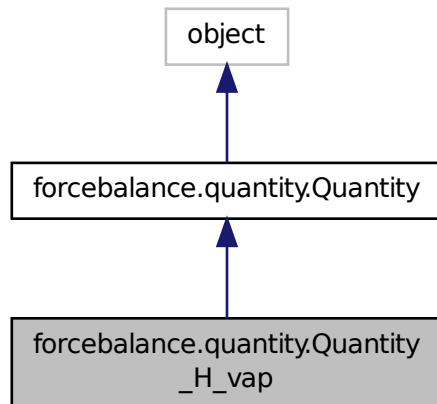
- [quantity.py](#)

8.62 forcebalance.quantity.Quantity_H_vap Class Reference

Inheritance diagram for forcebalance.quantity.Quantity_H_vap:



Collaboration diagram for forcebalance.quantity.Quantity_H_vap:



Public Member Functions

- def `__init__`
Enthalpy of vaporization.
- def `extract`
- def `__str__`

- def [extract](#)

Calculate and extract the quantity from MD results.

Public Attributes

- [name](#)
- [engname](#)
- [temperature](#)
- [pressure](#)

8.62.1 Detailed Description

Definition at line 201 of file `quantity.py`.

8.62.2 Constructor & Destructor Documentation

def forcebalance.quantity.Quantity.H_vap.__init__ (self, engname, temperature, pressure, name = None)
Enthalpy of vaporization.

Definition at line 204 of file `quantity.py`.

8.62.3 Member Function Documentation

def forcebalance.quantity.Quantity.__str__ (self) [inherited] Definition at line 95 of file `quantity.py`.

def forcebalance.quantity.Quantity.extract (self, engines, FF, mvals, h, AGrad = True) [inherited]
Calculate and extract the quantity from MD results.

How this is done depends on the quantity and the engine so this must be implemented in the subclass.

Parameters engines : list A list of Engine objects that are required to calculate the quantity. FF : FF Force field object. mvals : list Mathematical parameter values. h : float Finite difference step size. AGrad : Boolean Switch that turns derivatives on or off; if off, return all zeros.

Returns result : (float, float, np.array) The returned tuple is (Q, Qerr, Qgrad), where Q is the calculated quantity, Qerr is the calculated standard deviation of the quantity, and Qgrad is a M-array with the calculated gradients for the quantity, with M being the number of force field parameters that are being fitted.

Definition at line 126 of file `quantity.py`.

def forcebalance.quantity.Quantity.H_vap.extract (self, engines, FF, mvals, h, pgrad, AGrad = True)
Definition at line 209 of file `quantity.py`.

8.62.4 Member Data Documentation

forcebalance.quantity.Quantity.H_vap.engname Definition at line 229 of file `quantity.py`.

forcebalance.quantity.Quantity.H_vap.name Definition at line 207 of file `quantity.py`.

forcebalance.quantity.Quantity.pressure [inherited] Definition at line 93 of file `quantity.py`.

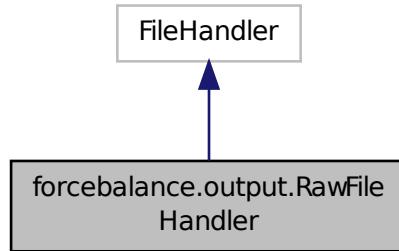
forcebalance.quantity.Quantity.temperature [inherited] Definition at line 92 of file `quantity.py`.

The documentation for this class was generated from the following file:

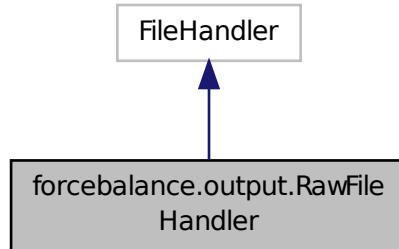
- [quantity.py](#)

8.63 forcebalance.output.RawFileHandler Class Reference

Exactly like output.FileHandler except it does no extra formatting before sending logging messages to the file.
Inheritance diagram for forcebalance.output.RawFileHandler:



Collaboration diagram for forcebalance.output.RawFileHandler:



Public Member Functions

- def [emit](#)

8.63.1 Detailed Description

Exactly like output.FileHandler except it does no extra formatting before sending logging messages to the file.
This is more compatible with how output has been displayed in ForceBalance.
Definition at line 47 of file [output.py](#).

8.63.2 Member Function Documentation

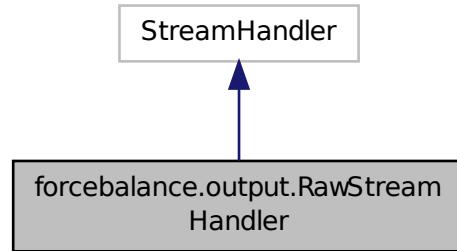
def forcebalance.output.RawFileHandler.emit (*self*, *record*) Definition at line 48 of file [output.py](#).

The documentation for this class was generated from the following file:

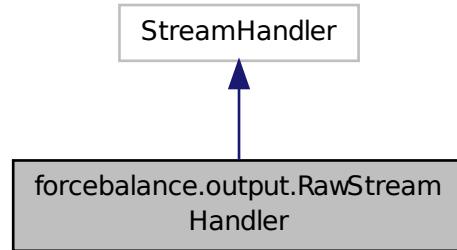
- [output.py](#)

8.64 forcebalance.output.RawStreamHandler Class Reference

Exactly like output.StreamHandler except it does no extra formatting before sending logging messages to the stream.
Inheritance diagram for forcebalance.output.RawStreamHandler:



Collaboration diagram for forcebalance.output.RawStreamHandler:



Public Member Functions

- def `__init__`
- def `emit`

8.64.1 Detailed Description

Exactly like output.StreamHandler except it does no extra formatting before sending logging messages to the stream.
This is more compatible with how output has been displayed in ForceBalance. Default stream has also been changed from stderr to stdout
Definition at line 34 of file output.py.

8.64.2 Constructor & Destructor Documentation

```
def forcebalance.output.RawStreamHandler.__init__ ( self, stream = sys.stdout ) Definition at line 35 of file output.py.
```

8.64.3 Member Function Documentation

```
def forcebalance.output.RawStreamHandler.emit ( self, record ) Definition at line 38 of file output.py.
```

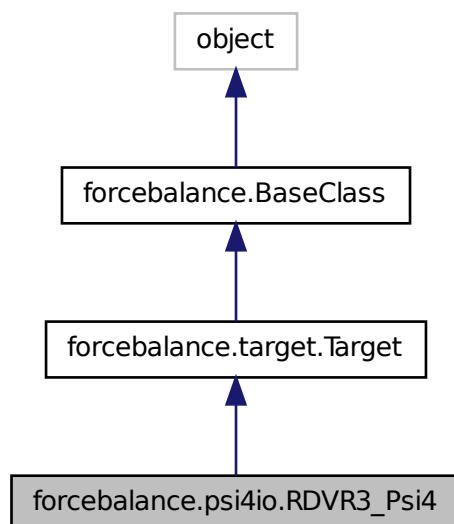
The documentation for this class was generated from the following file:

- [output.py](#)

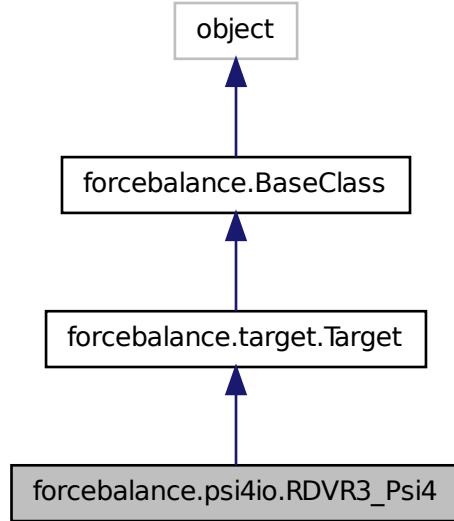
8.65 forcebalance.psi4io.RDVR3_Psi4 Class Reference

Subclass of Target for R-DVR3 grid fitting.

Inheritance diagram for forcebalance.psi4io.RDVR3_Psi4:



Collaboration diagram for forcebalance.psi4io.RDVR3_Psi4:



Public Member Functions

- def `_init_`
- def `indicate`
- def `submit_jobs`

Create a grid file and a psi4 input file in the absolute path and submit it to the work queue.

- def `driver`
- def `get`

LPW 04-17-2013.

- def `get_X`

Computes the objective function contribution without any parametric derivatives.

- def `read_0grads`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.

- def `write_0grads`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.

- def `get_G`

Computes the objective function contribution and its gradient.

- def `get_H`

Computes the objective function contribution and its gradient / Hessian.

- def `link_from_tempdir`

- def `refresh_temp_directory`

Back up the temporary directory if desired, delete it and then create a new one.

- def `check_files`

Check this directory for the presence of readable files when the 'read' option is set.

- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `objfiles`
Which parameters are differentiated?
- `objvals`
- `elements`
- `molecules`
- `callderivs`
- `factor`
- `bidirect`
- `tdir`
- `objd`
- `gradd`
- `hdiagd`
- `objective`
- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`
Relative directory of target.
- `tempdir`
- `rundir`
`self.tempdir = os.path.join('temp',self.name)` *The directory in which the simulation is running - this can be updated.*
- `FF`
Need the forcefield (here for now)
- `xct`
Counts how often the objective function was computed.
- `gct`

- **hct**
Counts how often the gradient was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**
Whether to write indicate.log at every iteration (true for all but remote.)
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

8.65.1 Detailed Description

Subclass of Target for R-DVR3 grid fitting.

Main features:

- Multiple molecules are treated as a single target.
- R-DVR3 can only print out the objective function, it cannot print out the residual vector.
- We should be smart enough to mask derivatives.

Definition at line 299 of file psi4io.py.

8.65.2 Constructor & Destructor Documentation

```
def forcebalance.psi4io.RDVR3_Psi4.__init__ ( self, options, tgt_opts, forcefield ) Definition at line 302 of file
psi4io.py.
```

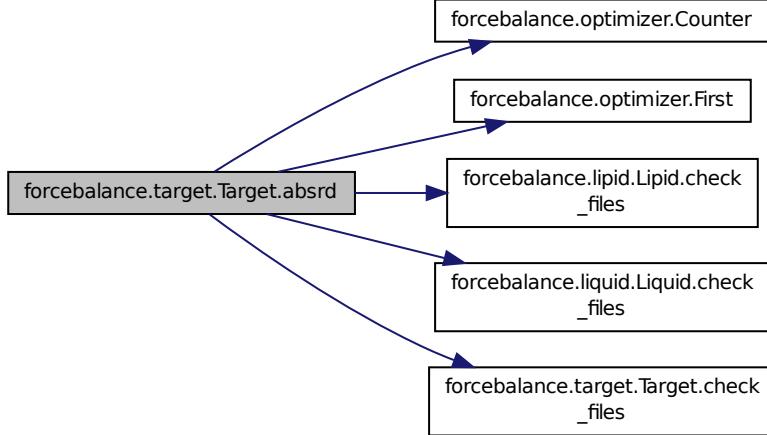
8.65.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory
specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:

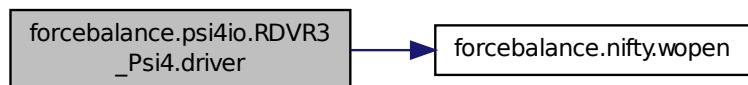


def forcebalance.target.Target.check_files(self, there) [inherited] Check this directory for the presence of readable files when the 'read' option is set.

Definition at line 364 of file target.py.

def forcebalance.psi4io.RDVR3.Psi4.driver(self, mvals, d) Definition at line 415 of file psi4io.py.

Here is the call graph for this function:



def forcebalance.psi4io.RDVR3.Psi4.get(self, mvals, AGrad=False, AHess=False) LPW 04-17-2013.

This subroutine builds the objective function from Psi4.

Parameters

in	<i>mvals</i>	Mathematical parameter values
in	<i>AGrad</i>	Switch to turn on analytic gradient

in	AHess	Switch to turn on analytic Hessian
----	-------	------------------------------------

Returns

Answer Contribution to the objective function

Definition at line 452 of file psi4io.py.

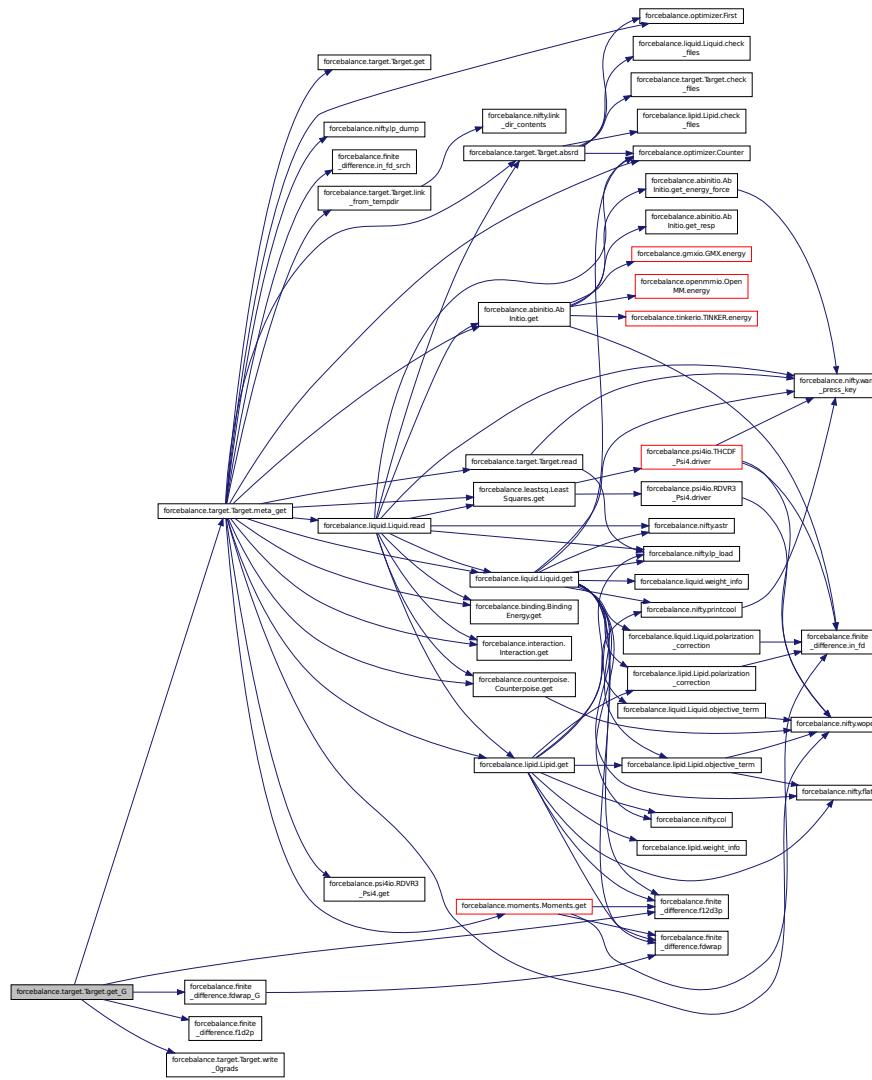
def forcebalance.target.Target.get_G (self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



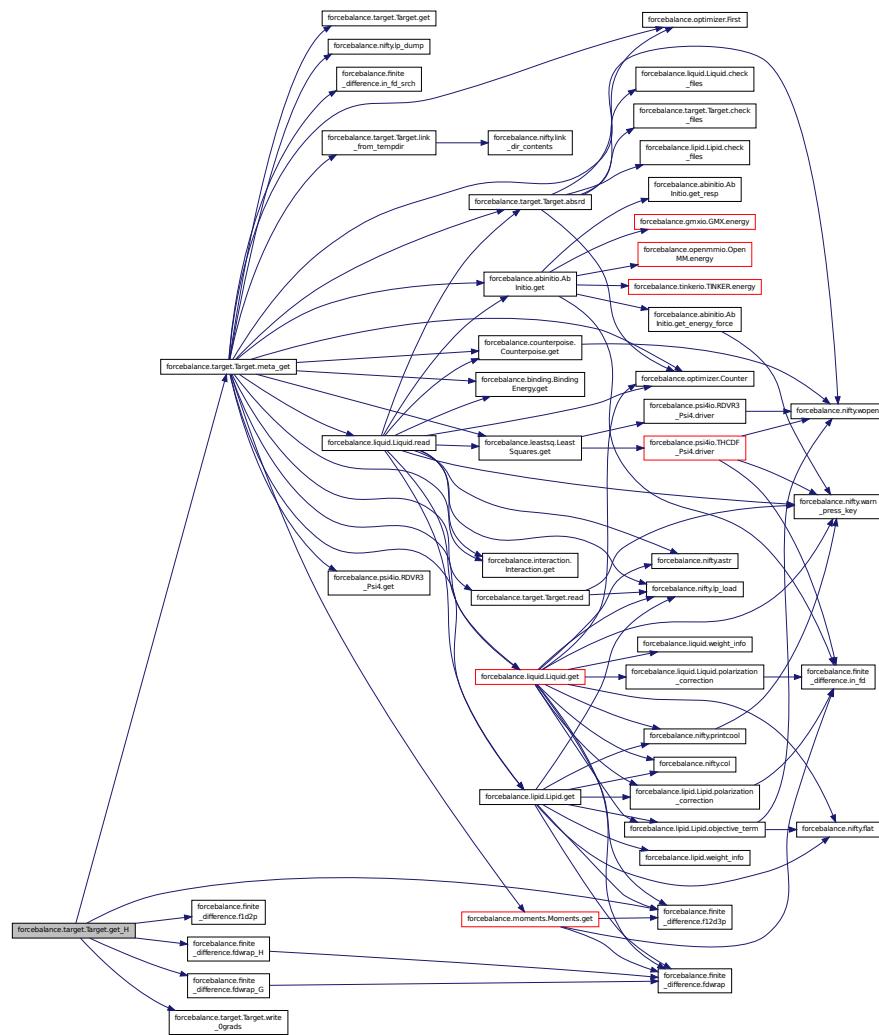
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

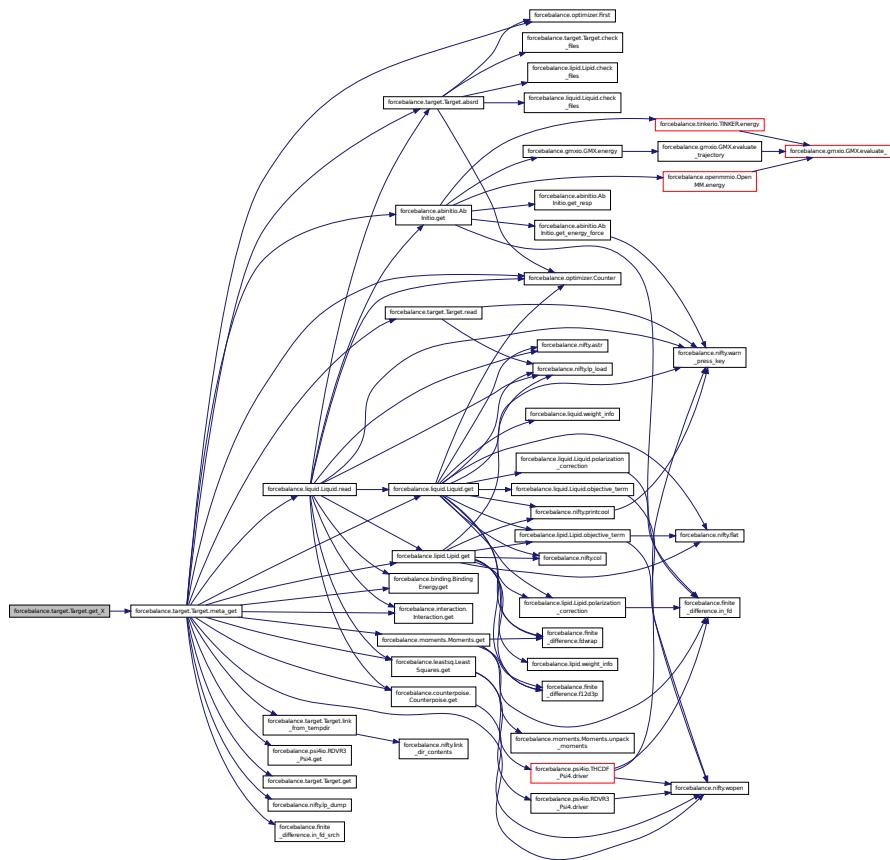
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

Here is the call graph for this function:



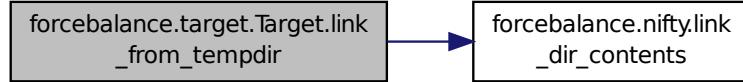
def forcebalance.ps4io.RDVR3_Psi4.indicate(self) Definition at line 342 of file ps4io.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

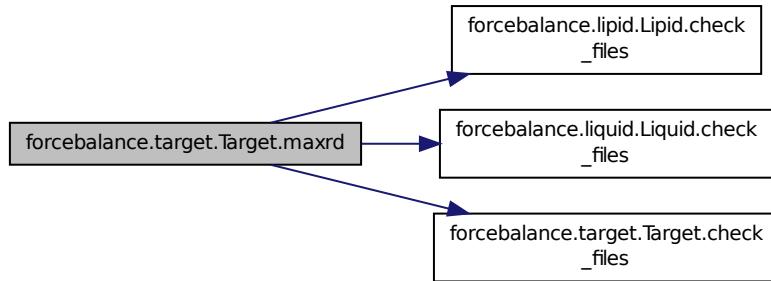
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

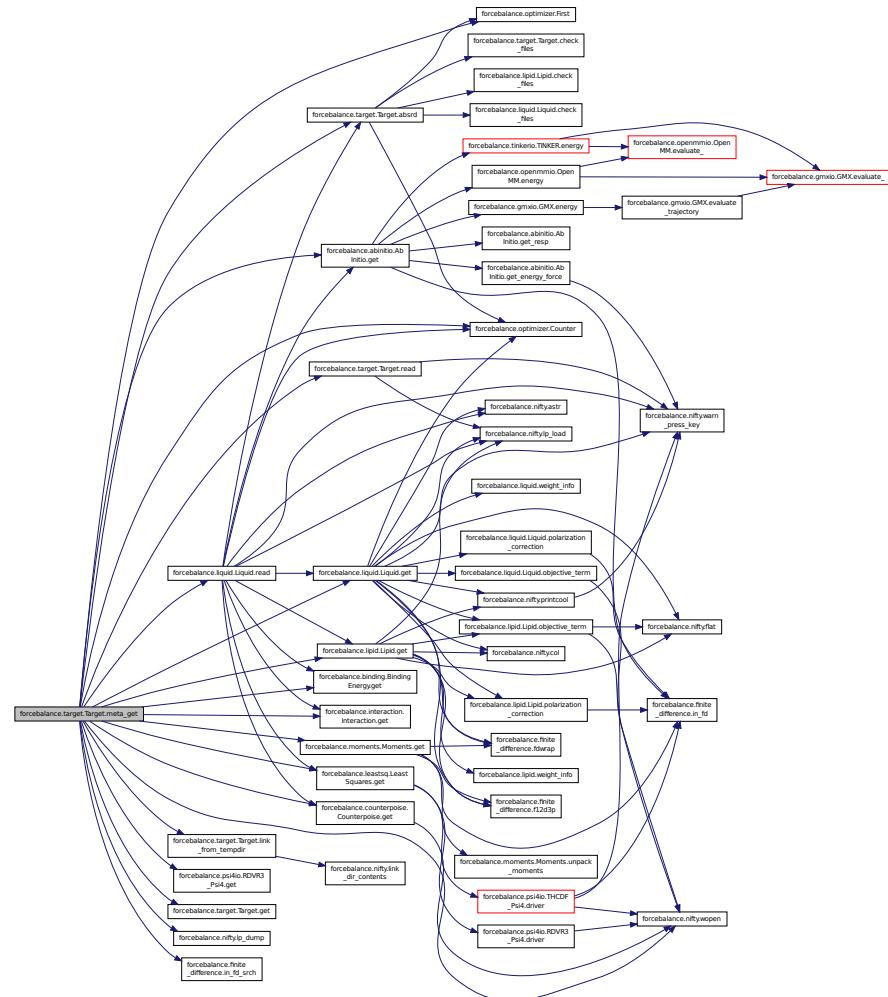


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

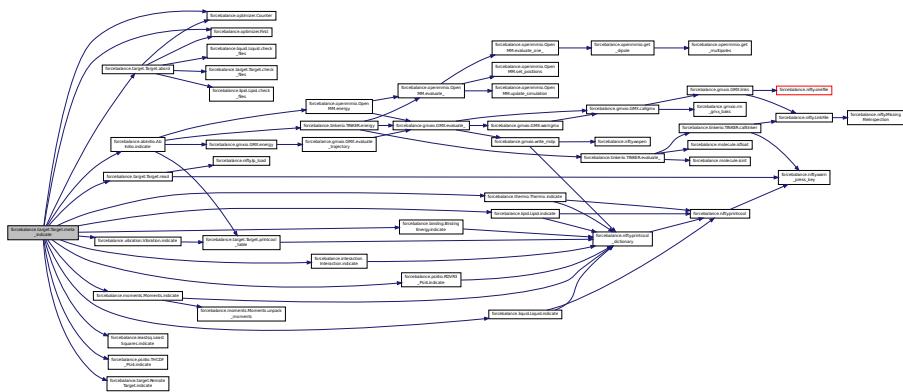
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

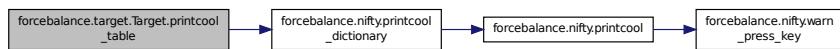
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

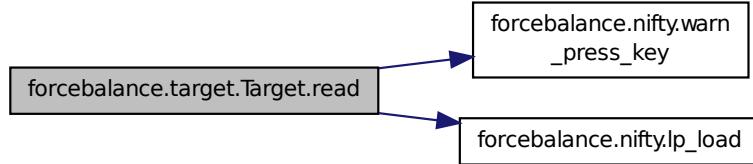
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

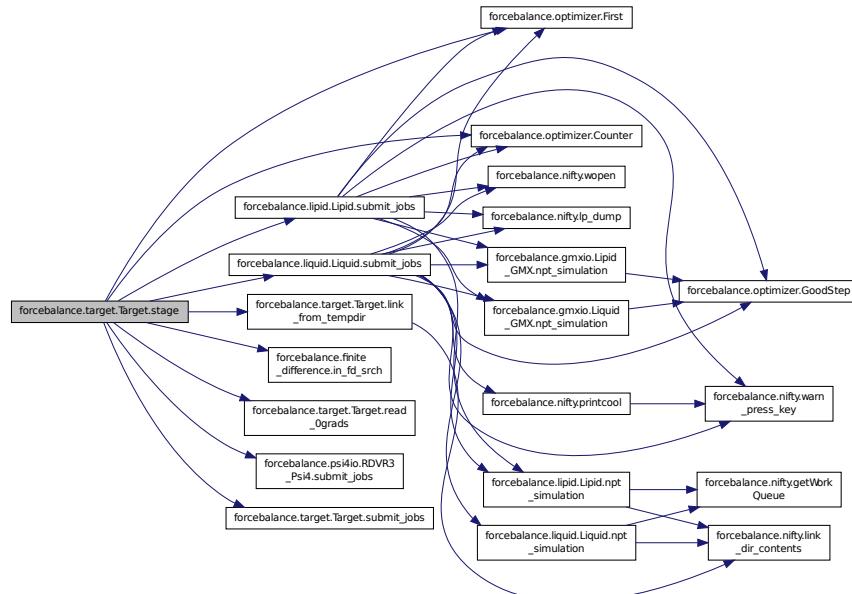
def forcebalance.BaseClass.set_option(self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage(self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



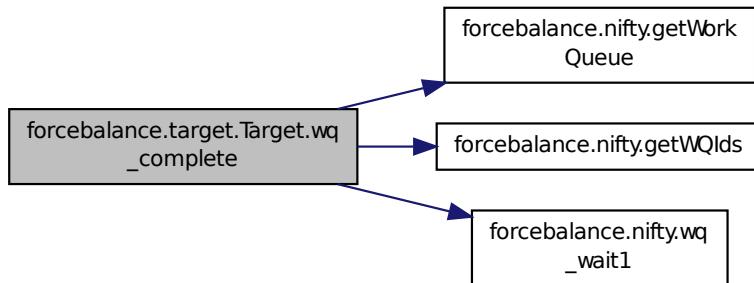
def forcebalance.psi4io.RDVR3.Psi4.submit_jobs (self, mvals, AGrad = True, AHess = True) Create a grid file and a psi4 input file in the absolute path and submit it to the work queue.

Definition at line 351 of file psi4io.py.

def forcebalance.target.Target.wq_complete (self) [inherited] This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.65.4 Member Data Documentation

forcebalance.psi4io.RDVR3_Psi4.bidirect Definition at line 314 of file psi4io.py.

forcebalance.psi4io.RDVR3_Psi4.callderivs Definition at line 312 of file psi4io.py.

forcebalance.psi4io.RDVR3_Psi4.elements Definition at line 310 of file psi4io.py.

forcebalance.psi4io.RDVR3_Psi4.factor Definition at line 313 of file psi4io.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.psi4io.RDVR3_Psi4.gradd Definition at line 462 of file psi4io.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.psi4io.RDVR3_Psi4.hdiagd Definition at line 463 of file psi4io.py.

forcebalance.psi4io.RDVR3_Psi4.molecules Definition at line 311 of file psi4io.py.

forcebalance.psi4io.RDVR3_Psi4.objd Definition at line 461 of file psi4io.py.

forcebalance.psi4io.RDVR3_Psi4.objective Definition at line 538 of file psi4io.py.

forcebalance.psi4io.RDVR3_Psi4.objfiles Which parameters are differentiated?

Definition at line 308 of file psi4io.py.

forcebalance.psi4io.RDVR3_Psi4.objvals Definition at line 309 of file psi4io.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [**inherited**] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [**inherited**] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [**inherited**] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number. The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.psi4io.RDVR3.Psi4.tdir Definition at line 355 of file psi4io.py.

forcebalance.target.Target.tempbase [**inherited**] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [**inherited**] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [**inherited**] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

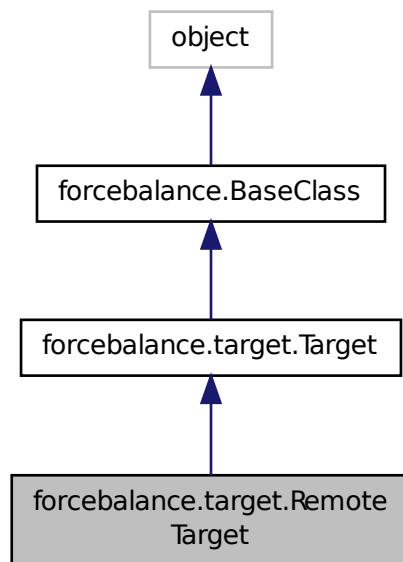
Definition at line 162 of file target.py.

The documentation for this class was generated from the following file:

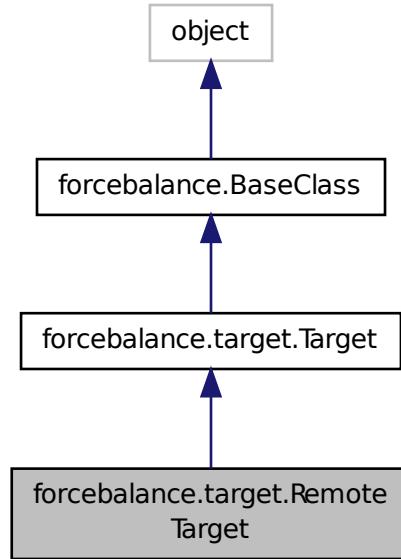
- [psi4io.py](#)

8.66 forcebalance.target.RemoteTarget Class Reference

Inheritance diagram for forcebalance.target.RemoteTarget:



Collaboration diagram for forcebalance.target.RemoteTarget:



Public Member Functions

- def `__init__`
- def `submit_jobs`
- def `read`
- def `get`
- def `indicate`
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`

Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`

Check this directory for the presence of readable files when the 'read' option is set.
- def `absrd`

- def `maxrd`
Supply the correct directory specified by user's "read" option.
- def `meta_indicate`
Supply the latest existing temp-directory containing valid data.
- def `meta_get`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `stage`
Wrapper around the get function.
- def `wq_complete`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `printcool_table`
This method determines whether the Work Queue tasks for the current target have completed.
- def `__setattr__`
Print target information in an organized table format.
- def `set_option`

Public Attributes

- `r_options`
- `r_tgt_opts`
- `remote_indicate`
- `read_indicate`
- `write_indicate`
- `write_objective`
- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`
Relative directory of target.
- `tempdir`
- `rundir`
`self.tempdir = os.path.join('temp',self.name)` *The directory in which the simulation is running - this can be updated.*
- `FF`
Need the forcefield (here for now)
- `xct`
Counts how often the objective function was computed.
- `gct`
Counts how often the gradient was computed.
- `hct`
Counts how often the Hessian was computed.
- `read_objective`
Whether to read objective.p from file when restarting an aborted run.
- `verbose_options`
- `PrintOptionDict`

8.66.1 Detailed Description

Definition at line 677 of file target.py.

8.66.2 Constructor & Destructor Documentation

```
def forcebalance.target.RemoteTarget.__init__ ( self, options, tgt_opts, forcefield ) Definition at line 678 of file target.py.
```

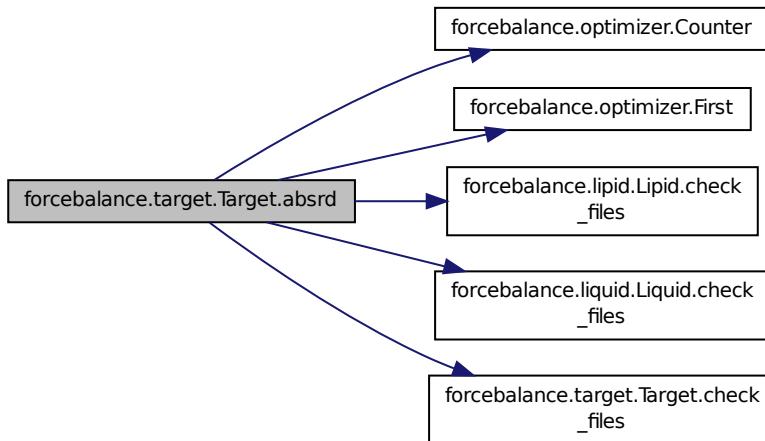
8.66.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.target.RemoteTarget.get ( self, mvals, AGrad = False, AHess = False ) Definition at line 729 of file target.py.
```

Here is the call graph for this function:



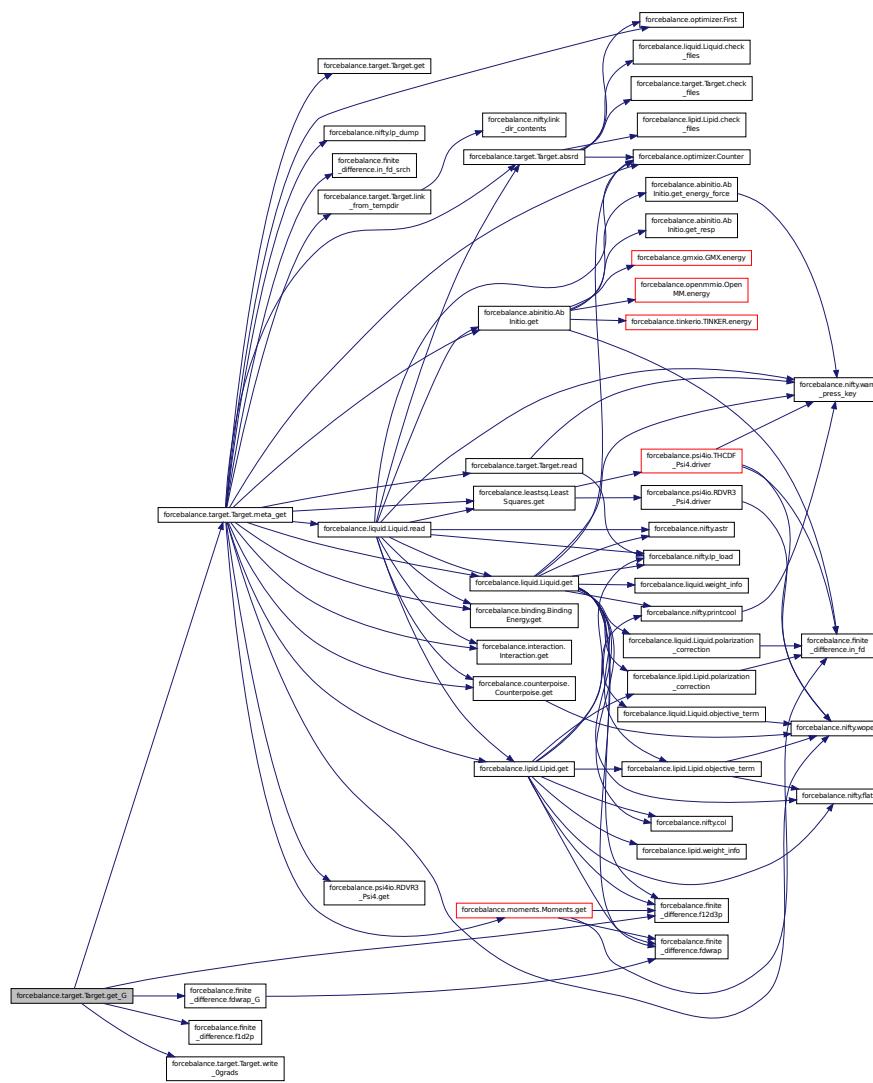
```
def forcebalance.target.Target.get_G ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.get_H ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient / Hessian.
```

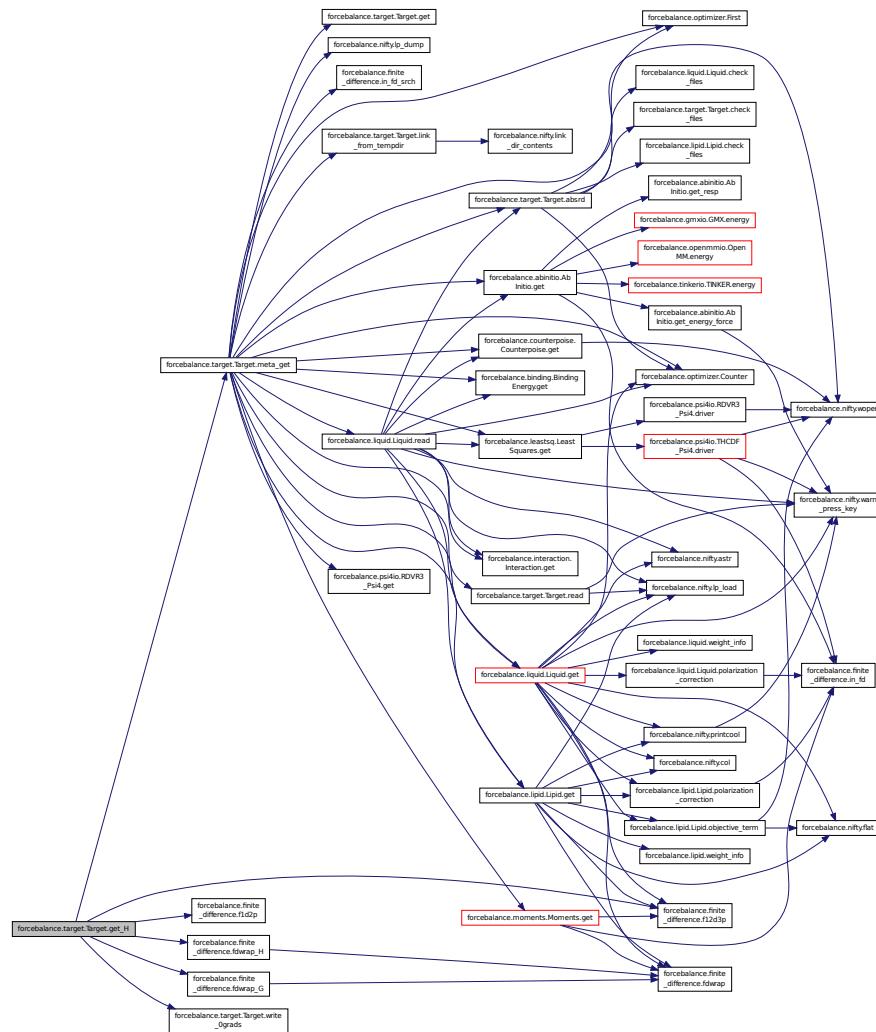
First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through

the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

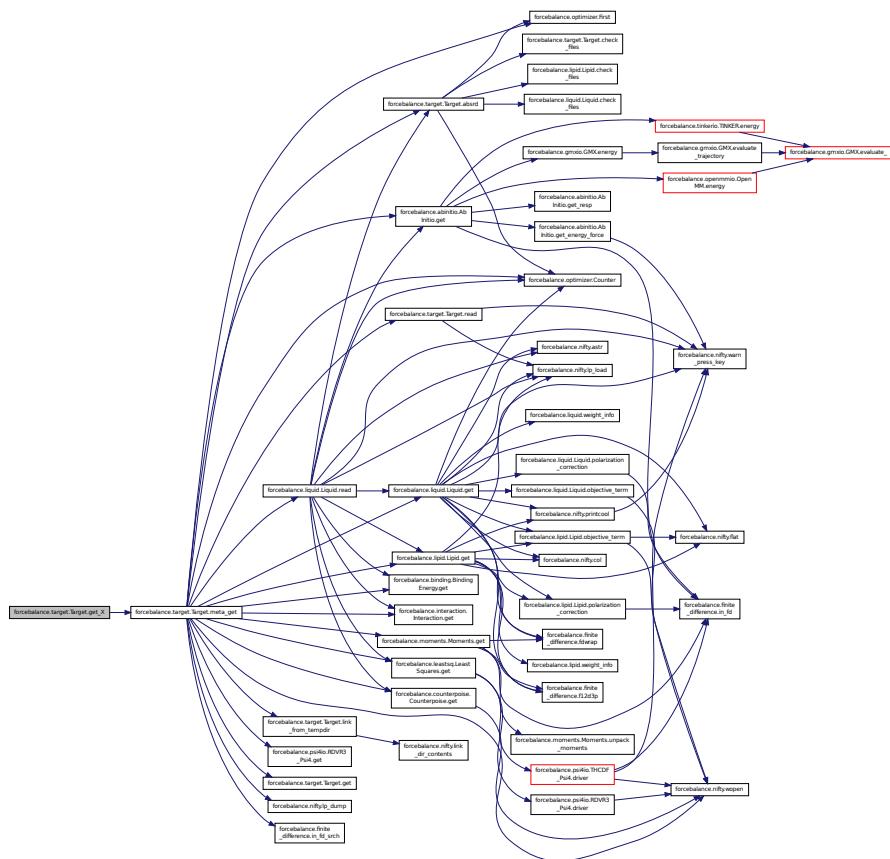
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

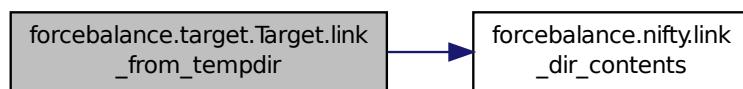
Here is the call graph for this function:



def forcebalance.target.RemoteTarget.indicate(self) Definition at line 735 of file target.py.

def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

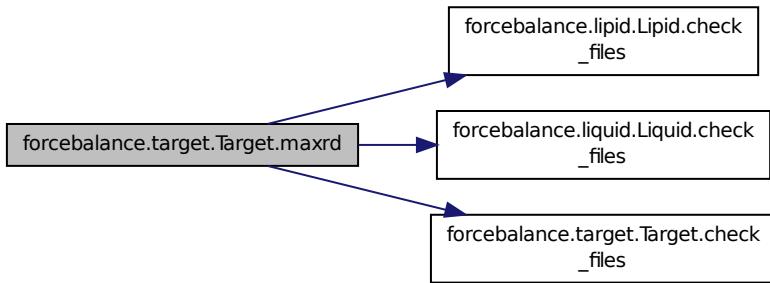
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

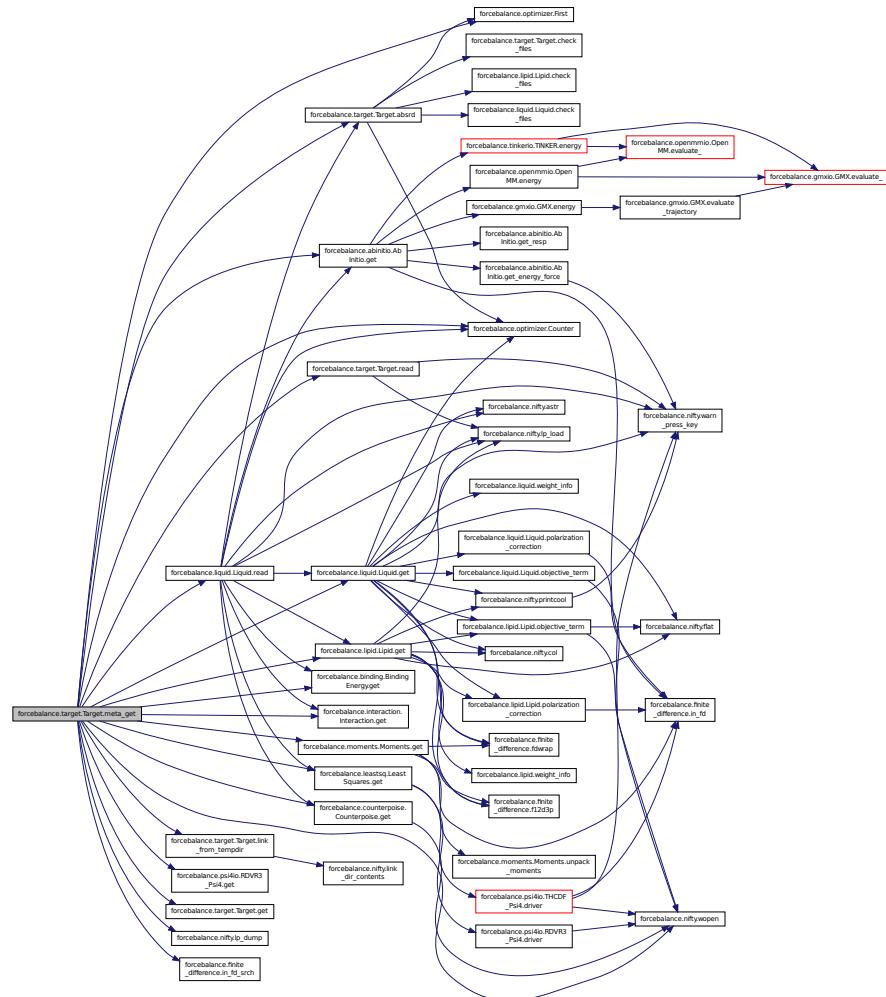
Definition at line 447 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.meta_get( self, mvals, AGrad=False, AHess=False, customdir=None ) [inherited] Wrapper around the get function.  
Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call read\(\) instead. The 'get' method should not worry about the directory that it's running in.  
Definition at line 511 of file target.py.
```

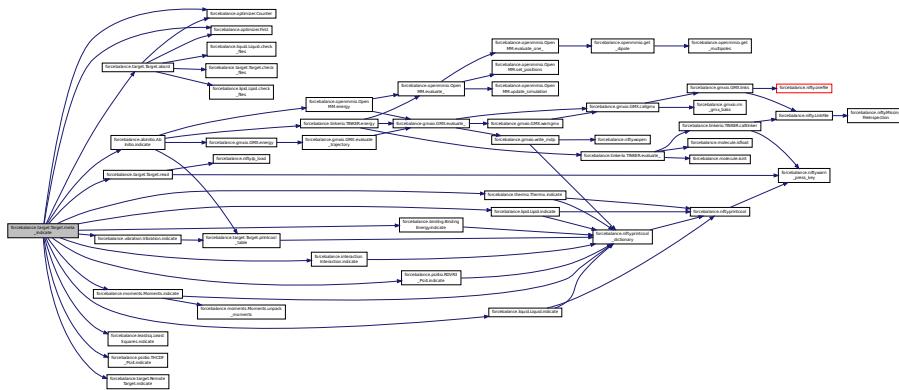
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

data	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
headings	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
banner	Optional heading line, which will be printed at the top in the title.
footnote	Optional footnote line, which will be printed at the bottom.

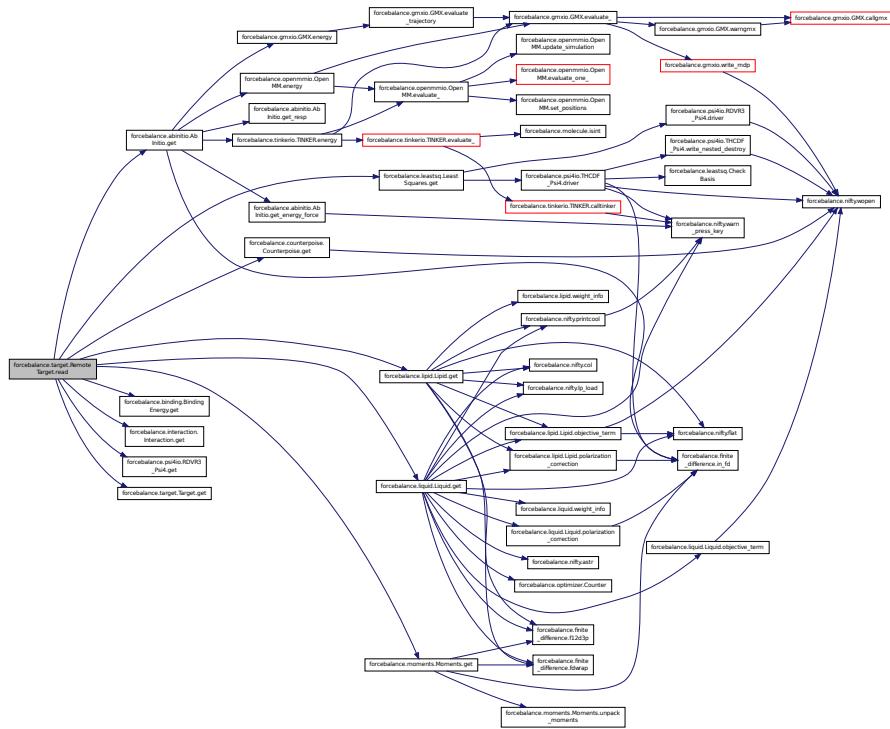
Definition at line 638 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.RemoteTarget.read( self, mvals, AGrad = False, AHess = False ) Definition at line 726 of file target.py.
```

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

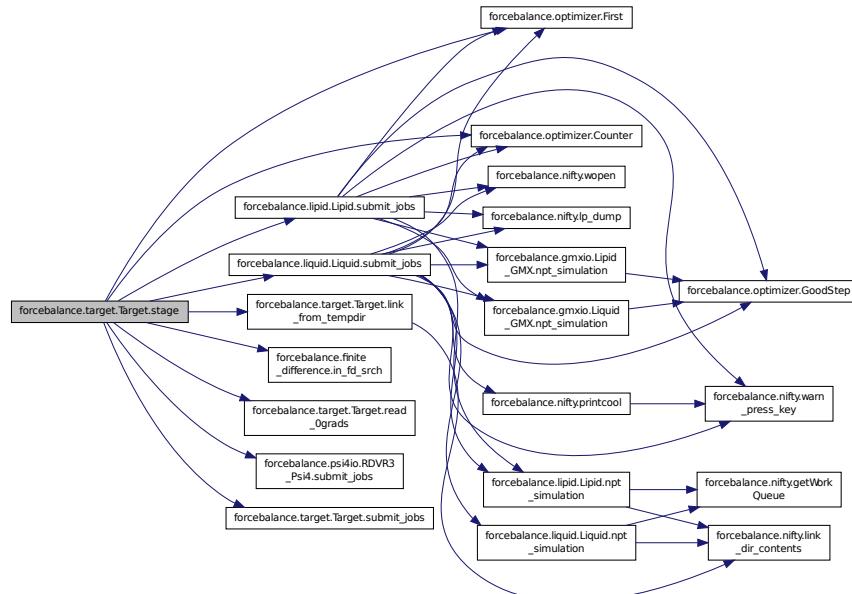
def forcebalance.BaseClass.set_option (self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

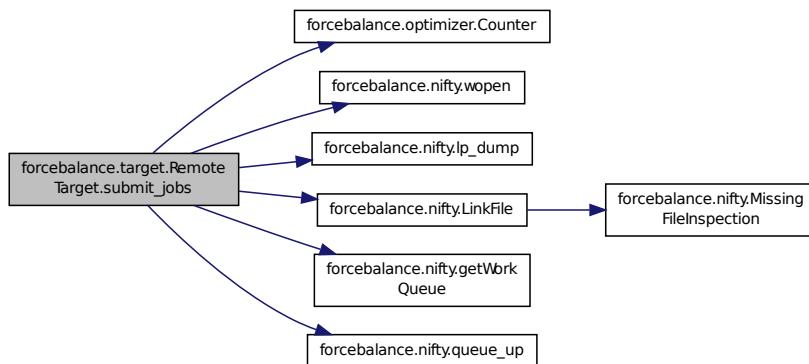
Definition at line 565 of file target.py.

Here is the call graph for this function:



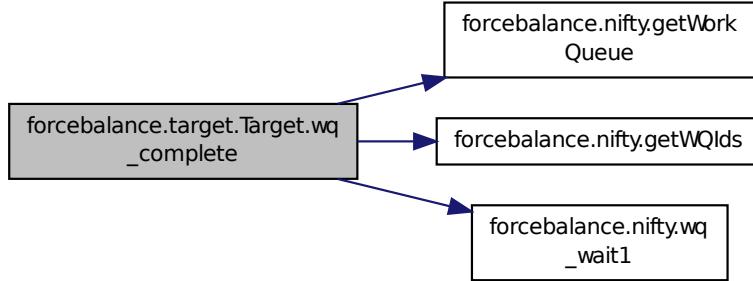
```
def forcebalance.target.RemoteTarget.submit_jobs ( self, mvals, AGrad = False, AHess = False )  
Definition at line 702 of file target.py.
```

Here is the call graph for this function:



```
def forcebalance.target.Target.wq_complete ( self ) [inherited] This method determines whether the Work  
Queue tasks for the current target have completed.  
Definition at line 602 of file target.py.
```

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.66.4 Member Data Documentation

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.RemoteTarget.r_options Definition at line 681 of file target.py.

forcebalance.target.RemoteTarget.r_tgt_opts Definition at line 684 of file target.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.RemoteTarget.read_indicate Definition at line 698 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.target.RemoteTarget.remote_indicate Definition at line 691 of file target.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number. The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.target.RemoteTarget.write_indicate Definition at line 699 of file target.py.

forcebalance.target.RemoteTarget.write_objective Definition at line 700 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

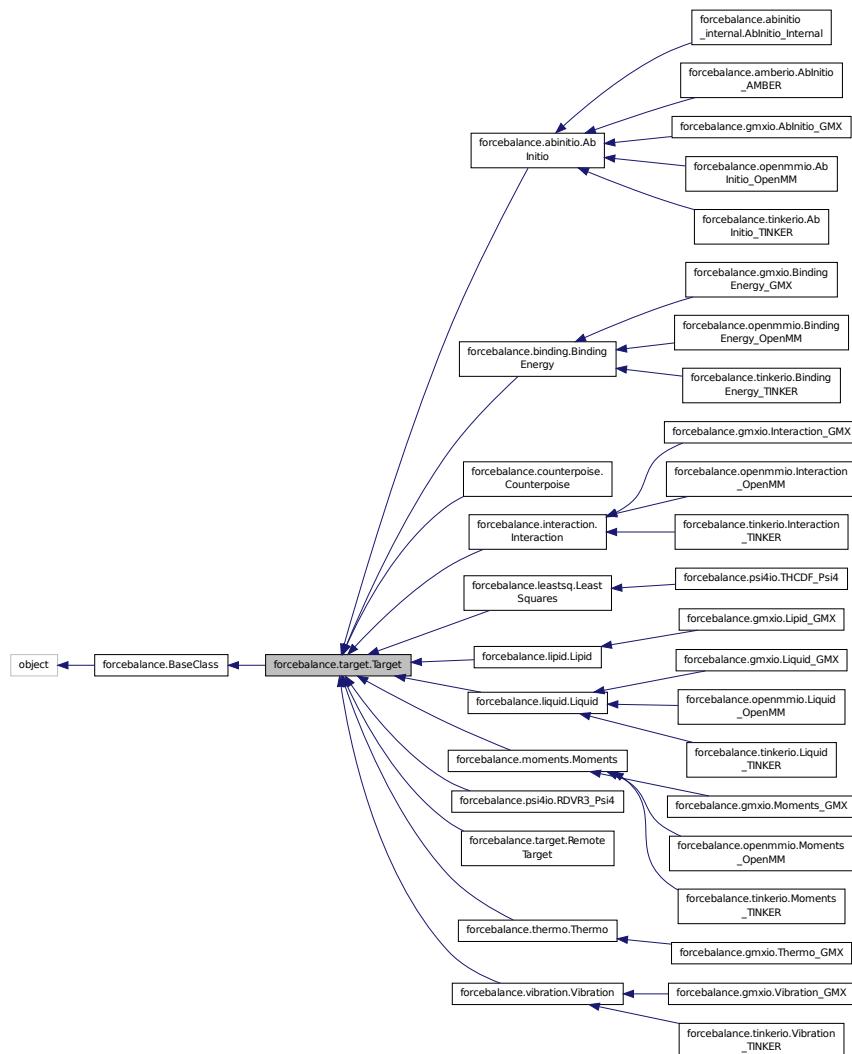
The documentation for this class was generated from the following file:

- [target.py](#)

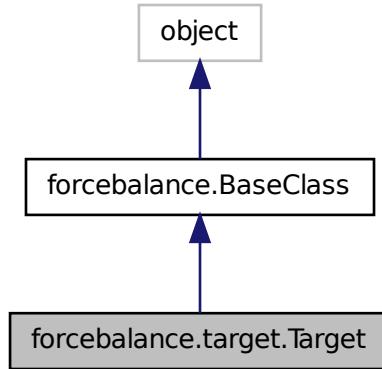
8.67 forcebalance.target.Target Class Reference

Base class for all fitting targets.

Inheritance diagram for forcebalance.target.Target:



Collaboration diagram for forcebalance.target.Target:



Public Member Functions

- def `_init_`

All options here are intended to be usable by every conceivable type of target (in other words, only add content here if it's widely applicable.)
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`

Back up the temporary directory if desired, delete it and then create a new one.
- def `get`

Every target must be able to return a contribution to the objective function - however, this must be implemented in the specific subclass.
- def `check_files`

Check this directory for the presence of readable files when the 'read' option is set.
- def `read`

Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`

Supply the correct directory specified by user's "read" option.
- def `maxrd`

Supply the latest existing temp-directory containing valid data.

- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`

Wrapper around the get function.

- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.

- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.

- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`
Relative directory of target.
- `tempdir`
`self.tempdir = os.path.join('temp', self.name)` The directory in which the simulation is running - this can be updated.
- `FF`
Need the forcefield (here for now)
- `xct`
Counts how often the objective function was computed.
- `gct`
Counts how often the gradient was computed.
- `hct`
Counts how often the Hessian was computed.
- `read_indicate`
Whether to read indicate.log from file when restarting an aborted run.
- `write_indicate`
Whether to write indicate.log at every iteration (true for all but remote.)
- `read_objective`
Whether to read objective.p from file when restarting an aborted run.
- `write_objective`
Whether to write objective.p at every iteration (true for all but remote.)
- `verbose_options`
- `PrintOptionDict`

8.67.1 Detailed Description

Base class for all fitting targets.

In ForceBalance a [Target](#) is defined as a set of reference data plus a corresponding method to simulate that data using the force field.

The 'computable quantities' may include energies and forces where the reference values come from QM calculations (energy and force matching), energies from an EDA analysis (Maybe in the future, FDA?), molecular properties (like polarizability, refractive indices, multipole moments or vibrational frequencies), relative entropies, and bulk properties. Single-molecule or bulk properties can even come from the experiment!

The central idea in ForceBalance is that each quantity makes a contribution to the overall objective function. So we can build force fields that fit several quantities at once, rather than putting all of our chips behind energy and force matching. In the future ForceBalance may even include multiobjective optimization into the optimizer.

The optimization is done by way of minimizing an 'objective function', which is comprised of squared differences between the computed and reference values. These differences are not computed in this file, but rather in subclasses that use [Target](#) as a base class. Thus, the contents of [Target](#) itself are meant to be as general as possible, because the pertinent variables apply to all types of fitting targets.

An important note: [Target](#) requires that all subclasses have a method `get(self,mvals,AGrad=False,AHess=False)` that does the following:

Inputs: `mvals` = The parameter vector, which modifies the force field (Note to self: We include `mvals` with each [Target](#) because we can create copies of the force field and do finite difference derivatives) `AGrad`, `AHess` = Boolean switches for computing analytic gradients and Hessians

Outputs: `Answer = { 'X': Number, 'G': array(NP), 'H': array((NP,NP)) }` 'X' = The objective function itself 'G' = The gradient, elements not computed analytically are zero 'H' = The Hessian, elements not computed analytically are zero

This is the only global requirement of a [Target](#). Obviously 'get' itself is not defined here, because its calculation will depend entirely on specifically which target we wish to use. However, this should give us a unified framework which will facilitate rapid implementation of Targets.

Future work: Robert suggested that I could enable automatic detection of which parameters need to be computed by finite difference. Not a bad idea. :)

Definition at line 75 of file target.py.

8.67.2 Constructor & Destructor Documentation

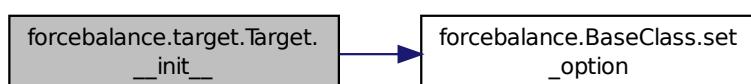
```
def forcebalance.target.Target.__init__ ( self, options, tgt_opts, forcefield )
```

All options here are intended to be usable by every conceivable type of target (in other words, only add content here if it's widely applicable.)

If we want to add attributes that are more specific (i.e. a set of reference forces for force matching), they are added in the subclass AblInitio that inherits from [Target](#).

Definition at line 92 of file target.py.

Here is the call graph for this function:



8.67.3 Member Function Documentation

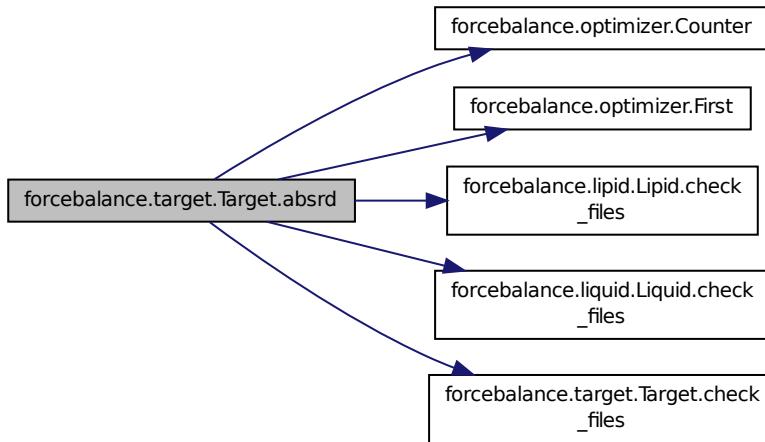
```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited]
```

Definition at line 28 of file __init__.py.

```
def forcebalance.target.Target.absrd ( self, inum = None ) Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files ( self, there ) Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.target.Target.get ( self, mvals, AGrad = False, AHess = False ) Every target must be able to return a contribution to the objective function - however, this must be implemented in the specific subclass.
```

See abinitio for an example.

Definition at line 357 of file target.py.

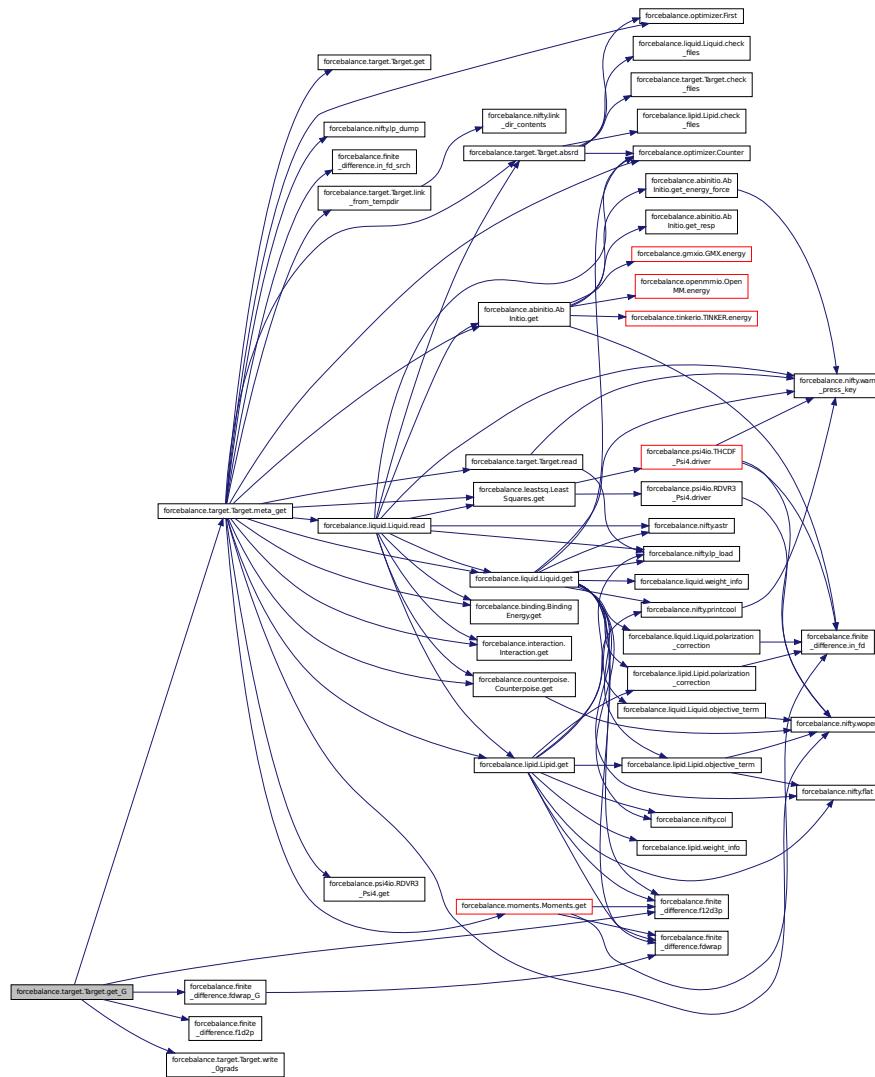
```
def forcebalance.target.Target.get_G ( self, mvals = None ) Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1.pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



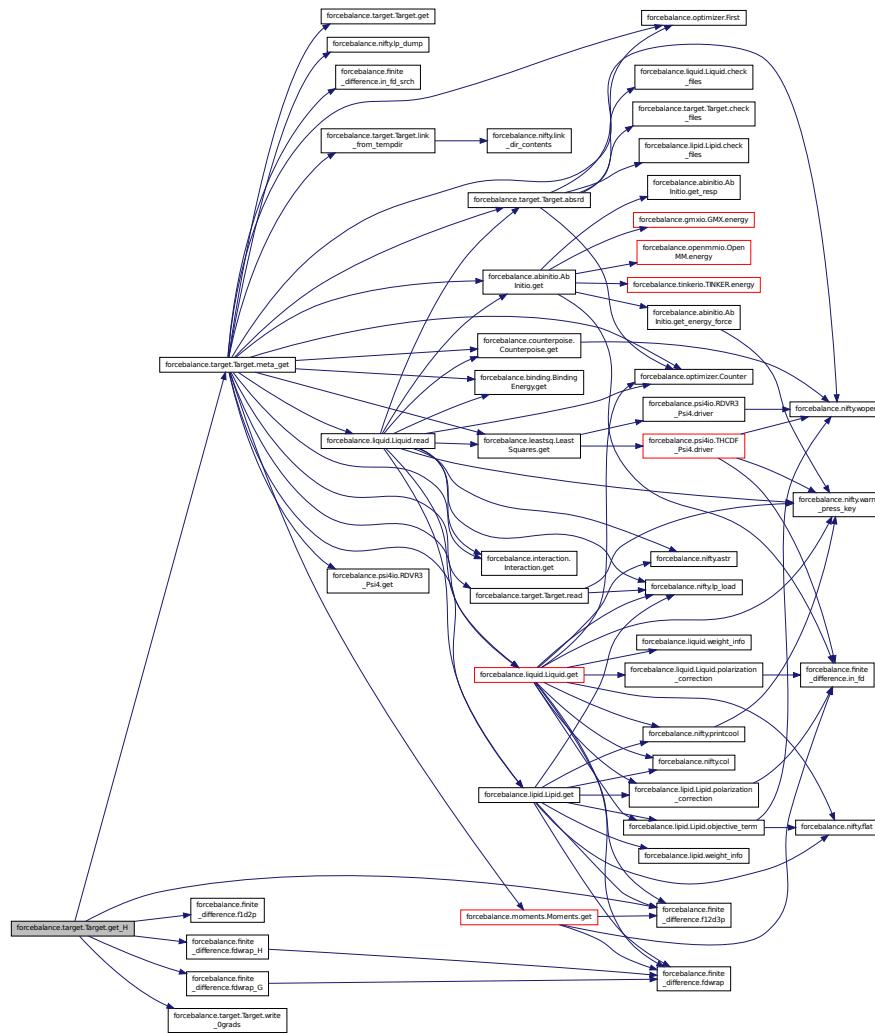
def forcebalance.target.Target.get_H (self, mvals = None) Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

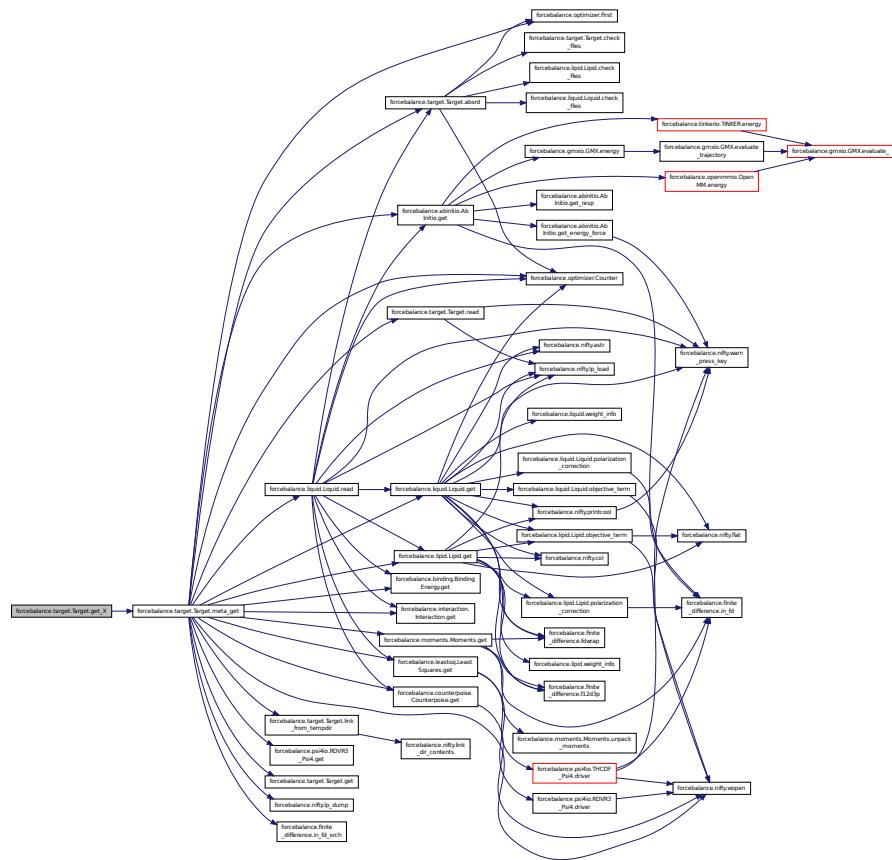
Here is the call graph for this function:



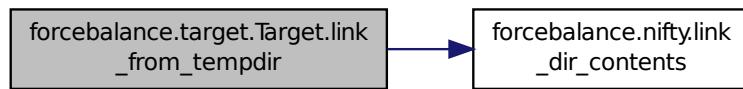
def forcebalance.target.Target.get_X (self, mvals = None) Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

Here is the call graph for this function:

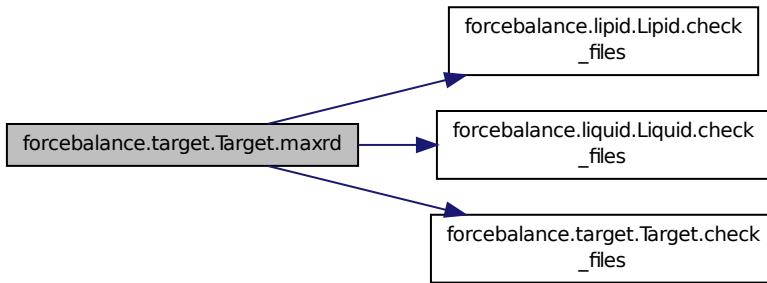


def forcebalance.target.Target.link_from_tempdir (self, absdestdir) Definition at line 315 of file target.py.
Here is the call graph for this function:



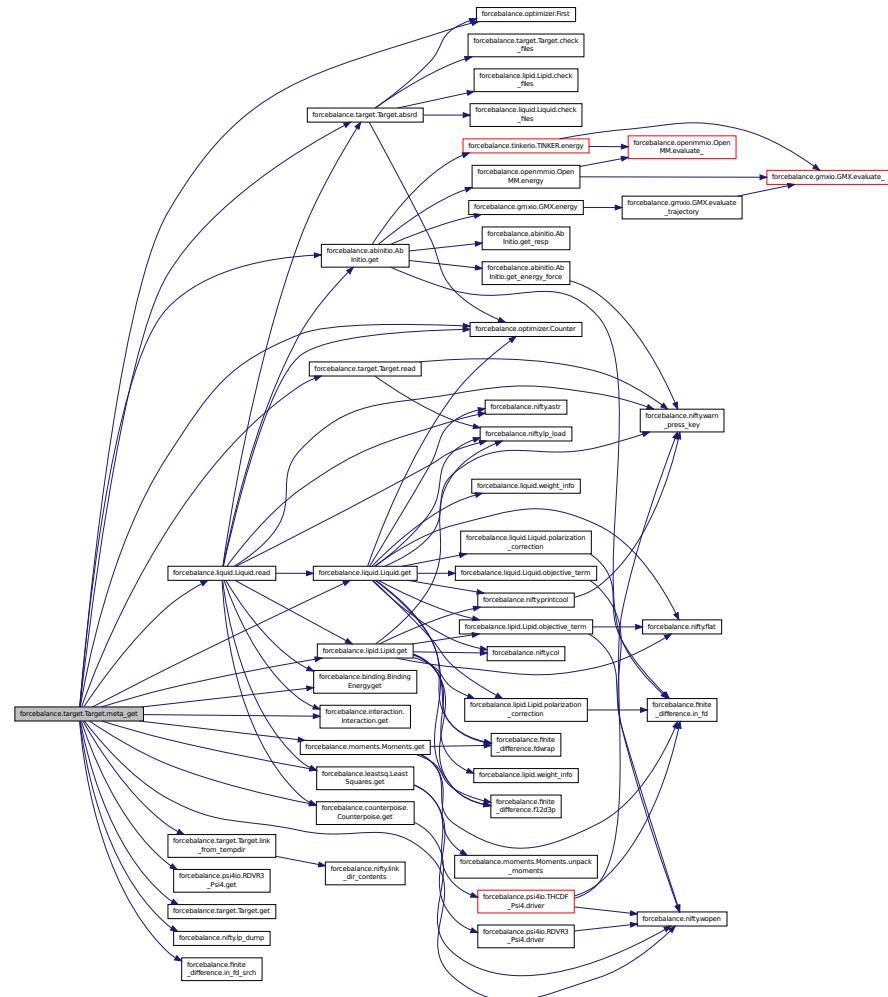
def forcebalance.target.Target.maxrd (self) Supply the latest existing temp-directory containing valid data.
Definition at line 447 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.meta_get( self, mvals, AGrad=False, AHess=False, customdir=None
) Wrapper around the get function.  
Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call read\(\) instead. The 'get' method should not worry about the directory that it's running in.  
Definition at line 511 of file target.py.
```

Here is the call graph for this function:

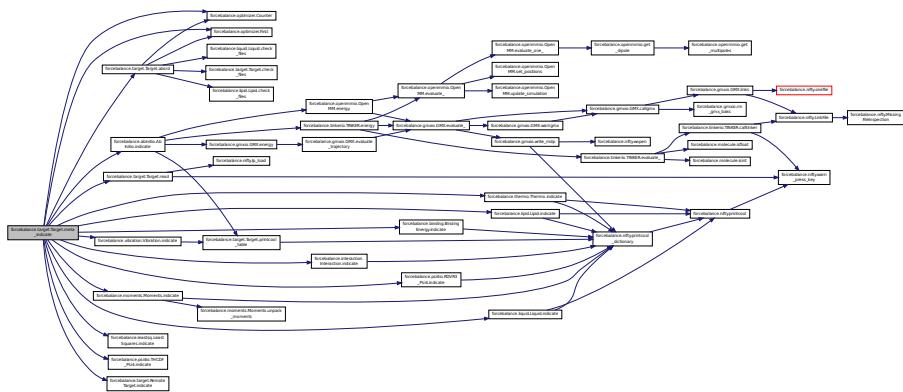


def forcebalance.target.Target.meta_indicate (self) Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.

Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

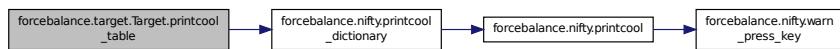
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

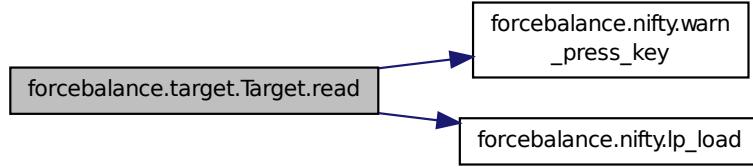
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory (self) Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

def forcebalance.BaseClass.set_option (self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

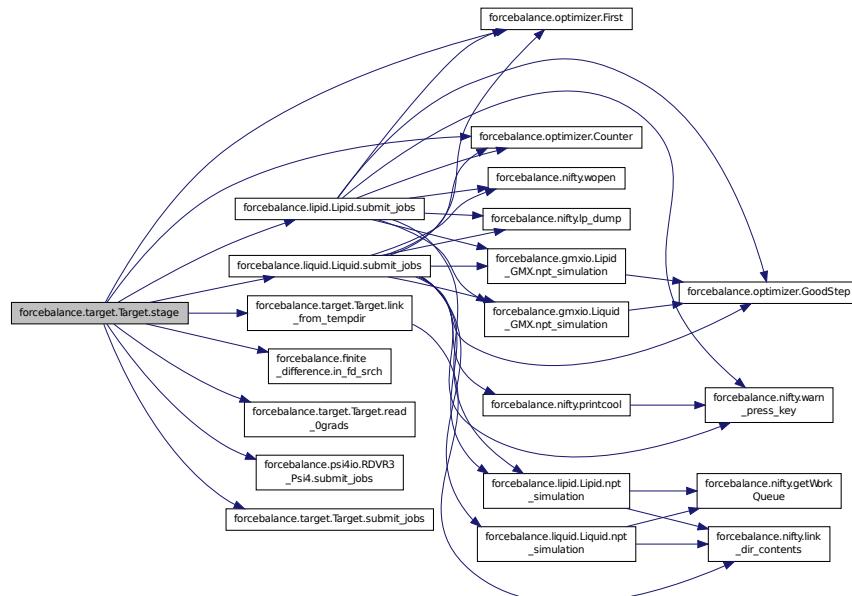
def forcebalance.target.Target.stage (self, mvals, AGrad = False, AHess = False, customdir = None)

Stages the directory for the target, and then launches Work Queue processes if any.

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

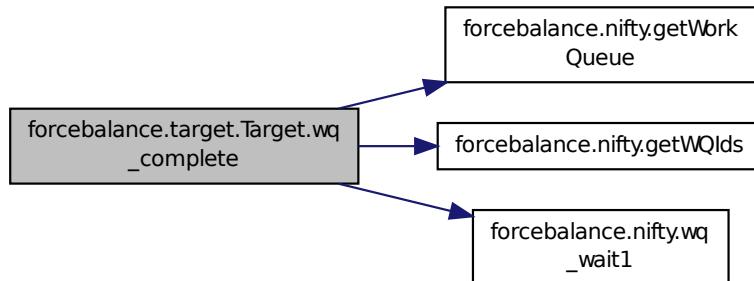


def forcebalance.target.Target.submit_jobs (self, mvals, AGrad = False, AHess = False) Definition at line 555 of file target.py.

def forcebalance.target.Target.wq_complete (self) This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.67.4 Member Data Documentation

forcebalance.target.Target.FF Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.target.Target.pgrad Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [**inherited**] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.target.Target.rundir self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [**inherited**] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate Whether to write indicate.log at every iteration (true for all but remote.)
Definition at line 170 of file target.py.

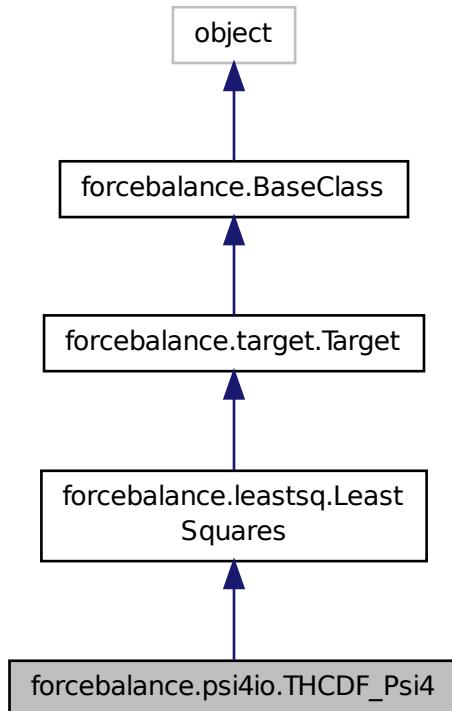
forcebalance.target.Target.write_objective Whether to write objective.p at every iteration (true for all but remote.)
Definition at line 174 of file target.py.

forcebalance.target.Target.xct Counts how often the objective function was computed.
Definition at line 162 of file target.py.
The documentation for this class was generated from the following file:

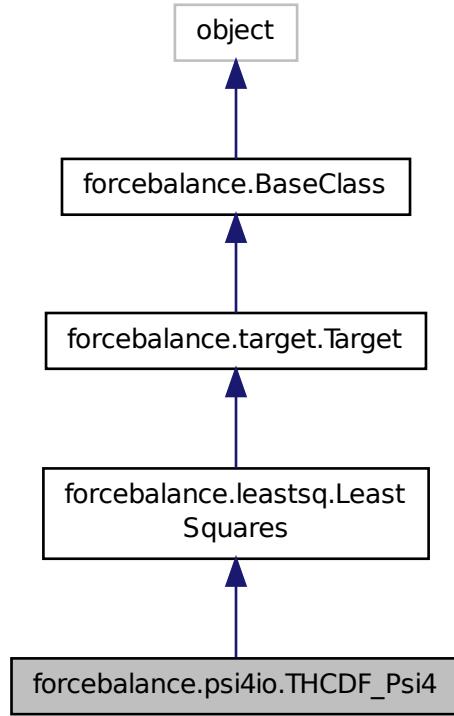
- [target.py](#)

8.68 forcebalance.psi4io.THCDF_Psi4 Class Reference

Inheritance diagram for forcebalance.psi4io.THCDF_Psi4:



Collaboration diagram for forcebalance.psi4io.THCDF_Psi4:



Public Member Functions

- def `_init_`
- def `prepare_temp_directory`
- def `indicate`
- def `write_nested_destroy`
- def `driver`
- def `get`
 LPW 05-30-2012.
- def `get_X`
 Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`
 Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`
 Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
 Computes the objective function contribution and its gradient.
- def `get_H`
 Computes the objective function contribution and its gradient / Hessian.

- def [link_from_tempdir](#)
- def [refresh_temp_directory](#)
Back up the temporary directory if desired, delete it and then create a new one.
- def [check_files](#)
Check this directory for the presence of readable files when the 'read' option is set.
- def [read](#)
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def [absrd](#)
Supply the correct directory specified by user's "read" option.
- def [maxrd](#)
Supply the latest existing temp-directory containing valid data.
- def [meta_indicate](#)
Wrap around the indicate function, so it can print to screen and also to a file.
- def [meta_get](#)
Wrapper around the get function.
- def [submit_jobs](#)
- def [stage](#)
Stages the directory for the target, and then launches Work Queue processes if any.
- def [wq_complete](#)
This method determines whether the Work Queue tasks for the current target have completed.
- def [printcool_table](#)
Print target information in an organized table format.
- def [__setattr__](#)
- def [set_option](#)

Public Attributes

- [Molecules](#)
- [throw_outs](#)
- [Elements](#)
- [GBSfnm](#)
Psi4 basis set file.
- [DATfnm](#)
Psi4 input file for calculation of linear dependencies This is actually a file in 'forcefield' until we can figure out a better system.
- [MP2_Energy](#)
Actually run PSI4.
- [DF_Energy](#)
- [MAQ](#)
Dictionary for derivative terms.
- [D](#)
- [objective](#)
- [rd](#)
Root directory of the whole project.
- [pgrad](#)
Iteration where we turn on zero-gradient skipping.
- [tempbase](#)
Relative directory of target.

- `tempdir`
`self.tempdir = os.path.join('temp',self.name)` The directory in which the simulation is running - this can be updated.
- `FF`
`Need the forcefield (here for now)`
- `xct`
`Counts how often the objective function was computed.`
- `gct`
`Counts how often the gradient was computed.`
- `hct`
`Counts how often the Hessian was computed.`
- `read_indicate`
`Whether to read indicate.log from file when restarting an aborted run.`
- `write_indicate`
`Whether to write indicate.log at every iteration (true for all but remote.)`
- `read_objective`
`Whether to read objective.p from file when restarting an aborted run.`
- `write_objective`
`Whether to write objective.p at every iteration (true for all but remote.)`
- `verbose_options`
- `PrintOptionDict`

8.68.1 Detailed Description

Definition at line 97 of file psi4io.py.

8.68.2 Constructor & Destructor Documentation

`def forcebalance.psi4io.THCDF_Psi4.__init__ (self, options, tgt_opts, forcefield)` Definition at line 99 of file psi4io.py.

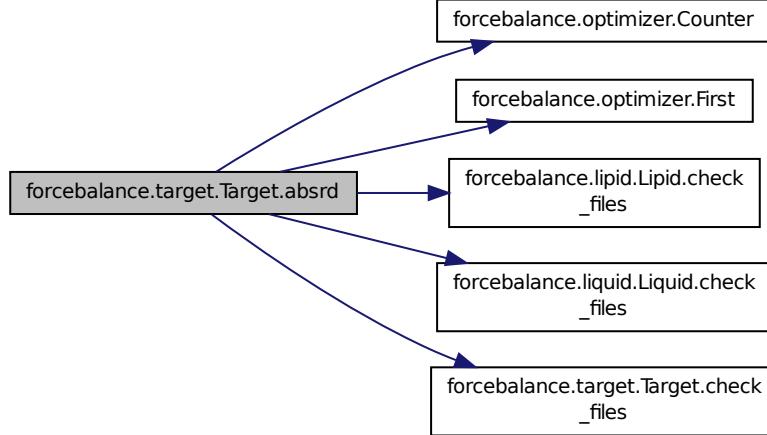
8.68.3 Member Function Documentation

`def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited]` Definition at line 28 of file __init__.py.

`def forcebalance.target.Target.absrd (self, inum = None) [inherited]` Supply the correct directory specified by user's "read" option.

Definition at line 393 of file target.py.

Here is the call graph for this function:

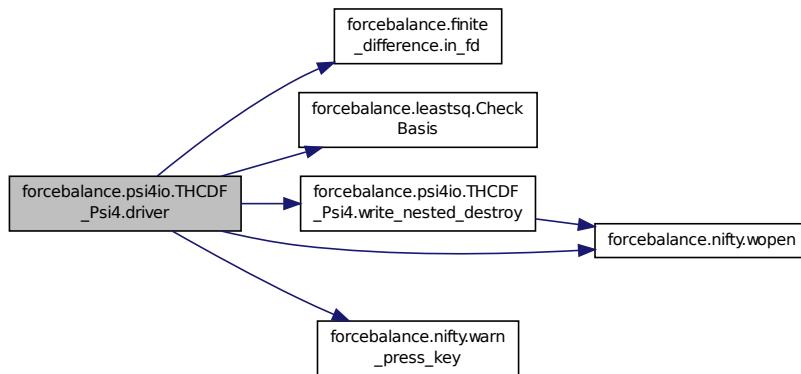


def forcebalance.target.Target.check_files(self, there) [inherited] Check this directory for the presence of readable files when the 'read' option is set.

Definition at line 364 of file target.py.

def forcebalance.psi4io.THCDF_Psi4.driver(self) Definition at line 175 of file psi4io.py.

Here is the call graph for this function:



def forcebalance.leastsq.LeastSquares.get(self, mvals, AGrad = False, AHess = False) [inherited] LPW 05-30-2012.

This subroutine builds the objective function (and optionally its derivatives) from a general software.

This subroutine interfaces with simulation software 'drivers'. The driver is expected to give exact values, fitting values, and weights.

Parameters

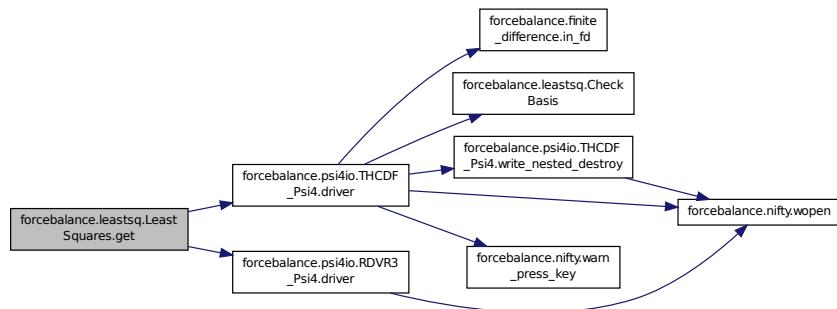
in	<i>mvals</i>	Mathematical parameter values
in	<i>AGrad</i>	Switch to turn on analytic gradient
in	<i>AHess</i>	Switch to turn on analytic Hessian

Returns

Answer Contribution to the objective function

Definition at line 62 of file leastsq.py.

Here is the call graph for this function:



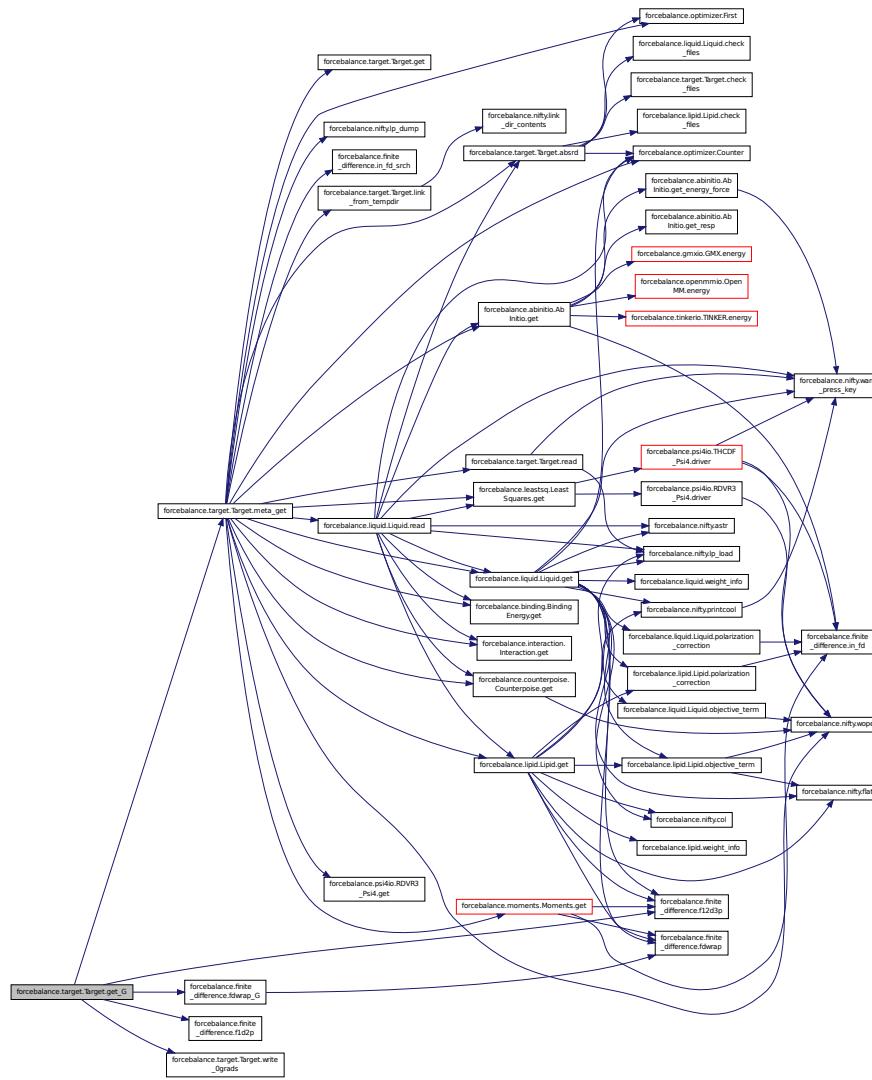
def forcebalance.target.Target.get_G (*self*, *mvals = None*) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



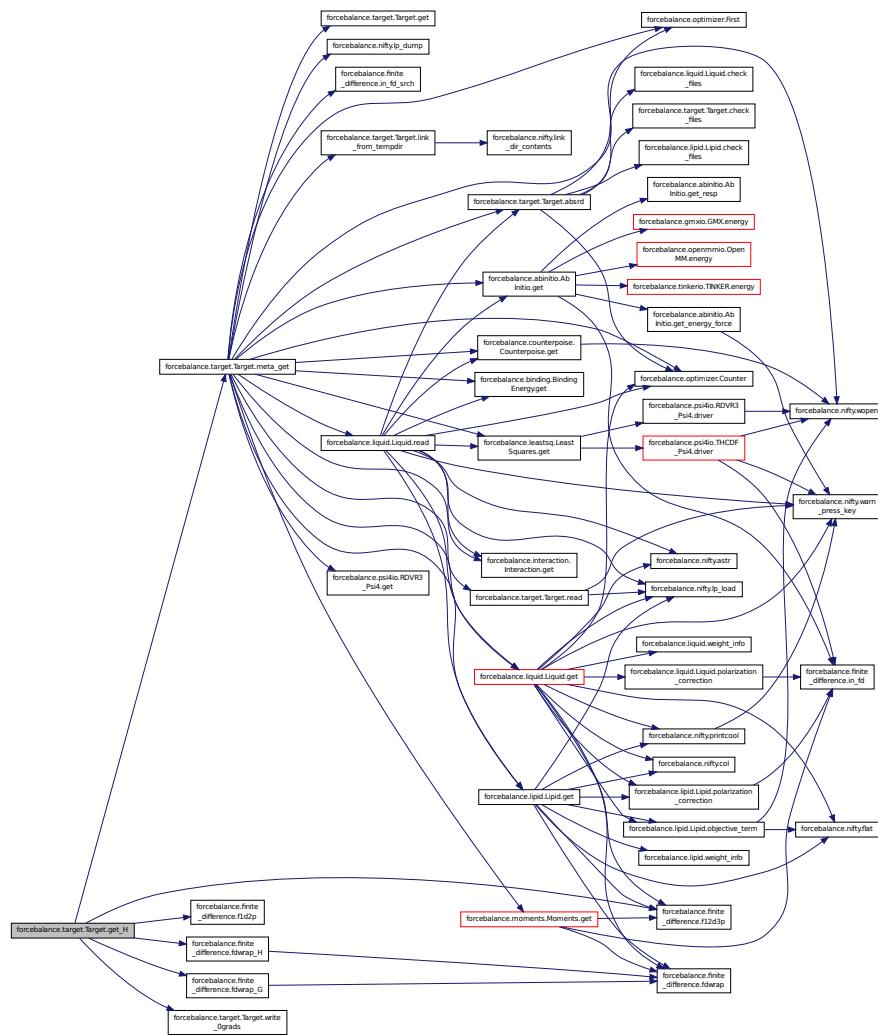
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

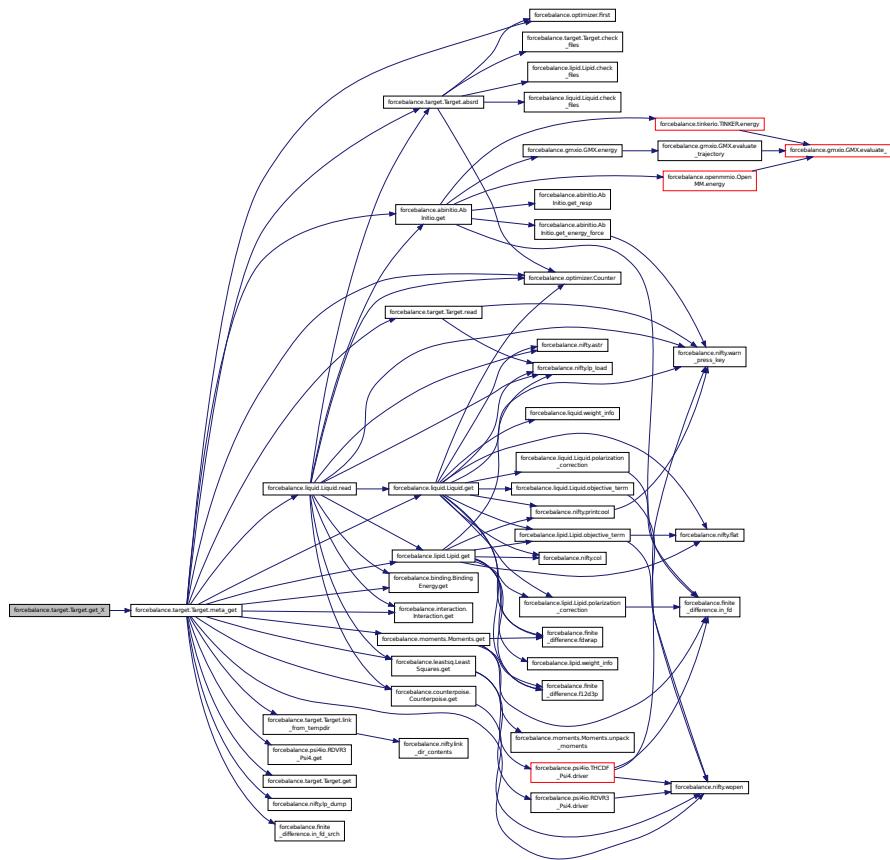
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

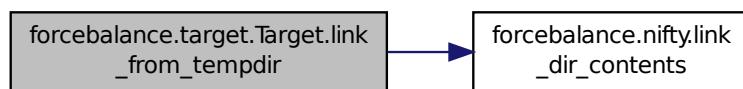
Here is the call graph for this function:



```
def forcebalance.psi4io.THCDF_Psi4.indicate ( self ) Definition at line 155 of file psi4io.py.
```

```
def forcebalance.target.Target.link_from_tempdir ( self, absdestdir ) [inherited] Definition at line 315 of file target.py.
```

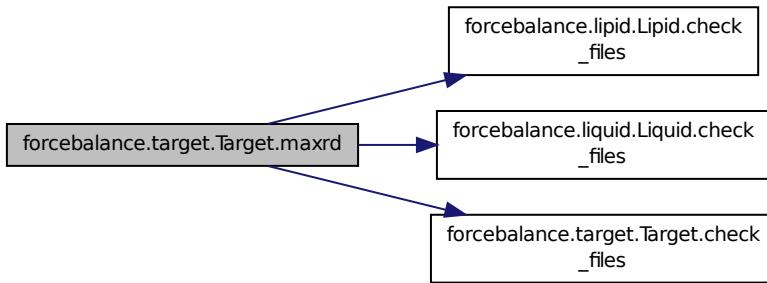
Here is the call graph for this function:



```
def forcebalance.target.Target.maxrd ( self ) [inherited] Supply the latest existing temp-directory containing valid data.
```

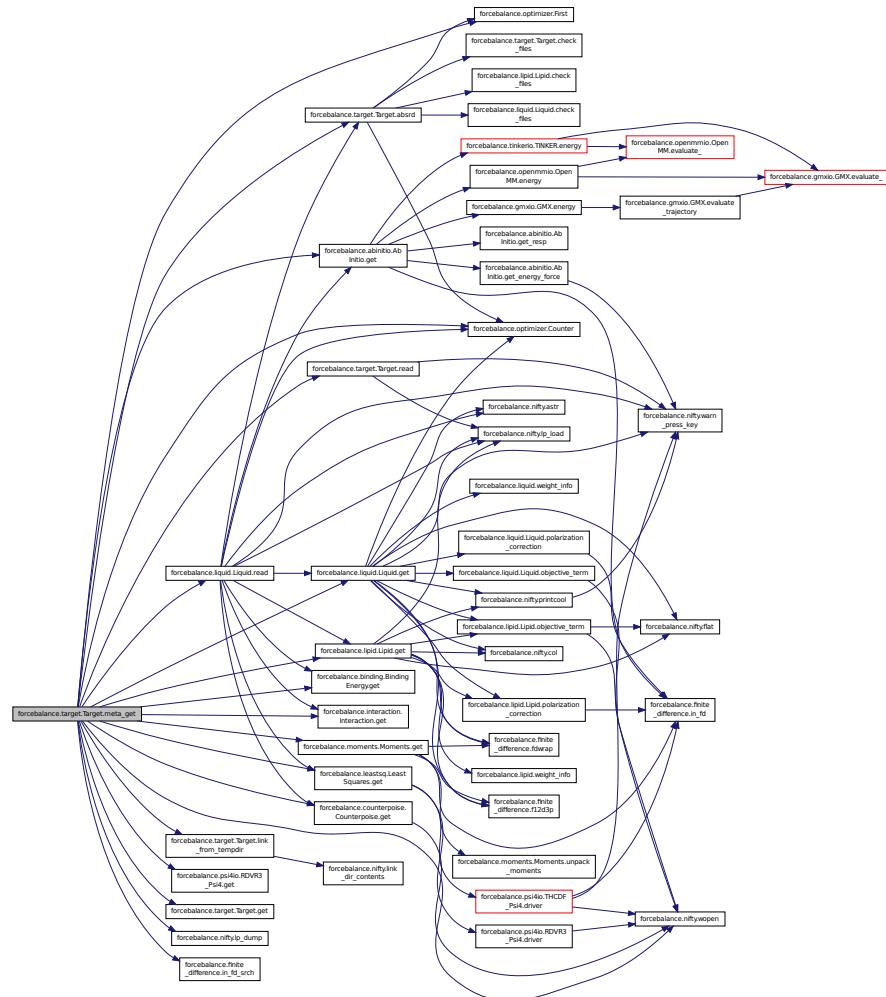
Definition at line 447 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.meta_get( self, mvals, AGrad=False, AHess=False, customdir=None ) [inherited] Wrapper around the get function.  
Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call read\(\) instead. The 'get' method should not worry about the directory that it's running in.  
Definition at line 511 of file target.py.
```

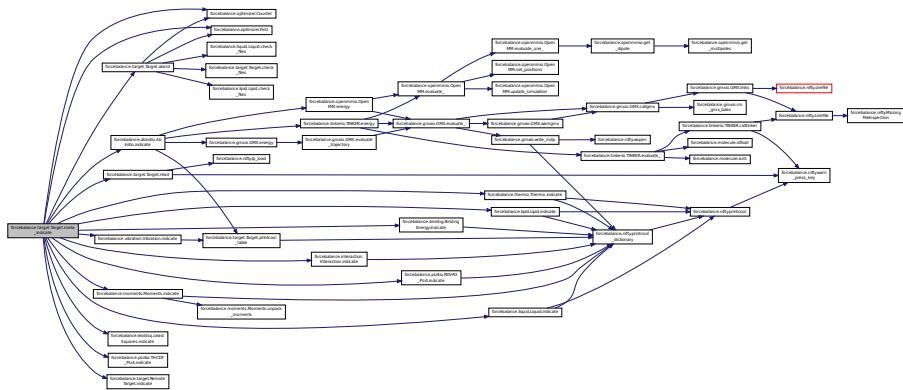
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



def forcebalance.psi4io.THCDF_Psi4.prepare_temp_directory (self, options, tgt_opts) Definition at line 144 of file psi4io.py.

Here is the call graph for this function:



def forcebalance.target.Target.printcool_table (self, data = OrderedDict ([]), headings = [], banner = None, footnote = None, color = 0) [inherited] Print target information in an organized table format.

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

Here is the call graph for this function:

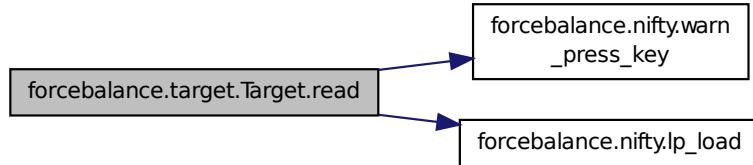


```
def forcebalance.target.Target.read ( self, mvals, AGrad = False, AHess = False ) [inherited]
```

Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.read_0grads ( self ) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.
```

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

```
def forcebalance.target.Target.refresh_temp_directory( self ) [inherited] Back up the temporary directory if desired, delete it and then create a new one.
```

Definition at line 321 of file target.py.

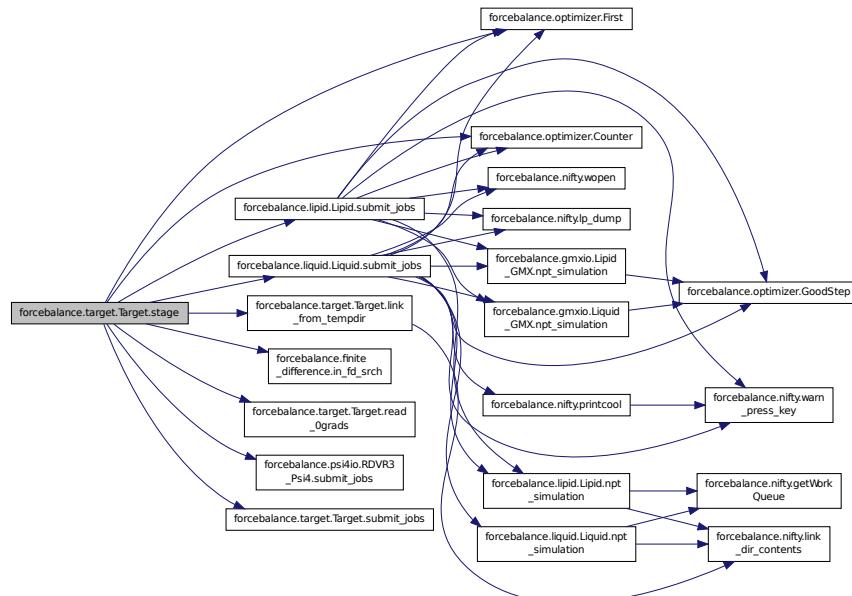
```
def forcebalance.BaseClass.set_option ( self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

```
def forcebalance.target.Target.stage ( self, mvals, AGrad = False, AHess = False, customdir = None ) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.
```

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:

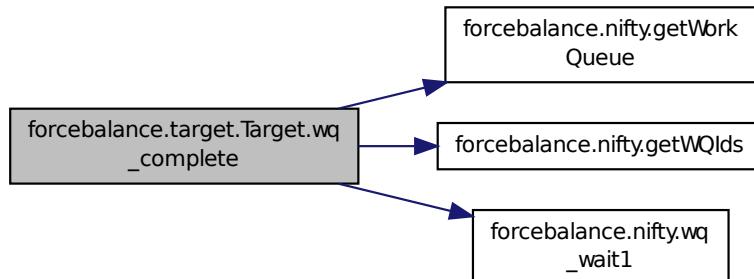


```
def forcebalance.target.Target.submit_jobs ( self, mvals, AGrad = False, AHess = False )
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:

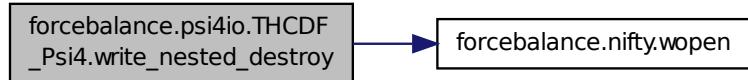


```
def forcebalance.target.Target.write_0grads( self, Ans ) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.
```

Definition at line 225 of file target.py.

def forcebalance.psi4io.THCDF_Psi4.write_nested_destroy (self, fnm, linedestroy) Definition at line 160 of file psi4io.py.

Here is the call graph for this function:



8.68.4 Member Data Documentation

forcebalance.leastsq.LeastSquares.D [inherited] Definition at line 126 of file leastsq.py.

forcebalance.psi4io.THCDF_Psi4.DATfnm Psi4 input file for calculation of linear dependencies This is actually a file in 'forcefield' until we can figure out a better system.

Definition at line 140 of file psi4io.py.

forcebalance.psi4io.THCDF_Psi4.DF_Energy Definition at line 241 of file psi4io.py.

forcebalance.psi4io.THCDF_Psi4.Elements Definition at line 117 of file psi4io.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.psi4io.THCDF_Psi4.GBSfnm Psi4 basis set file.

Definition at line 133 of file psi4io.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.leastsq.LeastSquares.MAQ [inherited] Dictionary for derivative terms.

Definition at line 88 of file leastsq.py.

forcebalance.psi4io.THCDF_Psi4.Molecules Definition at line 105 of file psi4io.py.

forcebalance.psi4io.THCDF_Psi4.MP2_Energy Actually run PSI4.

Read in the commented linindep.gbs file and ensure that these same lines are commented in the new .gbs file Now build a "Frankenstein" .gbs file composed of the original .gbs file but with data from the linindep.gbs file!

Definition at line 239 of file psi4io.py.

forcebalance.leastsq.LeastSquares.objective [inherited] Definition at line 127 of file leastsq.py.

forcebalance.target.Target.pgrad [**inherited**] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [**inherited**] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [**inherited**] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [**inherited**] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [**inherited**] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [**inherited**] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number. The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [**inherited**] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [**inherited**] Definition at line 155 of file target.py.

forcebalance.psi4io.THCDF_Psi4.throw_outs Definition at line 106 of file psi4io.py.

forcebalance.BaseClass.verbose_options [**inherited**] Definition at line 40 of file __init__.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

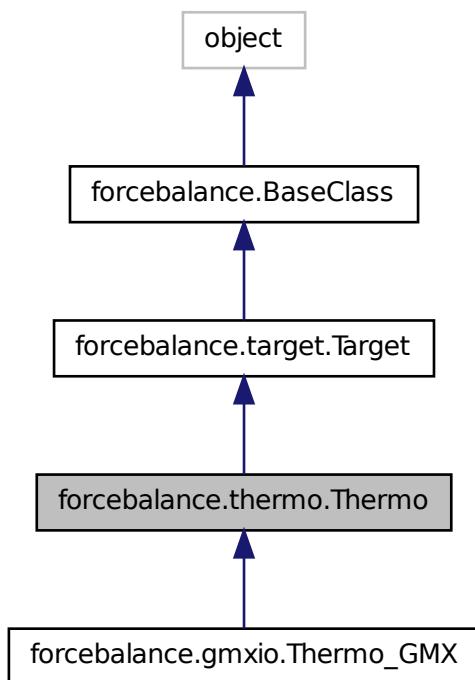
Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.
Definition at line 162 of file target.py.
The documentation for this class was generated from the following file:
• [psi4io.py](#)

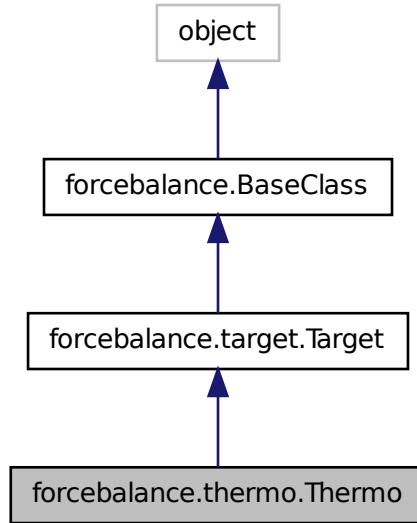
8.69 forcebalance.thermo.Thermo Class Reference

A target for fitting general experimental data sets.

Inheritance diagram for forcebalance.thermo.Thermo:



Collaboration diagram for forcebalance.thermo.Thermo:



Public Member Functions

- def `_init_`
- def `retrieve`

Retrieve the molecular dynamics (MD) results and store the calculated quantities in the [Point](#) object dp.
- def `submit_jobs`

This routine is called by [Objective.stage\(\)](#) and will run before "get".
- def `indicate`

Shows optimization state.
- def `objective_term`

Calculates the contribution to the objective function (the term) for a given quantity.
- def `get`

Return the contribution to the total objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.
- def `get_H`

Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`

- def [refresh_temp_directory](#)
Back up the temporary directory if desired, delete it and then create a new one.
- def [check_files](#)
Check this directory for the presence of readable files when the 'read' option is set.
- def [read](#)
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def [absrd](#)
Supply the correct directory specified by user's "read" option.
- def [maxrd](#)
Supply the latest existing temp-directory containing valid data.
- def [meta_indicate](#)
Wrap around the indicate function, so it can print to screen and also to a file.
- def [meta_get](#)
Wrapper around the get function.
- def [stage](#)
Stages the directory for the target, and then launches Work Queue processes if any.
- def [wq_complete](#)
This method determines whether the Work Queue tasks for the current target have completed.
- def [printcool_table](#)
Print target information in an organized table format.
- def [__setattr__](#)
- def [set_option](#)

Public Attributes

- [simpfx](#)
Initialize base class.
- [points](#)
- [denoms](#)
- [weights](#)
- [Xp](#)
- [Wp](#)
- [Pp](#)
- [Gp](#)
- [Objective](#)
- [rd](#)
Root directory of the whole project.
- [pgrad](#)
Iteration where we turn on zero-gradient skipping.
- [tempbase](#)
Relative directory of target.
- [tempdir](#)
- [rundir](#)
`self.tempdir = os.path.join('temp',self.name)` *The directory in which the simulation is running - this can be updated.*
- [FF](#)
Need the forcefield (here for now)
- [xct](#)
Counts how often the objective function was computed.

- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**
Whether to write indicate.log at every iteration (true for all but remote.)
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

8.69.1 Detailed Description

A target for fitting general experimental data sets.

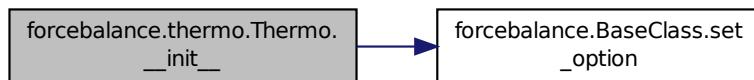
The experimental data is described in a .txt file and is handled with a `Quantity` subclass.

Definition at line 24 of file `thermo.py`.

8.69.2 Constructor & Destructor Documentation

def forcebalance.thermo.Thermo.__init__ (self, options, tgt_opts, forcefield) Definition at line 25 of file `thermo.py`.

Here is the call graph for this function:



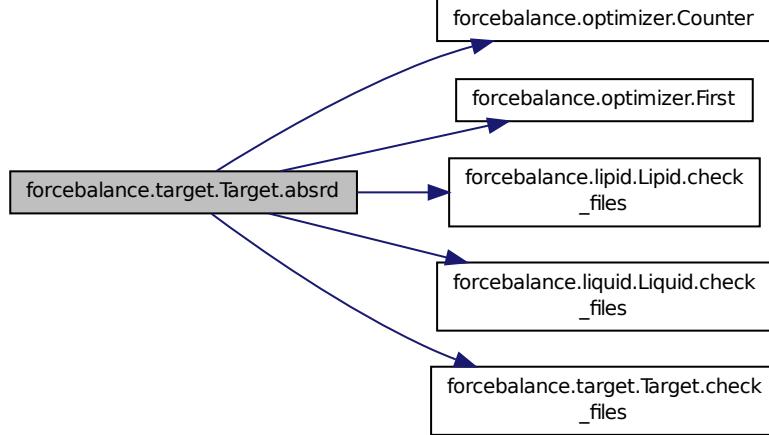
8.69.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited] Definition at line 28 of file `__init__.py`.

def forcebalance.target.Target.absrd (self, inum = None) [inherited] Supply the correct directory specified by user's "read" option.

Definition at line 393 of file `target.py`.

Here is the call graph for this function:



def forcebalance.target.Target.check_files(self, there) [inherited] Check this directory for the presence of readable files when the 'read' option is set.

Definition at line 364 of file target.py.

def forcebalance.thermo.Thermo.get(self, mvals, AGrad = True, AHess = True) Return the contribution to the total objective function.

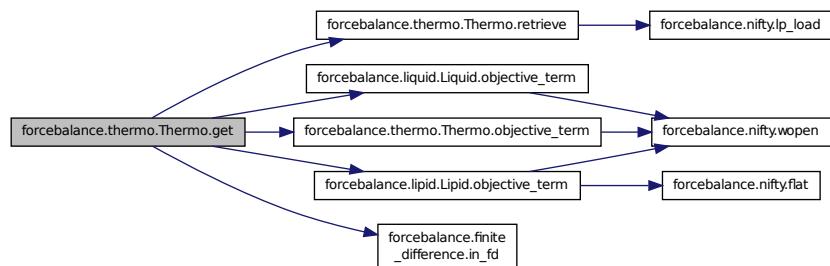
This is a weighted average of the calculated quantities.

Parameters mvals : list Mathematical parameter values. AGrad : Boolean Switch to turn on analytic gradient. AHess : Boolean Switch to turn on analytic Hessian.

Returns Answer : dict Contribution to the objective function. Answer is a dict with keys X for the objective function, G for its gradient and H for its Hessian.

Definition at line 361 of file thermo.py.

Here is the call graph for this function:



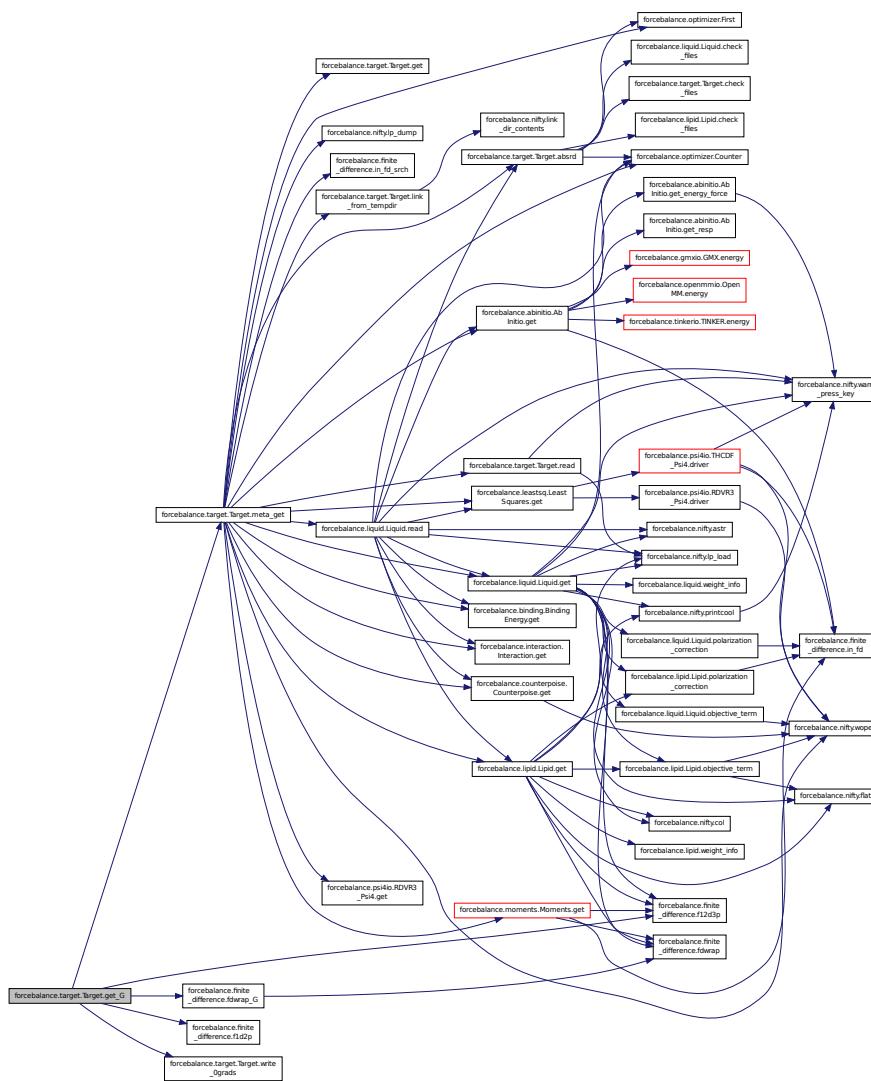
def forcebalance.target.Target.get_G(self, mvals = None) [inherited] Computes the objective function contribution and its gradient.

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the `fd1_pids` and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

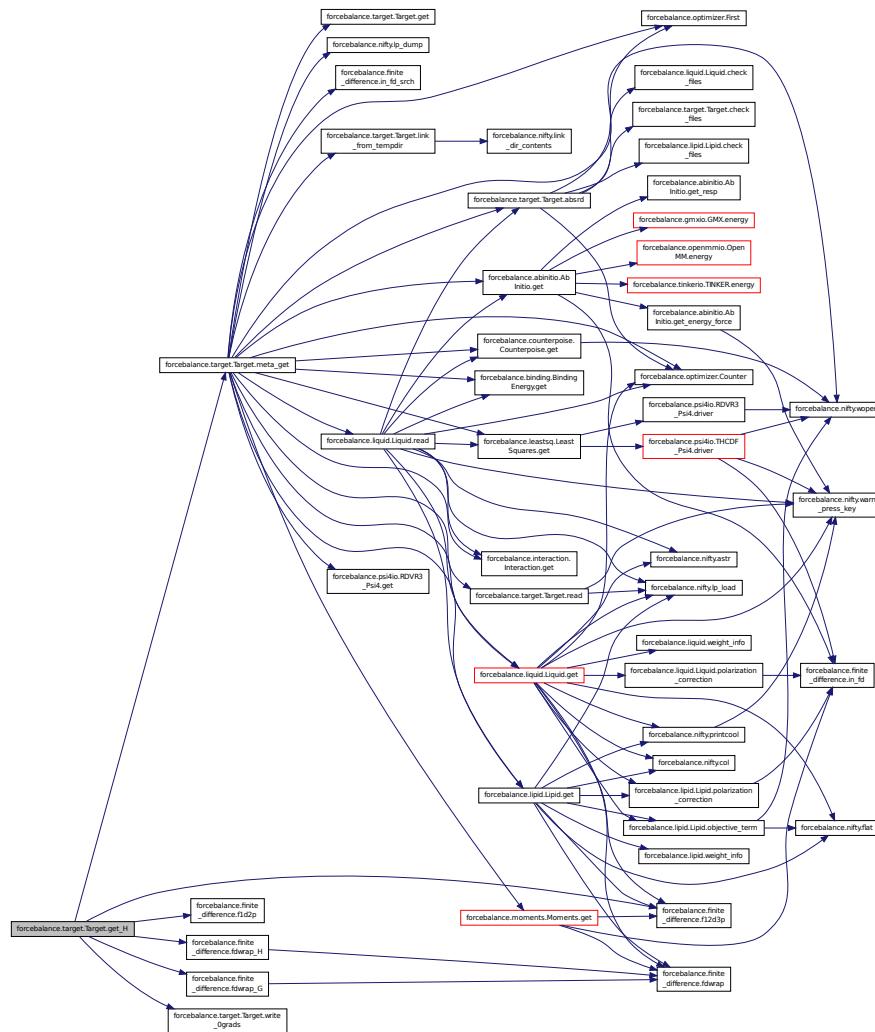
First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through

the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

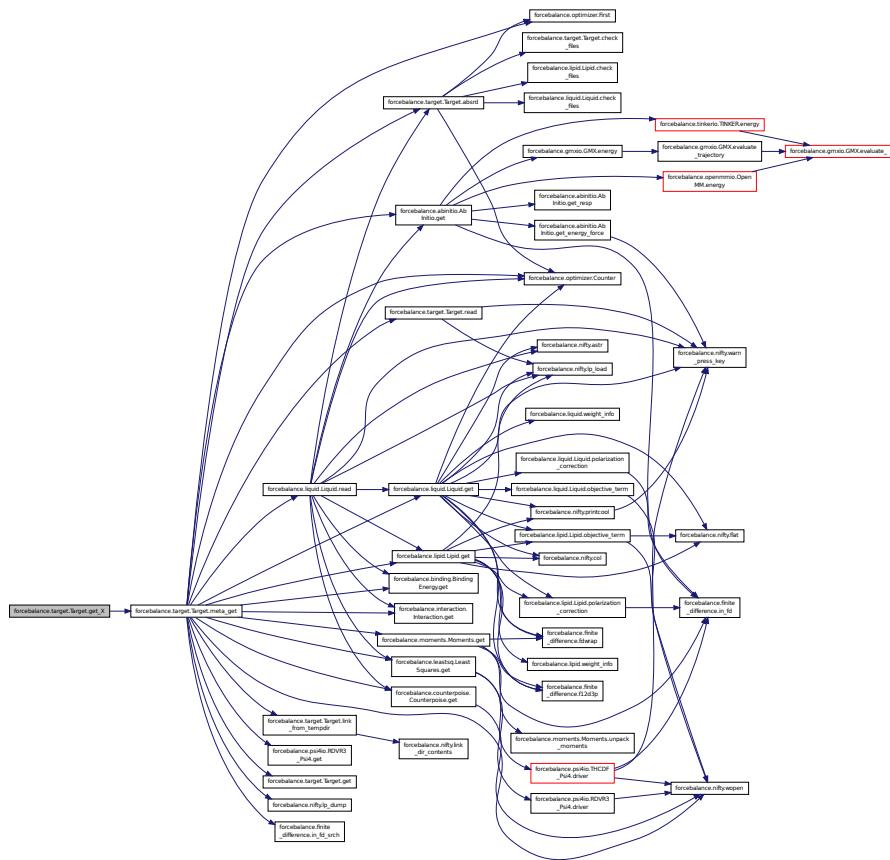
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

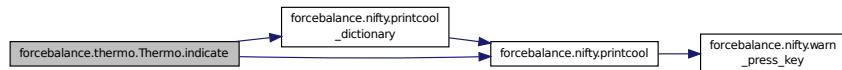
Here is the call graph for this function:



def forcebalance.thermo.Thermo.indicate (self) Shows optimization state.

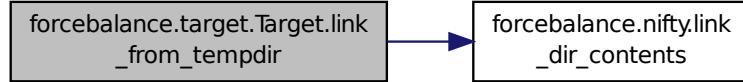
Definition at line 220 of file thermo.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

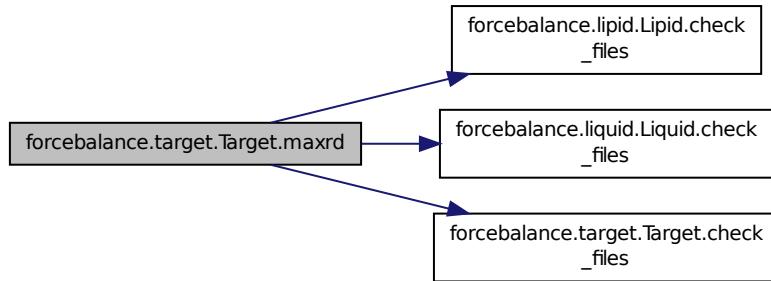
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

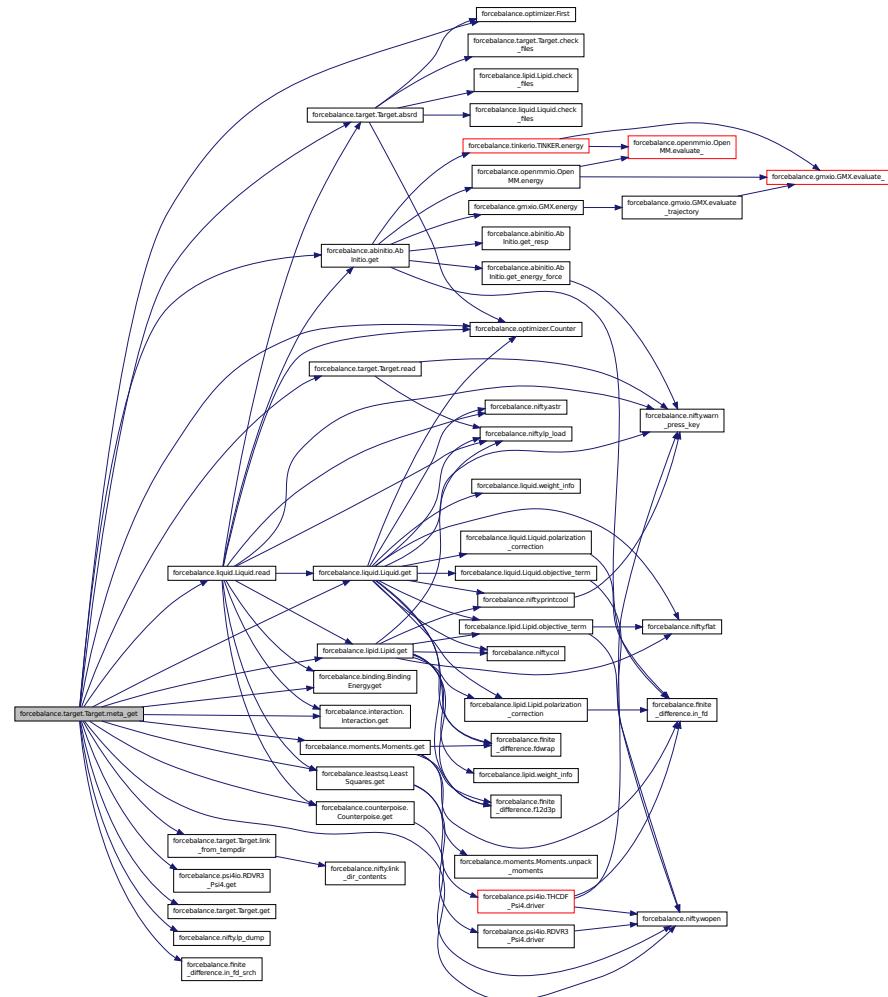


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

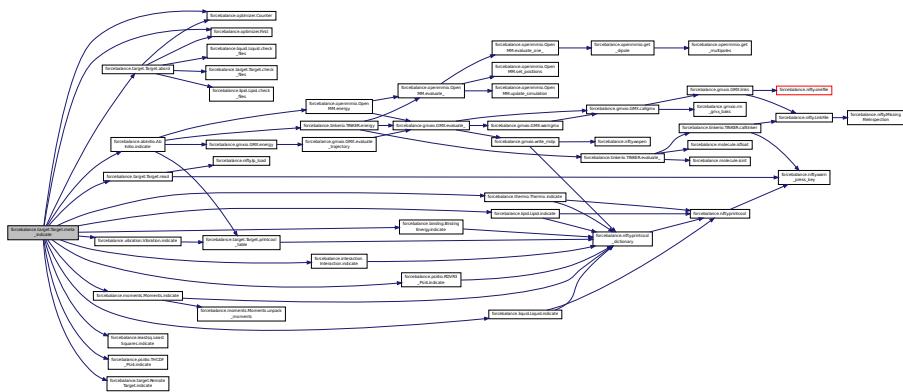
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



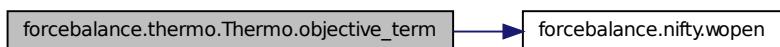
def forcebalance.thermo.Thermo.objective_term (self, quantity) Calculates the contribution to the objective function (the term) for a given quantity.

Parameters quantity : string Calculate the objective term for this quantity.

Returns term : dict term is a dict with keys X, G, H and info. The values of these keys are the objective term itself (X), its gradient (G), its Hessian (H), and an OrderedDict with print information on individual data points (info).

Definition at line 273 of file thermo.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

<code>data</code>	Column contents in the form of an <code>OrderedDict</code> , with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
-------------------	---

<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

Here is the call graph for this function:

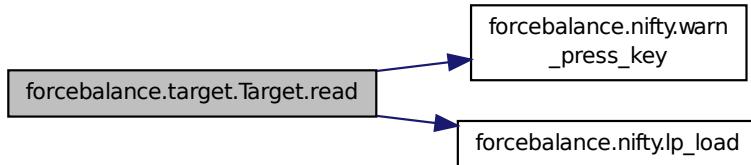


def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]

Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory(self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

def forcebalance.thermo.Thermo.retrieve (self, dp) Retrieve the molecular dynamics (MD) results and store the calculated quantities in the [Point](#) object dp.

Parameters dp : [Point](#) Store the calculated quantities in this point.

Returns Nothing

Definition at line 140 of file thermo.py.

Here is the call graph for this function:



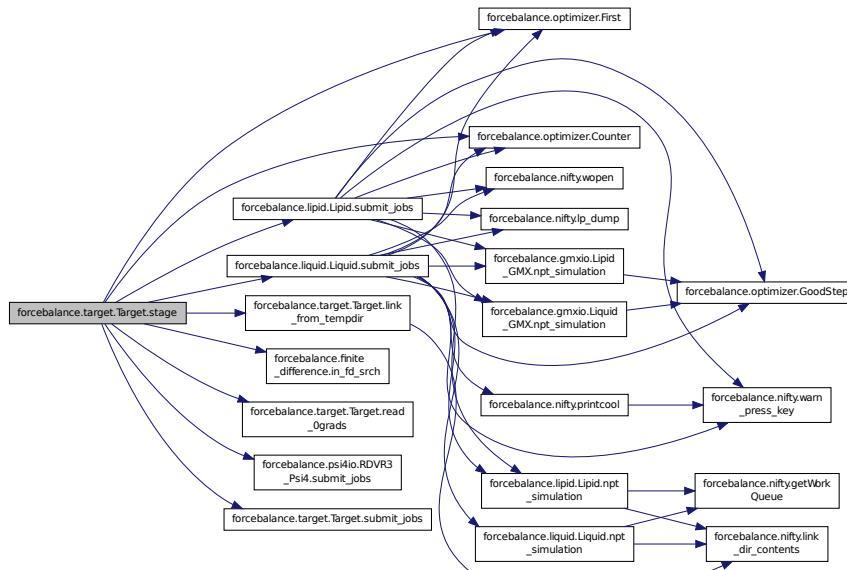
```
def forcebalance.BaseClass.set_option( self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

```
def forcebalance.target.Target.stage( self, mvals, AGrad = False, AHess = False, customdir = None ) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.
```

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



```
def forcebalance.thermo.Thermo.submit_jobs( self, mvals, AGrad = True, AHess = True ) This routine is called by Objective.stage() and will run before "get".
```

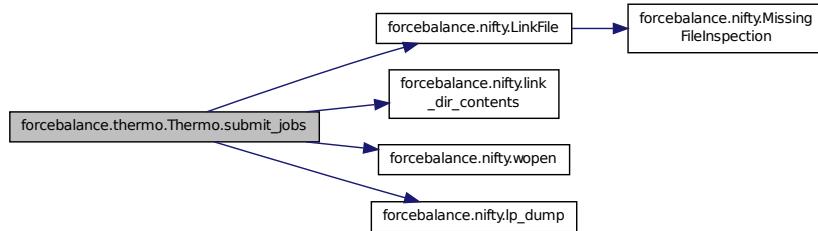
It submits the jobs and the [stage\(\)](#) function will wait for jobs to complete.

Parameters mvals : list Mathematical parameter values. AGrad : Boolean Switch to turn on analytic gradient. AHess : Boolean Switch to turn on analytic Hessian.

Returns Nothing.

Definition at line 179 of file thermo.py.

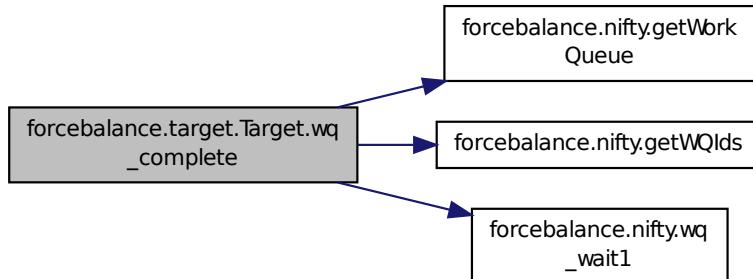
Here is the call graph for this function:



def forcebalance.target.Target.wq_complete(self) [inherited] This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads(self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.69.4 Member Data Documentation

forcebalance.thermo.Thermo.denoms Definition at line 47 of file thermo.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.thermo.Thermo.Gp Definition at line 418 of file thermo.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.thermo.Thermo.Objective Definition at line 420 of file thermo.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.
Dictionary of whether to call the derivatives.
Definition at line 127 of file target.py.

forcebalance.thermo.Thermo.points Definition at line 45 of file thermo.py.

forcebalance.thermo.Thermo.Pp Definition at line 415 of file thermo.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.
Submit jobs to the Work Queue.
Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.
Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.
Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.
Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number
The 'customdir' is customizable and can go below anything.
Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.
Definition at line 158 of file target.py.

forcebalance.thermo.Thermo.simpfx Initialize base class.
Parameters Reference experimental data Variables Prefix names for simulation data
Definition at line 43 of file thermo.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.
Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization
Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.thermo.Thermo.weights Definition at line 49 of file thermo.py.

forcebalance.thermo.Thermo.Wp Definition at line 413 of file thermo.py.

forcebalance.target.Target.write_indicate [inherited] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [inherited] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [inherited] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

forcebalance.thermo.Thermo.Xp Definition at line 412 of file thermo.py.

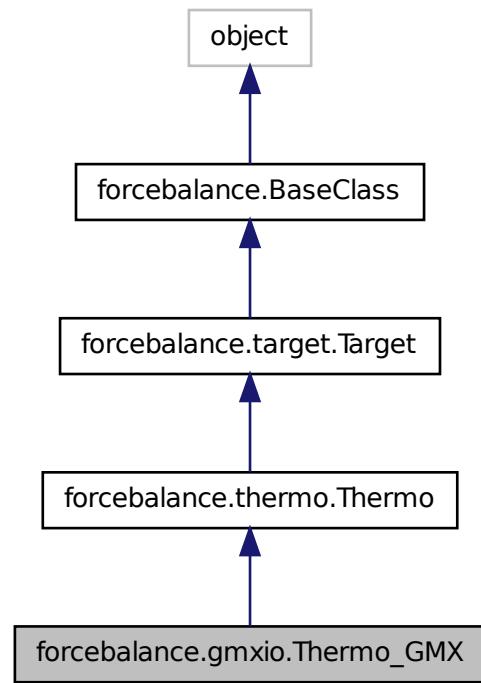
The documentation for this class was generated from the following file:

- [thermo.py](#)

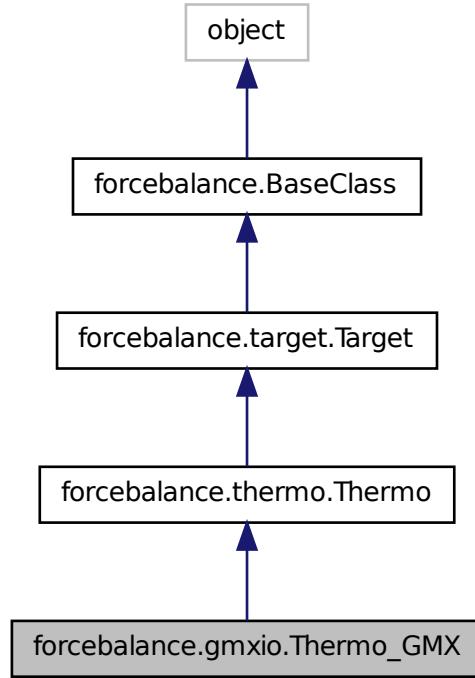
8.70 forcebalance.gmxio.Thermo_GMX Class Reference

Thermodynamical property matching using GROMACS.

Inheritance diagram for forcebalance.gmxio.Thermo_GMX:



Collaboration diagram for forcebalance.gmxio.Thermo_GMX:



Public Member Functions

- def `__init__`
- def `retrieve`

Retrieve the molecular dynamics (MD) results and store the calculated quantities in the `Point` object dp.
- def `submit_jobs`

This routine is called by `Objective.stage()` and will run before "get".
- def `indicate`

Shows optimization state.
- def `objective_term`

Calculates the contribution to the objective function (the term) for a given quantity.
- def `get`

Return the contribution to the total objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

- def `get_H`
Computes the objective function contribution and its gradient.
- def `link_from_tempdir`
Computes the objective function contribution and its gradient / Hessian.
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
- `engname`
- `mdpx`
- `scripts`
- `simpfx`
Initialize base class.
- `points`
- `denoms`
- `weights`
- `Xp`
- `Wp`
- `Pp`
- `Gp`
- `Objective`
- `rd`
Root directory of the whole project.
- `pgrad`
Iteration where we turn on zero-gradient skipping.
- `tempbase`

- Relative directory of target.*
- `tempdir`
 - `rundir`

self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
 - `FF`

Need the forcefield (here for now)
 - `xct`

Counts how often the objective function was computed.
 - `gct`

Counts how often the gradient was computed.
 - `hct`

Counts how often the Hessian was computed.
 - `read_indicate`

Whether to read indicate.log from file when restarting an aborted run.
 - `write_indicate`

Whether to write indicate.log at every iteration (true for all but remote.)
 - `read_objective`

Whether to read objective.p from file when restarting an aborted run.
 - `write_objective`

Whether to write objective.p at every iteration (true for all but remote.)
 - `verbose_options`
 - `PrintOptionDict`

8.70.1 Detailed Description

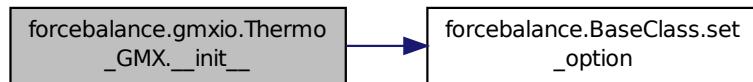
Thermodynamical property matching using GROMACS.

Definition at line 1503 of file gmxio.py.

8.70.2 Constructor & Destructor Documentation

def forcebalance.gmxio.Thermo_GMX.__init__(self, options, tgt_opts, forcefield) Definition at line 1504 of file gmxio.py.

Here is the call graph for this function:



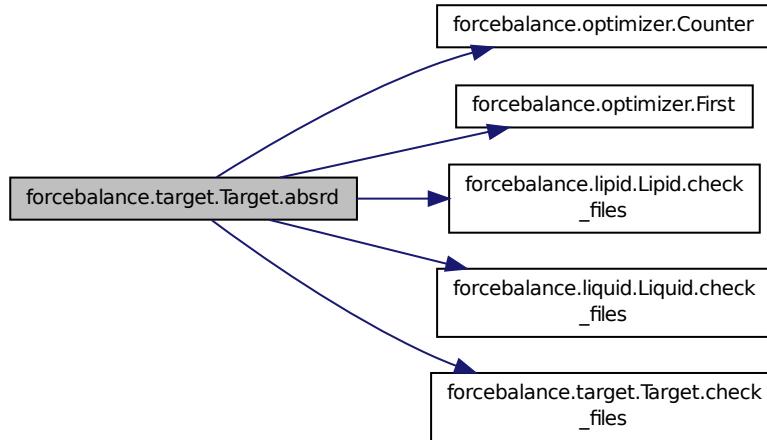
8.70.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__(self, key, value) [inherited] Definition at line 28 of file __init__.py.

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory  
specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence  
of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.thermo.Thermo.get ( self, mvals, AGrad = True, AHess = True ) [inherited]  
Return the contribution to the total objective function.
```

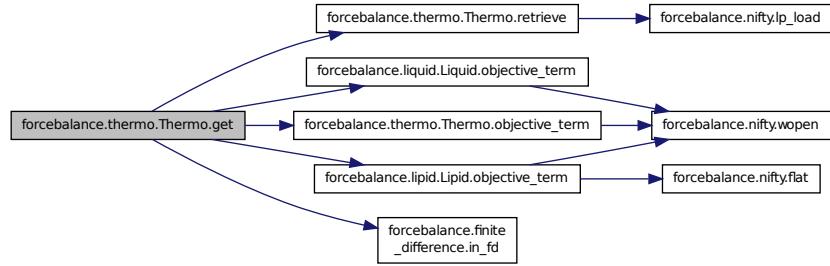
This is a weighted average of the calculated quantities.

Parameters mvals : list Mathematical parameter values. AGrad : Boolean Switch to turn on analytic gradient. AHess : Boolean Switch to turn on analytic Hessian.

Returns Answer : dict Contribution to the objective function. Answer is a dict with keys X for the objective function, G for its gradient and H for its Hessian.

Definition at line 361 of file thermo.py.

Here is the call graph for this function:



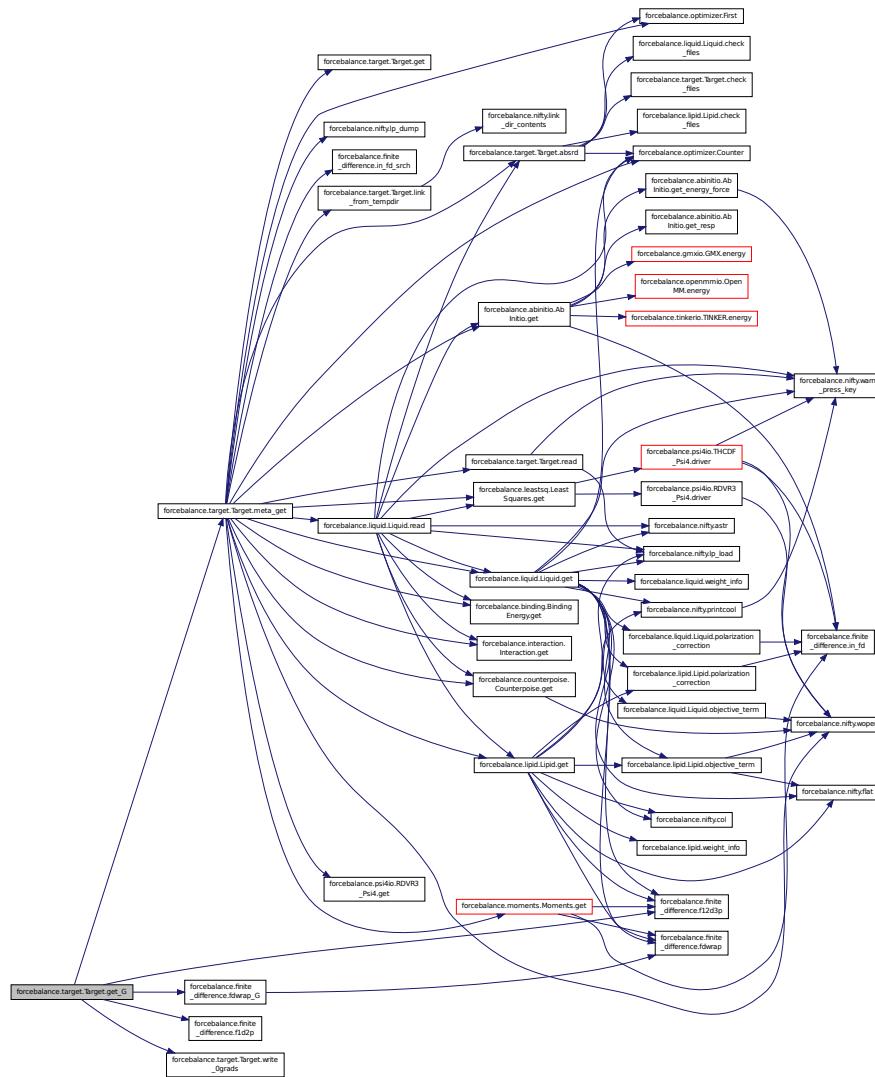
```
def forcebalance.target.Target.get_G( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the `fd1.pids` and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



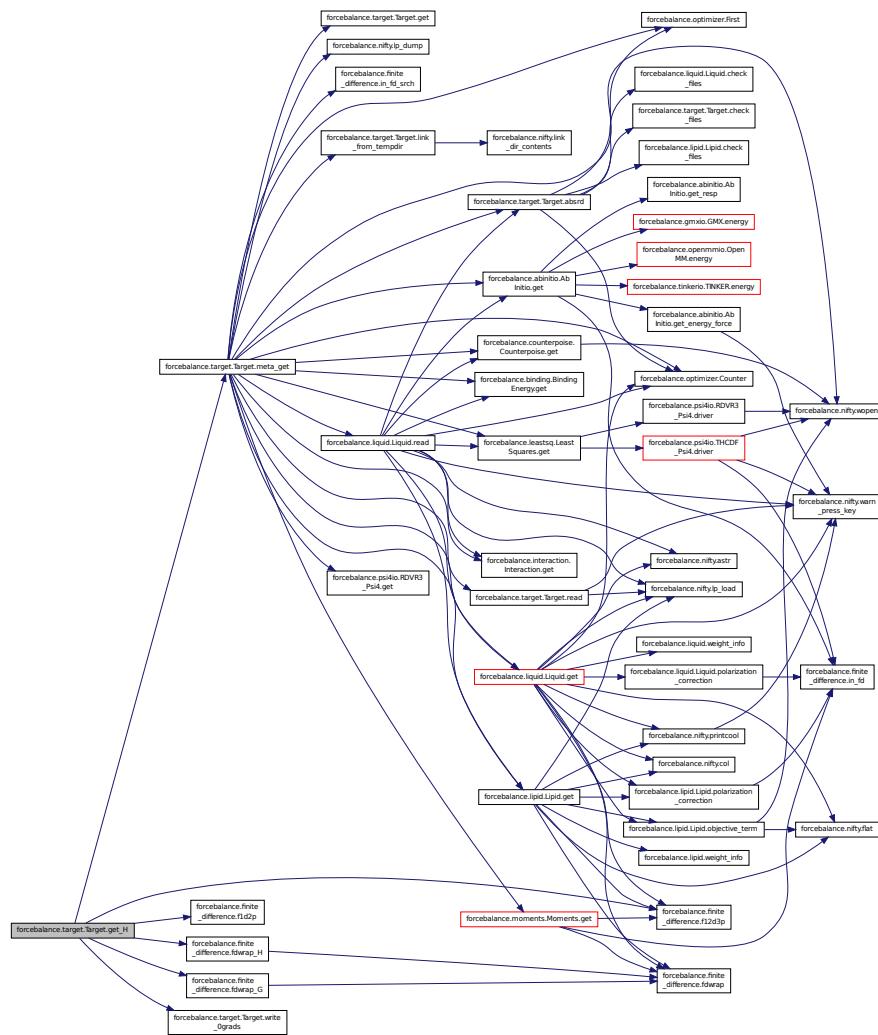
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

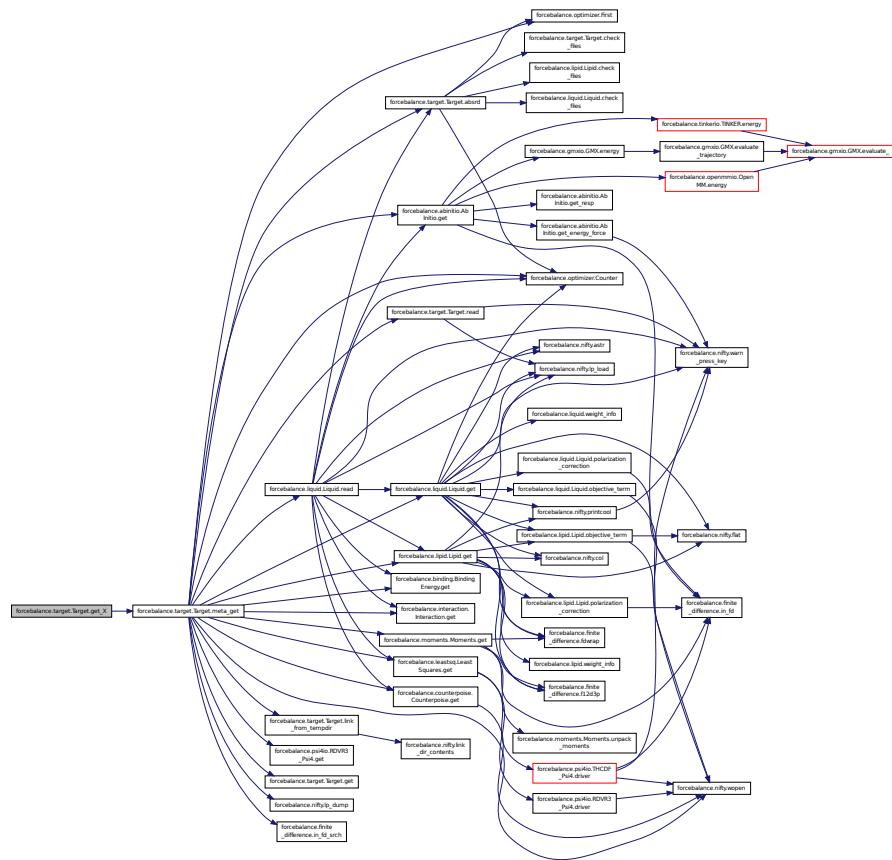
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

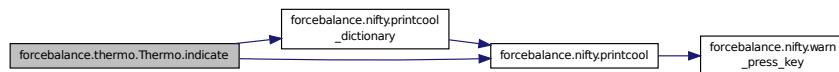
Here is the call graph for this function:



def forcebalance.thermo.Thermo.indicate (self) [inherited] Shows optimization state.

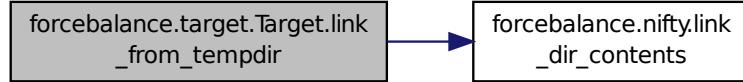
Definition at line 220 of file thermo.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

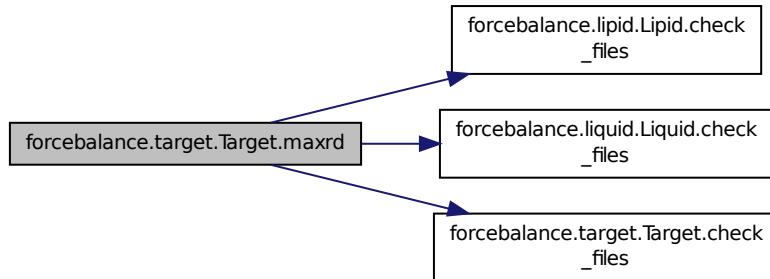
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

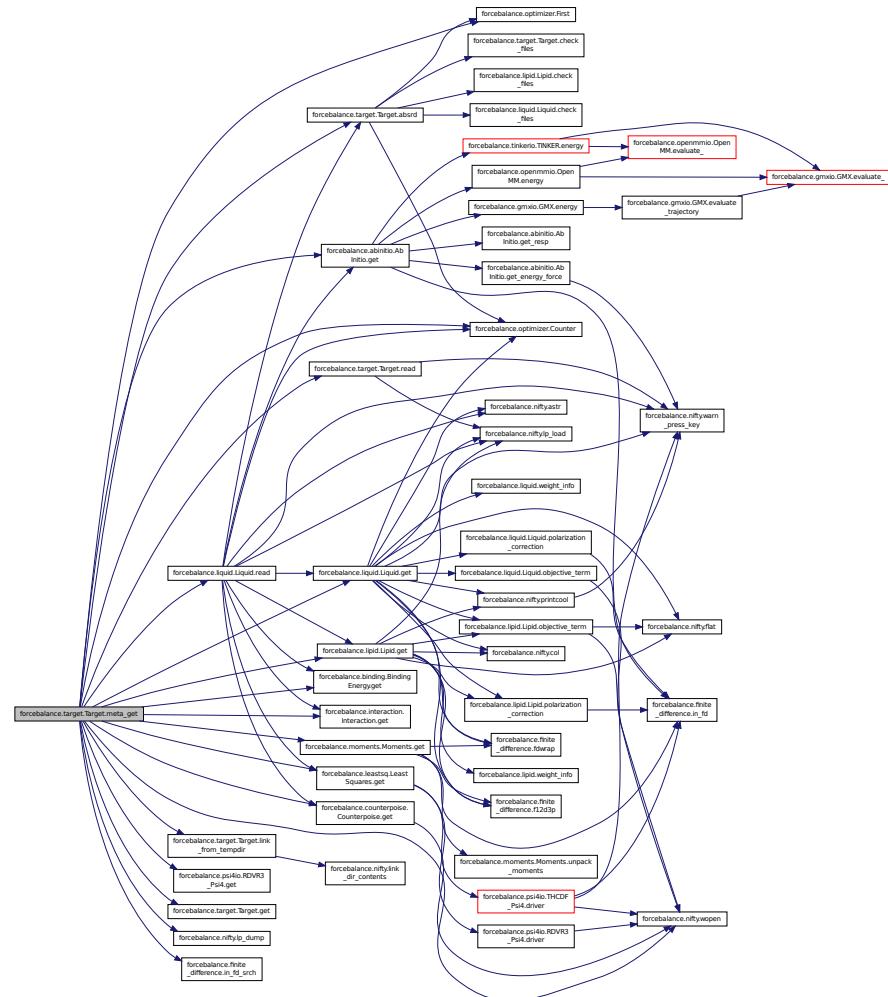


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

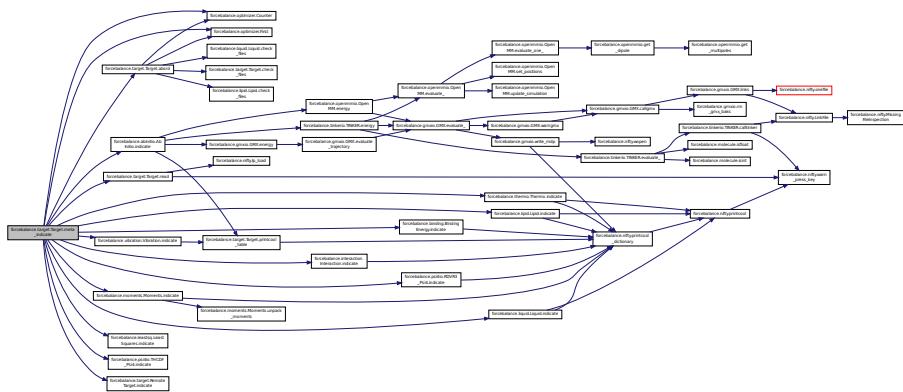
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



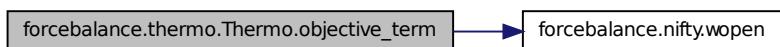
def forcebalance.thermo.Thermo.objective_term (self, quantity) [inherited] Calculates the contribution to the objective function (the term) for a given quantity.

Parameters quantity : string Calculate the objective term for this quantity.

Returns term : dict term is a dict with keys X, G, H and info. The values of these keys are the objective term itself (X), its gradient (G), its Hessian (H), and an OrderedDict with print information on individual data points (info).

Definition at line 273 of file thermo.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

<code>data</code>	Column contents in the form of an <code>OrderedDict</code> , with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
-------------------	---

<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

Here is the call graph for this function:

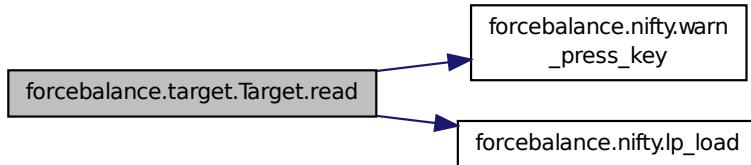


def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]

Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

def forcebalance.thermo.Thermo.retrieve (self, dp) [inherited] Retrieve the molecular dynamics (MD) results and store the calculated quantities in the [Point](#) object dp.

Parameters dp : [Point](#) Store the calculated quantities in this point.

Returns Nothing

Definition at line 140 of file thermo.py.

Here is the call graph for this function:



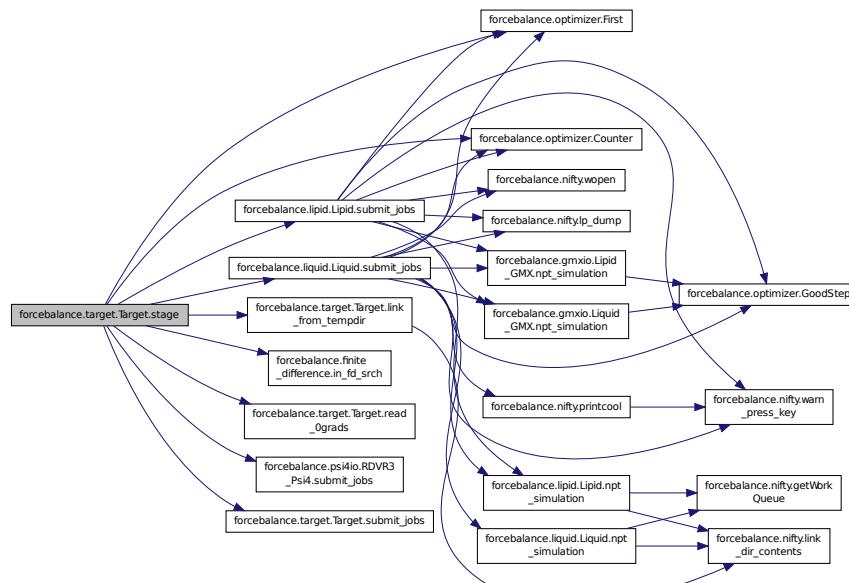
```
def forcebalance.BaseClass.set_option( self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False ) [inherited] Definition at line 42 of file __init__.py.
```

```
def forcebalance.target.Target.stage( self, mvals, AGrad = False, AHess = False, customdir = None ) [inherited] Stages the directory for the target, and then launches Work Queue processes if any.
```

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



```
def forcebalance.thermo.Thermo.submit_jobs( self, mvals, AGrad = True, AHess = True ) [inherited] This routine is called by Objective.stage() and will run before "get".
```

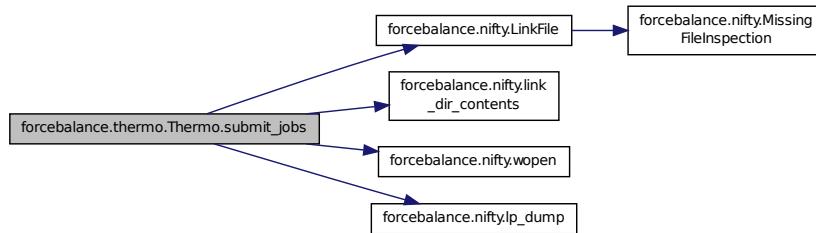
It submits the jobs and the [stage\(\)](#) function will wait for jobs to complete.

Parameters mvals : list Mathematical parameter values. AGrad : Boolean Switch to turn on analytic gradient. AHess : Boolean Switch to turn on analytic Hessian.

Returns Nothing.

Definition at line 179 of file thermo.py.

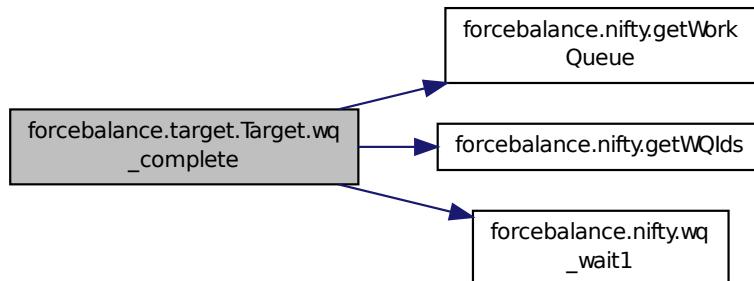
Here is the call graph for this function:



def forcebalance.target.Target.wq_complete(self) [inherited] This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads(self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.70.4 Member Data Documentation

forcebalance.thermo.Thermo.denoms [inherited] Definition at line 47 of file thermo.py.

forcebalance.gmxio.Thermo_GMX.engine_ Definition at line 1509 of file gmxio.py.

forcebalance.gmxio.Thermo_GMX.engname Definition at line 1511 of file gmxio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)
Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.
Definition at line 164 of file target.py.

forcebalance.thermo.Thermo.Gp [inherited] Definition at line 418 of file thermo.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.
Definition at line 166 of file target.py.

forcebalance.gmxio.Thermo_GMX.mdpfx Definition at line 1513 of file gmxio.py.

forcebalance.thermo.Thermo.Objective [inherited] Definition at line 420 of file thermo.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.
Dictionary of whether to call the derivatives.
Definition at line 127 of file target.py.

forcebalance.thermo.Thermo.points [inherited] Definition at line 45 of file thermo.py.

forcebalance.thermo.Thermo.Pp [inherited] Definition at line 415 of file thermo.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.
Submit jobs to the Work Queue.
Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.
Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.
Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.
Definition at line 172 of file target.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number
The 'customdir' is customizable and can go below anything.
Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.
Definition at line 158 of file target.py.

forcebalance.gmxio.Thermo_GMX.scripts Definition at line 1515 of file gmxio.py.

forcebalance.thermo.Thermo.simpfx [**inherited**] Initialize base class.

Parameters Reference experimental data Variables Prefix names for simulation data
Definition at line 43 of file thermo.py.

forcebalance.target.Target.tempbase [**inherited**] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [**inherited**] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [**inherited**] Definition at line 40 of file __init__.py.

forcebalance.thermo.Thermo.weights [**inherited**] Definition at line 49 of file thermo.py.

forcebalance.thermo.Thermo.Wp [**inherited**] Definition at line 413 of file thermo.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

forcebalance.thermo.Thermo.Xp [**inherited**] Definition at line 412 of file thermo.py.

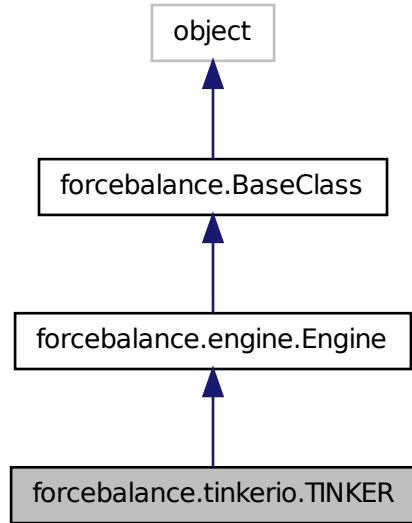
The documentation for this class was generated from the following file:

- [gmxio.py](#)

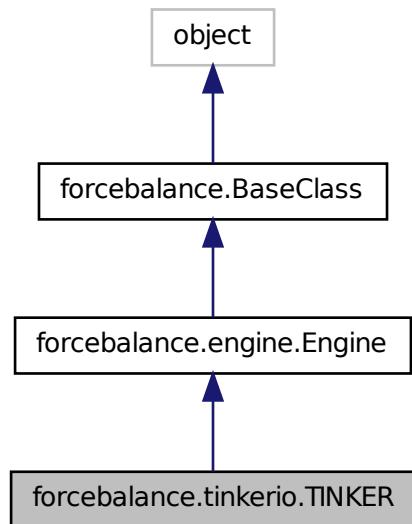
8.71 forcebalance.tinkerio.TINKER Class Reference

Engine for carrying out general purpose TINKER calculations.

Inheritance diagram for forcebalance.tinkerio.TINKER:



Collaboration diagram for forcebalance.tinkerio.TINKER:



Public Member Functions

- def `_init_`
Called by `init` ; Set TINKER-specific options.
- def `readsrc`
Called by `init` ; read files from the source directory.
- def `calltinker`
Call TINKER; prepend the tinkerpath to calling the TINKER program.
- def `prepare`
Called by `init` ; prepare the temp directory and figure out the topology.
- def `optimize`
Optimize the geometry and align the optimized geometry to the starting geometry.
- def `evaluate_`
Utility function for computing energy, and (optionally) forces and dipoles using TINKER.
- def `energy_force_one`
Computes the energy and force using TINKER for one snapshot.
- def `energy`
Computes the energy using TINKER over a trajectory.
- def `energy_force`
Computes the energy and force using TINKER over a trajectory.
- def `energy_dipole`
Computes the energy and dipole using TINKER over a trajectory.
- def `normal_modes`
- def `multipole_moments`
Return the multipole moments of the 1st snapshot in Debye and Buckingham units.
- def `energy_rmsd`
Calculate energy of the selected structure (optionally minimize and return the minimized energy and RMSD).
- def `interaction_energy`
Calculate the interaction energy for two fragments.
- def `molecular_dynamics`
Method for running a molecular dynamics simulation.
- def `prepare`
- def `__setattr__`
- def `set_option`

Public Attributes

- `valkwds`
Keyword args that aren't in this list are filtered out.
- `warn_vn`
- `tinkerpath`
The directory containing TINKER executables (e.g.
- `key`
- `prm`
- `mol`
- `rigid`
Attempt to set some TINKER options.
- `pbc`

- `abskey`
- `AtomMask`
If the coordinates do not come with TINKER suffixes then throw an error.
- `AtomLists`
- `A`
- `B`
- `mdtraj`
- `name`
- `verbose`
- `target`

Engines can get properties from the Target that creates them.

- `root`
- `srcdir`
- `tempdir`
- `FF`
- `verbose_options`
- `PrintOptionDict`

8.71.1 Detailed Description

Engine for carrying out general purpose TINKER calculations.

Definition at line 304 of file tinkerio.py.

8.71.2 Constructor & Destructor Documentation

```
def forcebalance.tinkerio.TINKER.__init__ ( self, name = "tinker", kwargs )
```

Definition at line 307 of file tinkerio.py.

8.71.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited]
```

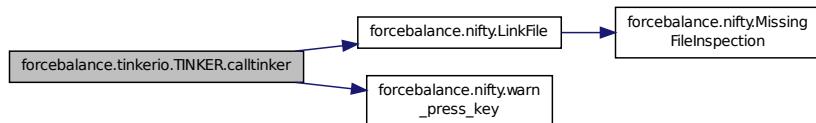
Definition at line 28 of file __init__.py.

```
def forcebalance.tinkerio.TINKER.calltinker ( self, command, stdin = None, print_to_screen = False, print_command = False, kwargs )
```

Call TINKER; prepend the tinkerpath to calling the TINKER program.

Definition at line 351 of file tinkerio.py.

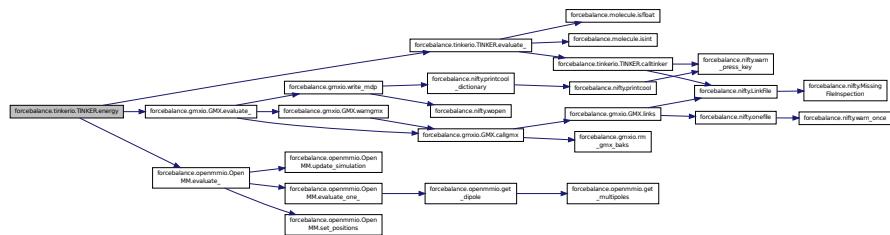
Here is the call graph for this function:



def forcebalance.tinkerio.TINKER.energy (self) Computes the energy using TINKER over a trajectory.

Definition at line 654 of file tinkerio.py.

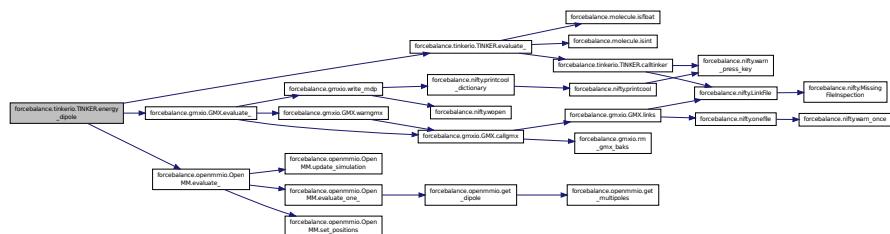
Here is the call graph for this function:



def forcebalance.tinkerio.TINKER.energy_dipole (self) Computes the energy and dipole using [TINKER](#) over a trajectory.

Definition at line 679 of file tinkerio.py.

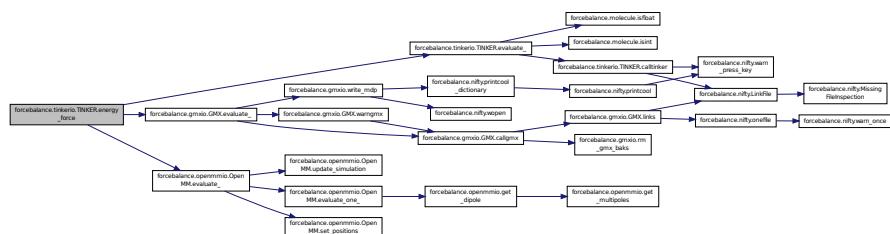
Here is the call graph for this function:



def forcebalance.tinkerio.TINKER.energy_force (self) Computes the energy and force using [TINKER](#) over a trajectory.

Definition at line 666 of file tinkerio.py.

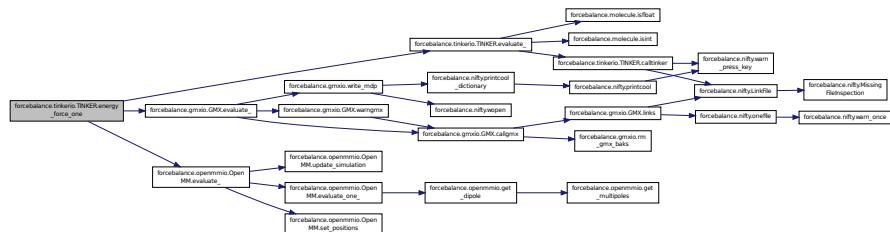
Here is the call graph for this function:



def forcebalance.tinkerio.TINKER.energy_force_one(self, shot) Computes the energy and force using TINKER for one snapshot.

Definition at line 645 of file tinkerio.py.

Here is the call graph for this function:

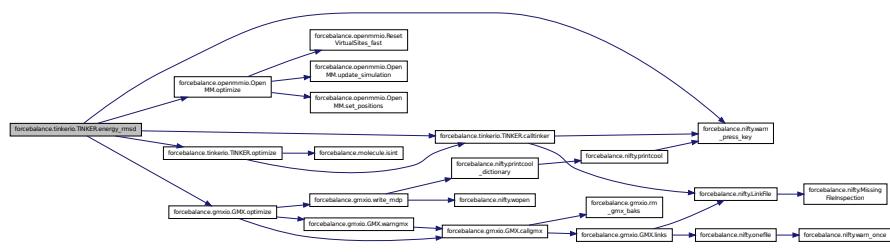


def forcebalance.tinkerio.TINKER.energy_rmsd (self, shot = 0, optimize = True) Calculate energy of the selected structure (optionally minimize and return the minimized energy and RMSD).

In kcal/mol.

Definition at line 791 of file tinkerio.py.

Here is the call graph for this function:



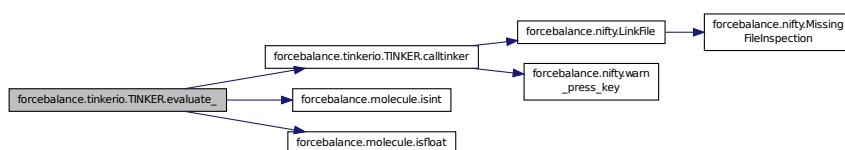
def forcebalance.tinkerio.TINKER.evaluate_(self, xyzin, force = False, dipole = False) Utility function for computing energy, and (optionally) forces and dipoles using TINKER.

Inputs: xyzin: TINKER .xyz file name. force: Switch for calculating the force. dipole: Switch for calculating the dipole.

Outputs: Result: Dictionary containing energies, forces and/or dipoles.

Definition at line 596 of file tinkerio.py.

Here is the call graph for this function:



```
def forcebalance.tinkerio.TINKER.interaction.energy ( self, fraga, fragb ) Calculate the interaction energy for  
two fragments.
```

Definition at line 829 of file tinkerio.py.

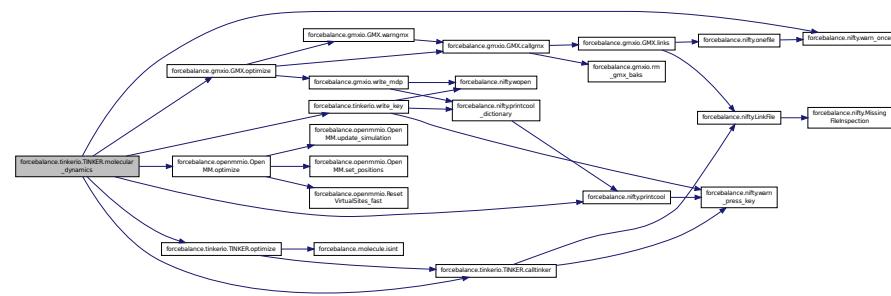
```
def forcebalance.tinkerio.TINKER.molecular_dynamics ( self, nsteps, timestep, temperature = None, pressure = None, nequil = 0, nsave = 1000, minimize = True, anisotropic = False, threads = 1, verbose = False, kwargs ) Method for running a molecular dynamics simulation.
```

Required arguments: nsteps = (int) Number of total time steps timestep = (float) Time step in FEMTOSECOND-S temperature = (float) Temperature control (Kelvin) pressure = (float) Pressure control (atmospheres) nequil = (int) Number of additional time steps at the beginning for equilibration nsave = (int) Step interval for saving and printing data minimize = (bool) Perform an energy minimization prior to dynamics threads = (int) Specify how many OpenMP threads to use

Returns simulation data: Rhos = (array) Density in kilogram m⁻³ Potentials = (array) Potential energies Kinetics = (array) Kinetic energies Volumes = (array) Box volumes Dips = (3xN array) Dipole moments EComps = (dict) Energy components

Definition at line 860 of file tinkerio.py.

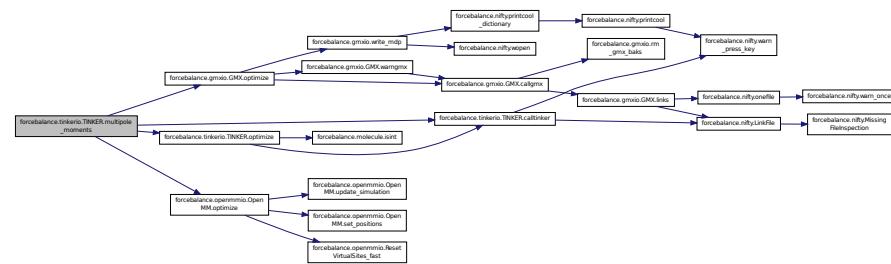
Here is the call graph for this function:



```
def forcebalance.tinkerio.TINKER.multipole_moments ( self, shot = 0, optimize = True, polarizability = False ) Return the multipole moments of the 1st snapshot in Debye and Buckingham units.
```

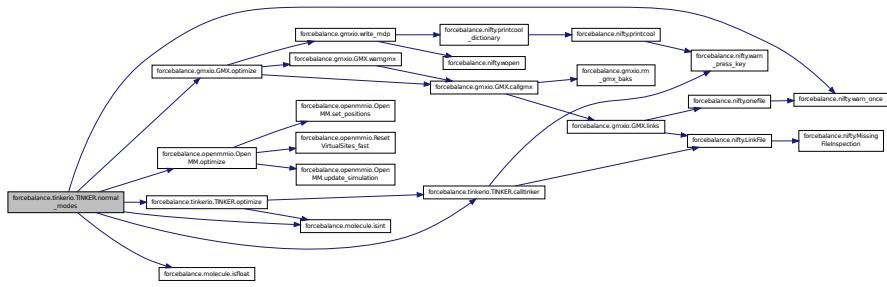
Definition at line 728 of file tinkerio.py.

Here is the call graph for this function:



```
def forcebalance.tinkerio.TINKER.normal_modes ( self, shot = 0, optimize = True ) Definition at line 690 of file tinkerio.py.
```

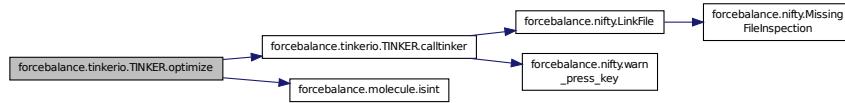
Here is the call graph for this function:



def forcebalance.tinkerio.TINKER.optimize (self, shot = 0, method = "newton", crit = 1e-4) Optimize the geometry and align the optimized geometry to the starting geometry.

Definition at line 543 of file tinkerio.py.

Here is the call graph for this function:



def forcebalance.engine.Engine.prepare (self, kwargs) [inherited] Definition at line 95 of file engine.py.

def forcebalance.tinkerio.TINKER.prepare (self, pbc = False, kwargs) Called by **init** ; prepare the temp directory and figure out the topology.

Definition at line 393 of file tinkerio.py.

Here is the call graph for this function:



def forcebalance.tinkerio.TINKER.readsrc (self, kwargs) Called by **init** ; read files from the source directory.

Definition at line 332 of file tinkerio.py.

def forcebalance.BaseClass.set_option (self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

def forcebalance.tinkerio.TINKER.setopts (self, kwargs) Called by **init** ; Set TINKER-specific options.

Definition at line 315 of file tinkerio.py.

8.71.4 Member Data Documentation

forcebalance.tinkerio.TINKER.A Definition at line 832 of file tinkerio.py.

forcebalance.tinkerio.TINKER.abskey Definition at line 481 of file tinkerio.py.

forcebalance.tinkerio.TINKER.AtomLists Definition at line 494 of file tinkerio.py.

forcebalance.tinkerio.TINKER.AtomMask If the coordinates do not come with TINKER suffixes then throw an error.

Call analyze to read information needed to build the atom lists. Parse the output of analyze.

Definition at line 493 of file tinkerio.py.

forcebalance.tinkerio.TINKER.B Definition at line 833 of file tinkerio.py.

forcebalance.engine.Engine.FF [inherited] Definition at line 65 of file engine.py.

forcebalance.tinkerio.TINKER.key Definition at line 335 of file tinkerio.py.

forcebalance.tinkerio.TINKER.mdtraj Definition at line 929 of file tinkerio.py.

forcebalance.tinkerio.TINKER.mol Definition at line 338 of file tinkerio.py.

forcebalance.engine.Engine.name [inherited] Definition at line 48 of file engine.py.

forcebalance.tinkerio.TINKER.pbc Definition at line 458 of file tinkerio.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.tinkerio.TINKER.prm Definition at line 336 of file tinkerio.py.

forcebalance.tinkerio.TINKER.rigid Attempt to set some TINKER options.

Definition at line 399 of file tinkerio.py.

forcebalance.engine.Engine.root [inherited] Definition at line 56 of file engine.py.

forcebalance.engine.Engine.srkdir [inherited] Definition at line 57 of file engine.py.

forcebalance.engine.Engine.target [inherited] Engines can get properties from the Target that creates them.

Definition at line 55 of file engine.py.

forcebalance.engine.Engine.tempdir [inherited] Definition at line 58 of file engine.py.

forcebalance.tinkerio.TINKER.tinkerpath The directory containing TINKER executables (e.g. dynamic)

Definition at line 320 of file tinkerio.py.

forcebalance.tinkerio.TINKER.valkwrd Keyword args that aren't in this list are filtered out.

Definition at line 309 of file tinkerio.py.

`forcebalance.engine.Engine.verbose` [inherited] Definition at line 50 of file engine.py.

`forcebalance.BaseClass.verbose_options` [inherited] Definition at line 40 of file __init__.py.

`forcebalance.tinkerio.TINKER.warn_vn` Definition at line 310 of file tinkerio.py.

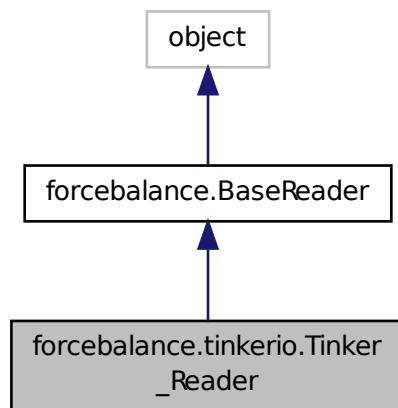
The documentation for this class was generated from the following file:

- `tinkerio.py`

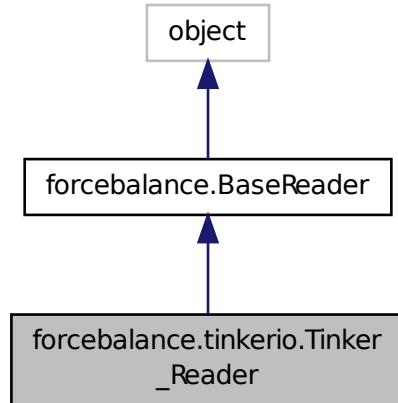
8.72 forcebalance.tinkerio.Tinker_Reader Class Reference

Finite state machine for parsing TINKER force field files.

Inheritance diagram for forcebalance.tinkerio.Tinker_Reader:



Collaboration diagram for forcebalance.tinkerio.Tinker_Reader:



Public Member Functions

- def `__init__`
- def `feed`

Given a line, determine the interaction type and the atoms involved (the suffix).
- def `Split`
- def `Whites`
- def `build.pid`

Returns the parameter type (e.g.

Public Attributes

- `pdict`

The parameter dictionary (defined in this file)
- `atom`

The atom numbers in the interaction (stored in the TINKER parser)
- `itype`
- `suffix`
- `In`
- `adict`

The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.
- `molatom`

The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.
- `Molecules`
- `AtomTypes`

8.72.1 Detailed Description

Finite state machine for parsing [TINKER](#) force field files.

This class is instantiated when we begin to read in a file. The `feed(line)` method updates the state of the machine, informing it of the current interaction type. Using this information we can look up the interaction type and parameter type for building the parameter ID.

Definition at line 92 of file `tinkerio.py`.

8.72.2 Constructor & Destructor Documentation

`def forcebalance.tinkerio.Tinker_Reader.__init__ (self, fnm)` Definition at line 94 of file `tinkerio.py`.

8.72.3 Member Function Documentation

`def forcebalance.BaseReader.build_pid (self, pfd) [inherited]` Returns the parameter type (e.g. K in BONDSK) based on the current interaction type.

Both the 'pdct' dictionary (see `gmlio.pdict`) and the interaction type 'state' (here, BONDS) are needed to get the parameter type.

If, however, 'pdct' does not contain the ptype value, a suitable substitute is simply the field number.

Note that if the interaction type state is not set, then it defaults to the file name, so a generic parameter ID is 'filename.line_num.field_num'

Definition at line 124 of file `__init__.py`.

`def forcebalance.tinkerio.Tinker_Reader.feed (self, line)` Given a line, determine the interaction type and the atoms involved (the suffix).

[TINKER](#) generally has stuff like this:

bond-cubic		-2.55			
bond-quartic		3.793125			
vdw	1	3.4050	0.1100		
vdw	2	2.6550	0.0135	0.910 # PRM 4	
multipole	2	1	2		
			0.25983		
			-0.03859	0.00000	-0.05818
			-0.03673		
			0.00000	-0.10739	
			-0.00203	0.00000	0.14412

The '#PRM 4' has no effect on [TINKER](#) but it indicates that we are tuning the fourth field on the line (the 0.910 value).

Todo Put the rescaling factors for [TINKER](#) parameters in here. Currently we're using the initial value to determine the rescaling factor which is not very good.

Every parameter line is prefaced by the interaction type except for 'multipole' which is on multiple lines. Because the lines that come after 'multipole' are predictable, we just determine the current line using the previous line.

Random note: Unit of force is kcal / mole / angstrom squared.

Definition at line 135 of file `tinkerio.py`.

`def forcebalance.BaseReader.Split (self, line) [inherited]` Definition at line 99 of file `__init__.py`.

`def forcebalance.BaseReader.Whites (self, line) [inherited]` Definition at line 102 of file `__init__.py`.

8.72.4 Member Data Documentation

forcebalance.BaseReader.adict [inherited] The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

Definition at line 89 of file `__init__.py`.

forcebalance.tinkerio.Tinker_Reader.atom The atom numbers in the interaction (stored in the **TINKER** parser)

Definition at line 99 of file `tinkerio.py`.

forcebalance.BaseReader.AtomTypes [inherited] Definition at line 97 of file `__init__.py`.

forcebalance.tinkerio.Tinker_Reader.itype Definition at line 143 of file `tinkerio.py`.

forcebalance.BaseReader.In [inherited] Definition at line 84 of file `__init__.py`.

forcebalance.BaseReader.molatom [inherited] The mapping of (molecule name) to a dictionary of atom types for the atoms in that residue.

`self.moleculerdict = OrderedDict()` The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.

Definition at line 94 of file `__init__.py`.

forcebalance.BaseReader.Molecules [inherited] Definition at line 96 of file `__init__.py`.

forcebalance.tinkerio.Tinker_Reader.pdict The parameter dictionary (defined in this file)

Definition at line 97 of file `tinkerio.py`.

forcebalance.tinkerio.Tinker_Reader.suffix Definition at line 165 of file `tinkerio.py`.

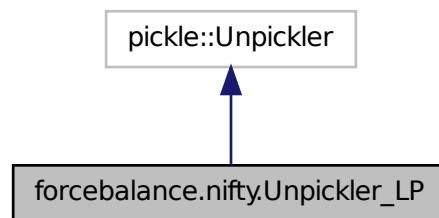
The documentation for this class was generated from the following file:

- [tinkerio.py](#)

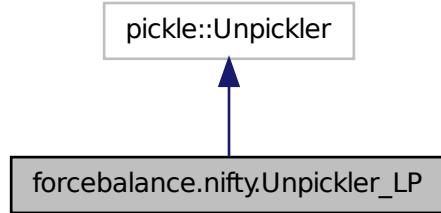
8.73 forcebalance.nifty.Unpickler_LP Class Reference

A subclass of the python Unpickler that implements unpickling of `_ElementTree` types.

Inheritance diagram for `forcebalance.nifty.Unpickler_LP`:



Collaboration diagram for forcebalance.nifty.Unpickler_LP:



Public Member Functions

- def `__init__`

8.73.1 Detailed Description

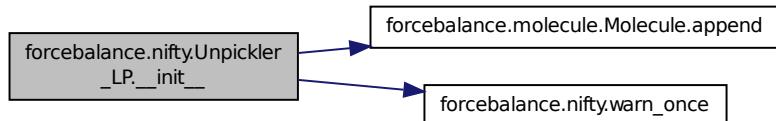
A subclass of the python Unpickler that implements unpickling of _ElementTree types.

Definition at line 587 of file nifty.py.

8.73.2 Constructor & Destructor Documentation

`def forcebalance.nifty.Unpickler_LP.__init__ (self, file)` Definition at line 588 of file nifty.py.

Here is the call graph for this function:



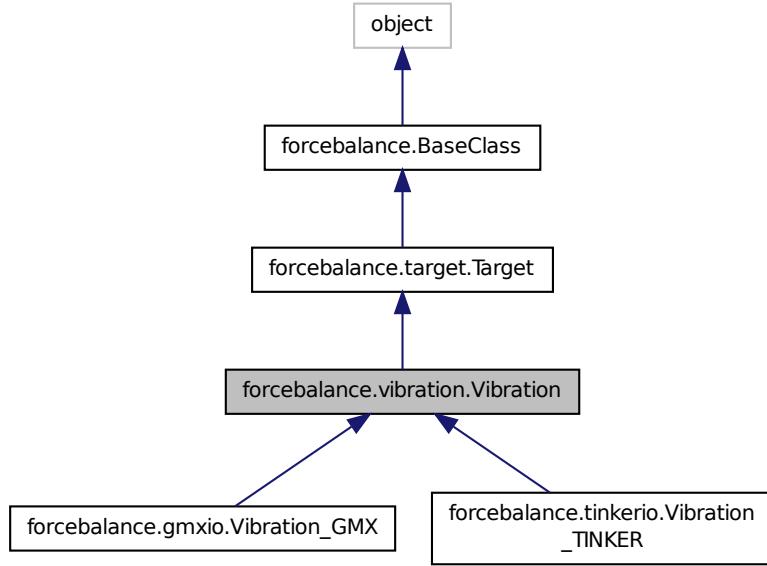
The documentation for this class was generated from the following file:

- [nifty.py](#)

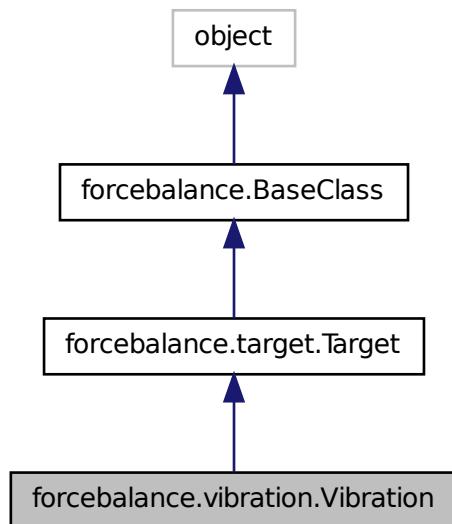
8.74 forcebalance.vibration.Vibration Class Reference

Subclass of Target for fitting force fields to vibrational spectra (from experiment or theory).

Inheritance diagram for forcebalance.vibration.Vibration:



Collaboration diagram for forcebalance.vibration.Vibration:



Public Member Functions

- def `_init_`
Initialization.
- def `read.reference_data`
Read the reference vibrational data from a file.
- def `indicate`
Print qualitative indicator.
- def `vibration_driver`
- def `process_vectors`
Return a set of normal and mass-weighted eigenvectors such that their outer product is the identity.
- def `get`
Evaluate objective function.
- def `get_X`
Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`
Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`
Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`
Computes the objective function contribution and its gradient.
- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- **vfnm**
The vdata.txt file that contains the vibrations.
- **engine**
Read in the reference data.
- **na**
Number of atoms.
- **ref_eigvals**
- **ref_eigvecs**
- **ref_eigvecs_nrm_mw**
- **reassign**
- **c2r**
- **overlaps**
- **calc_eigvals**
- **objective**
- **rd**
Root directory of the whole project.
- **pgrad**
Iteration where we turn on zero-gradient skipping.
- **tempbase**
Relative directory of target.
- **tempdir**
- **rundir**
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**
Whether to write indicate.log at every iteration (true for all but remote.)
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

8.74.1 Detailed Description

Subclass of Target for fitting force fields to vibrational spectra (from experiment or theory).

Currently Tinker is supported.

Definition at line 36 of file vibration.py.

8.74.2 Constructor & Destructor Documentation

```
def forcebalance.vibration.Vibration.__init__ ( self, options, tgt_opts, forcefield ) Initialization.
```

Definition at line 41 of file vibration.py.

Here is the call graph for this function:



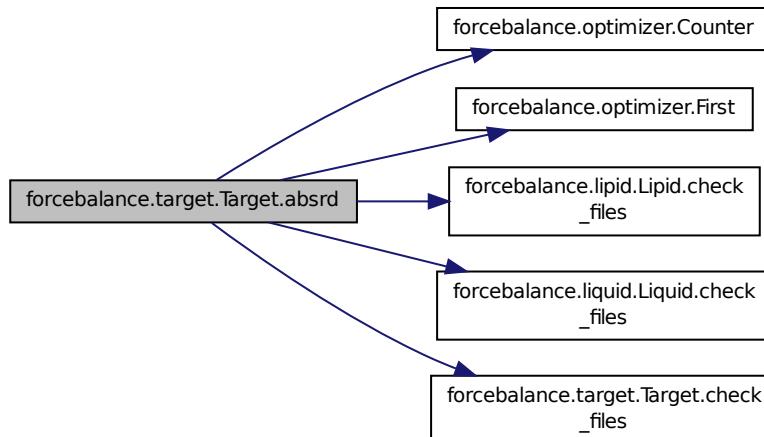
8.74.3 Member Function Documentation

```
def forcebalance.BaseClass.__setattr__ ( self, key, value ) [inherited] Definition at line 28 of file __init__.py.
```

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.vibration.Vibration.get ( self, mvals, AGrad=False, AHess=False ) Evaluate objective function.
```

Definition at line 151 of file vibration.py.

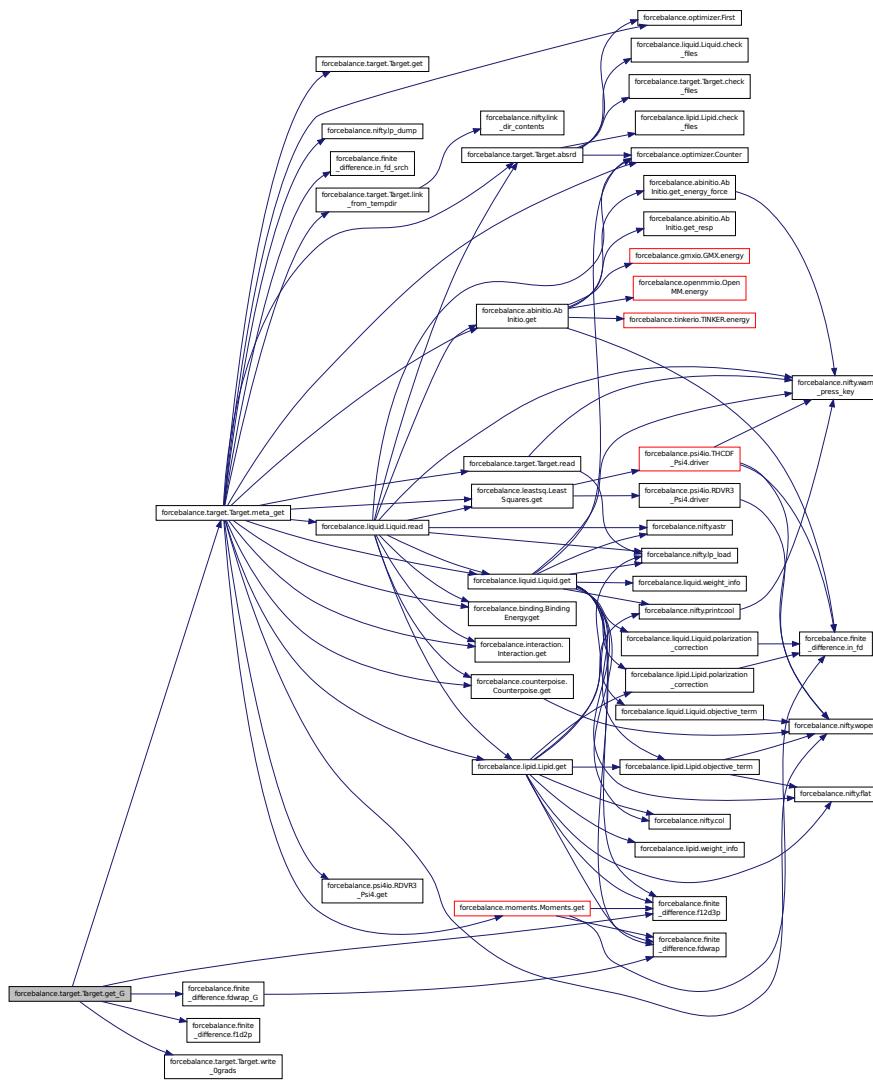
```
def forcebalance.target.Target.get_G ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.get_H ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient / Hessian.
```

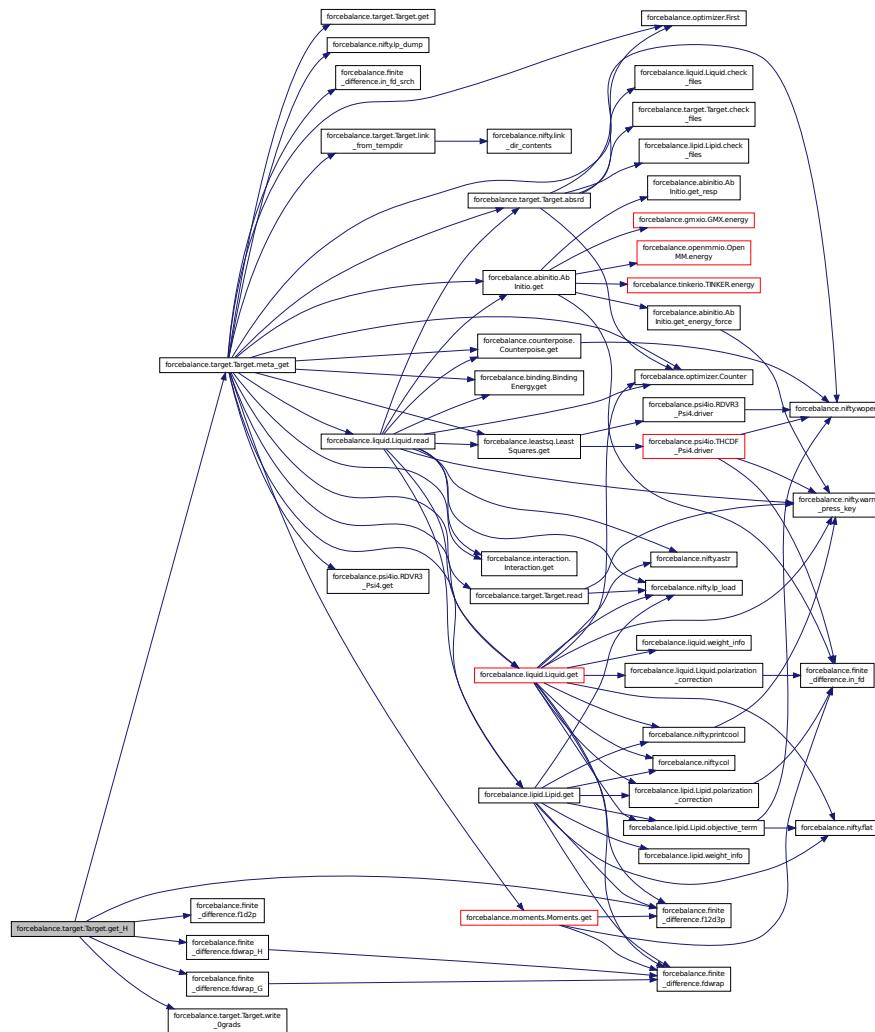
First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through

the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

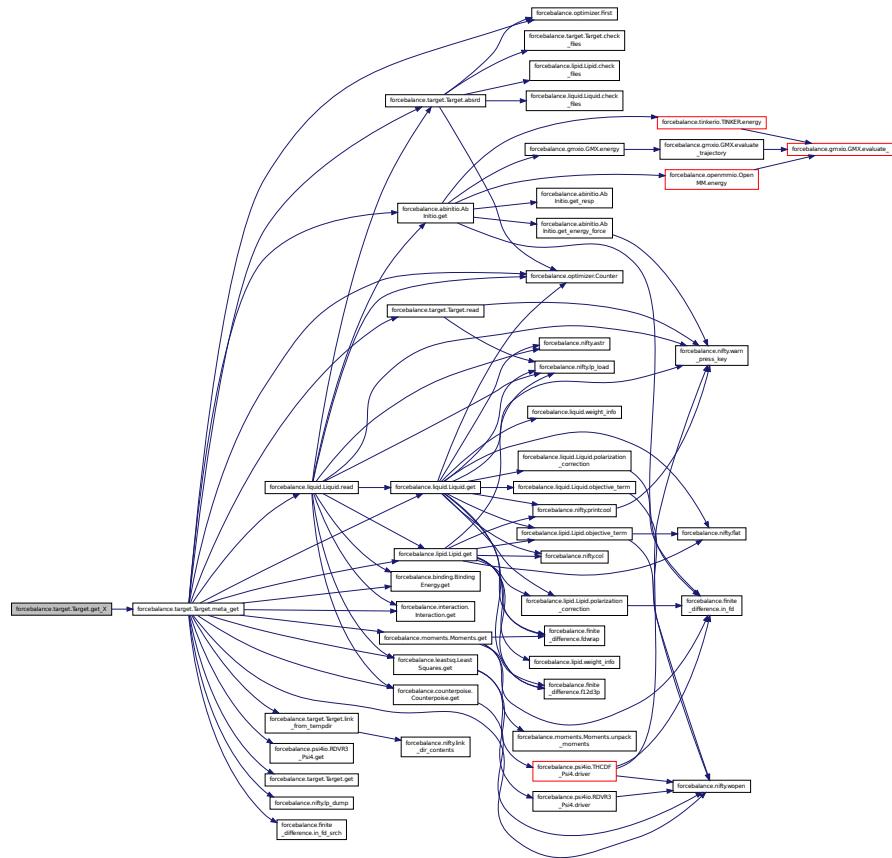
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

Here is the call graph for this function:



def forcebalance.vibration.Vibration.indicate (self) Print qualitative indicator.

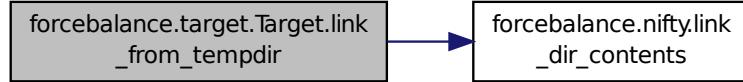
Definition at line 110 of file vibration.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

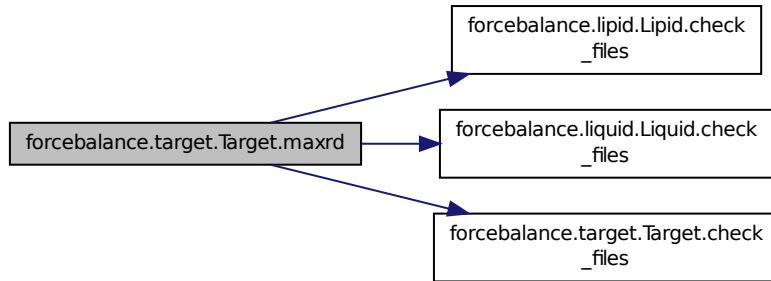
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

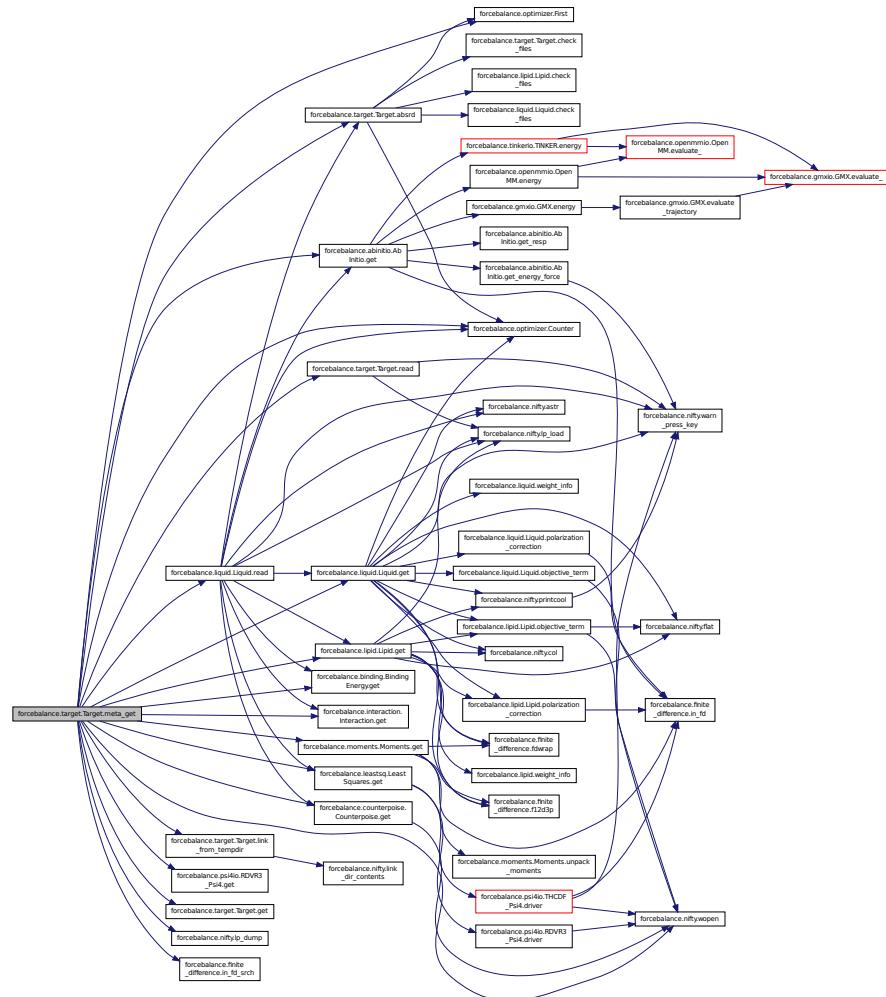


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

Here is the call graph for this function:

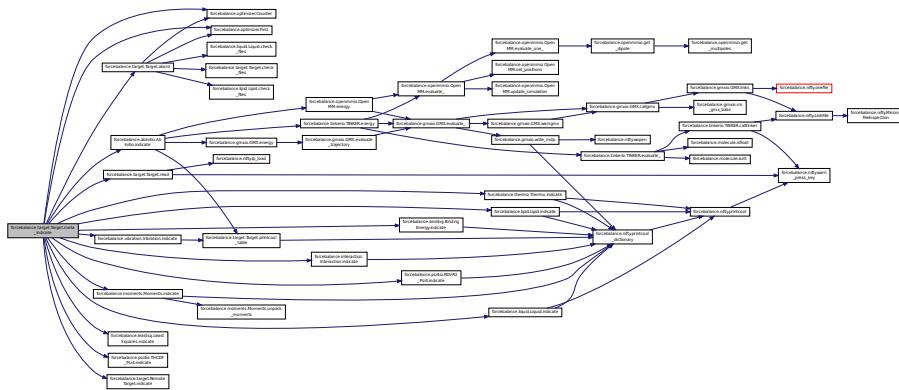


def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.

Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around `printcool_dictionary`.

The input should be something like:

Parameters

<code>data</code>	Column contents in the form of an <code>OrderedDict</code> , with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<code>headings</code>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in <code>OrderedDict</code> , plus one. Use "\n" characters to specify long column names that may take up more than one line.
<code>banner</code>	Optional heading line, which will be printed at the top in the title.
<code>footnote</code>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file `target.py`.

Here is the call graph for this function:

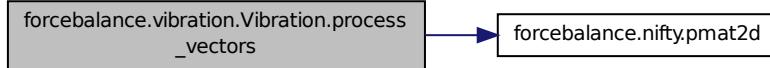


```
def forcebalance.vibration.Vibration.process_vectors( self, vecs, verbose = False, check = False )
```

Return a set of normal and mass-weighted eigenvectors such that their outer product is the identity.

Definition at line 127 of file `vibration.py`.

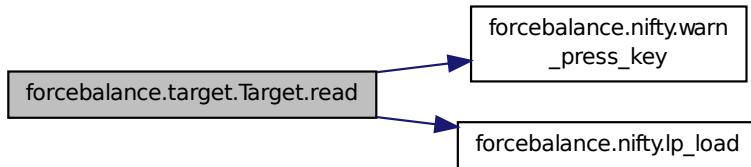
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.vibration.Vibration.read_reference_data (self) Read the reference vibrational data from a file.
Definition at line 69 of file vibration.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

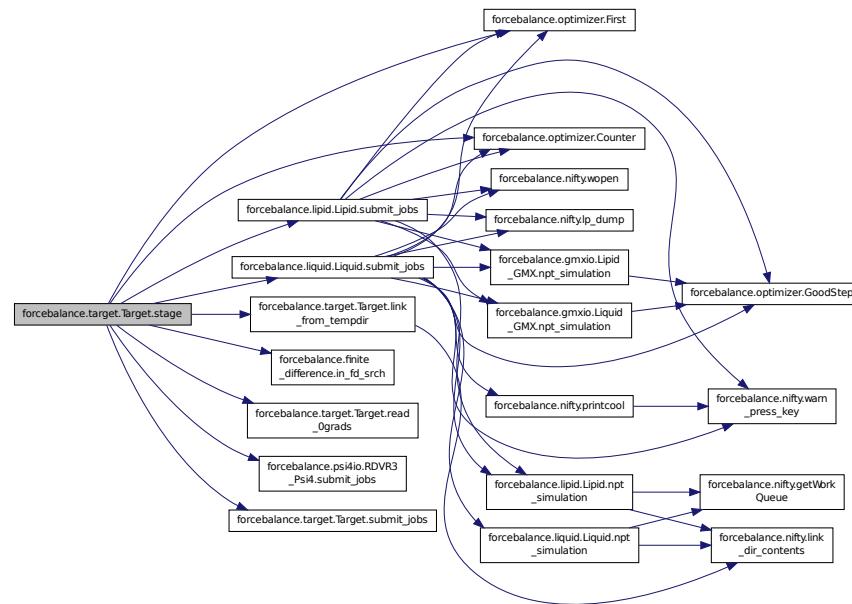
def forcebalance.BaseClass.set_option (self, in_dict, src.key, dest.key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

```
def forcebalance.target.Target.stage( self, mvals, AGrad = False, AHess = False, customdir = None )  
[inherited] Stages the directory for the target, and then launches Work Queue processes if any.
```

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



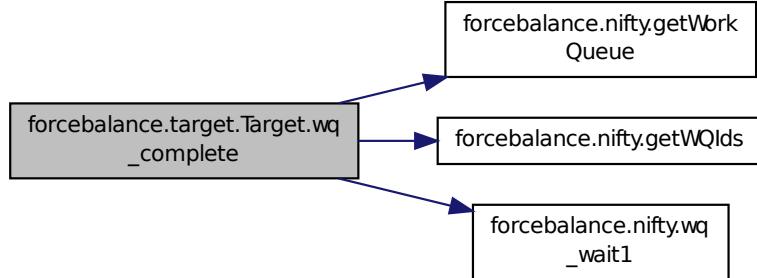
```
def forcebalance.target.Target.submit_jobs( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.vibration.Vibration.vibration_driver( self ) Definition at line 118 of file vibration.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.74.4 Member Data Documentation

forcebalance.vibration.Vibration.c2r Definition at line 178 of file vibration.py.

forcebalance.vibration.Vibration.calc_eigvals Definition at line 198 of file vibration.py.

forcebalance.vibration.Vibration.engine Read in the reference data.

Build keyword dictionaries to pass to engine. Create engine object.

Definition at line 63 of file vibration.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.vibration.Vibration.na Number of atoms.

Definition at line 71 of file vibration.py.

forcebalance.vibration.Vibration.objective Definition at line 199 of file vibration.py.

forcebalance.vibration.Vibration.overlaps Definition at line 183 of file vibration.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [**inherited**] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [**inherited**] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [**inherited**] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [**inherited**] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.vibration.Vibration.reassign Definition at line 165 of file vibration.py.

forcebalance.vibration.Vibration.ref_eigvals Definition at line 72 of file vibration.py.

forcebalance.vibration.Vibration.ref_eigvecs Definition at line 73 of file vibration.py.

forcebalance.vibration.Vibration.ref_eigvecs_nrm_mw Definition at line 155 of file vibration.py.

forcebalance.target.Target.rundir [**inherited**] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target_name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [**inherited**] Relative directory of target.

Temporary (working) directory; it is temp/(target_name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [**inherited**] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [**inherited**] Definition at line 40 of file __init__.py.

forcebalance.vibration.Vibration.vfnm The vdata.txt file that contains the vibrations.

Definition at line 56 of file vibration.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

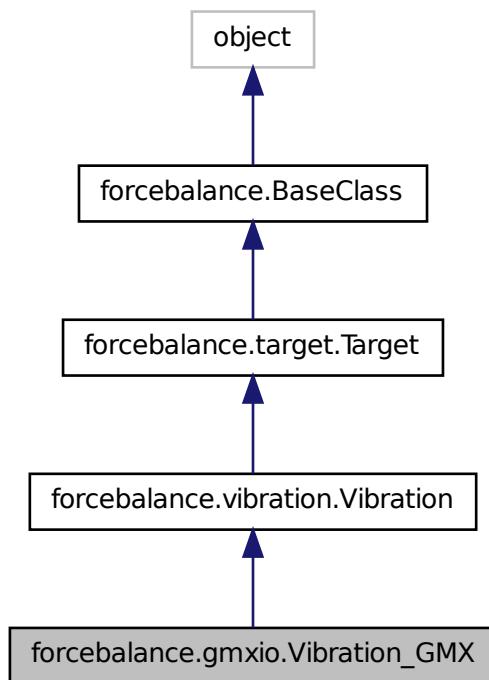
The documentation for this class was generated from the following file:

- [vibration.py](#)

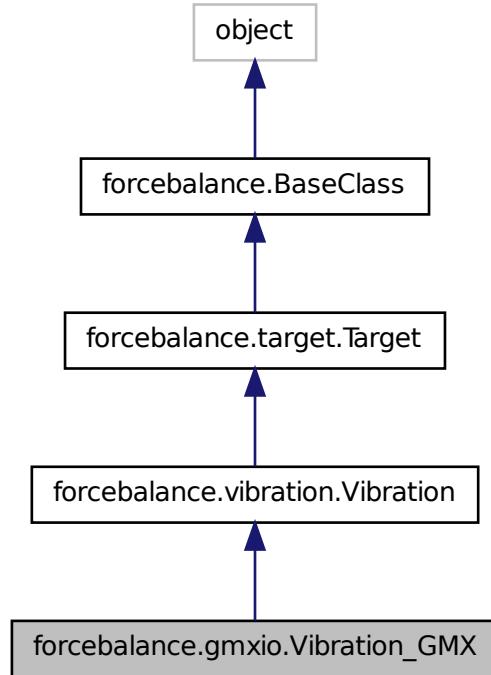
8.75 forcebalance.gmxio.Vibration_GMX Class Reference

Vibrational frequency matching using GROMACS.

Inheritance diagram for forcebalance.gmxio.Vibration_GMX:



Collaboration diagram for forcebalance.gmxio.Vibration_GMX:



Public Member Functions

- def `__init__`
- def `read_reference_data`

Read the reference vibrational data from a file.
- def `indicate`

Print qualitative indicator.
- def `vibration_driver`
- def `process_vectors`

Return a set of normal and mass-weighted eigenvectors such that their outer product is the identity.
- def `get`

Evaluate objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_0grads`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_0grads`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

Computes the objective function contribution and its gradient.

- def `get_H`
Computes the objective function contribution and its gradient / Hessian.
- def `link_from_tempdir`
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
Default file names for coordinates and key file.
- `vfnm`
The vdata.txt file that contains the vibrations.
- `engine`
Read in the reference data.
- `na`
Number of atoms.
- `ref_eigvals`
- `ref_eigvecs`
- `ref_eigvecs_nrm_mw`
- `reassign`
- `c2r`
- `overlaps`
- `calc_eigvals`
- `objective`
- `rd`
Root directory of the whole project.
- `pgrad`

Iteration where we turn on zero-gradient skipping.

- **tempbase**
Relative directory of target.
- **tempdir**
- **rundir**
self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**
Whether to write indicate.log at every iteration (true for all but remote.)
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

8.75.1 Detailed Description

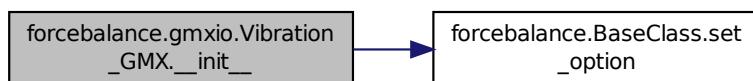
Vibrational frequency matching using GROMACS.

Definition at line 1493 of file gmxio.py.

8.75.2 Constructor & Destructor Documentation

def forcebalance.gmxio.Vibration_GMX.__init__ (self, options, tgt_opts, forcefield) Definition at line 1494 of file gmxio.py.

Here is the call graph for this function:



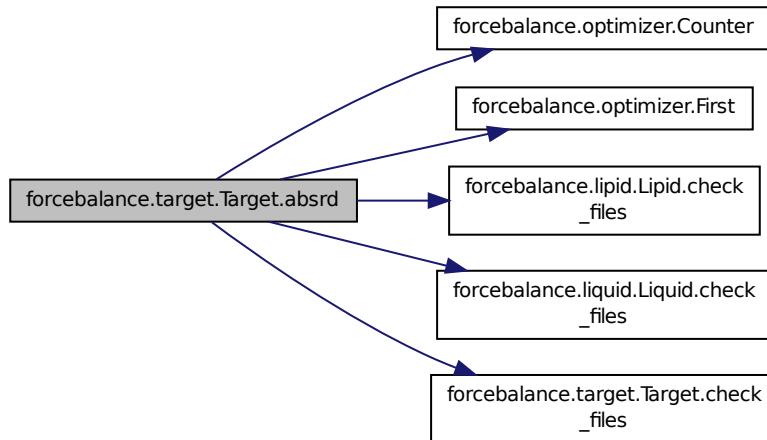
8.75.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (self, key, value) [inherited] Definition at line 28 of file __init__.py.

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.vibration.Vibration.get ( self, mvals, AGrad=False, AHess=False ) [inherited]  
Evaluate objective function.
```

Definition at line 151 of file vibration.py.

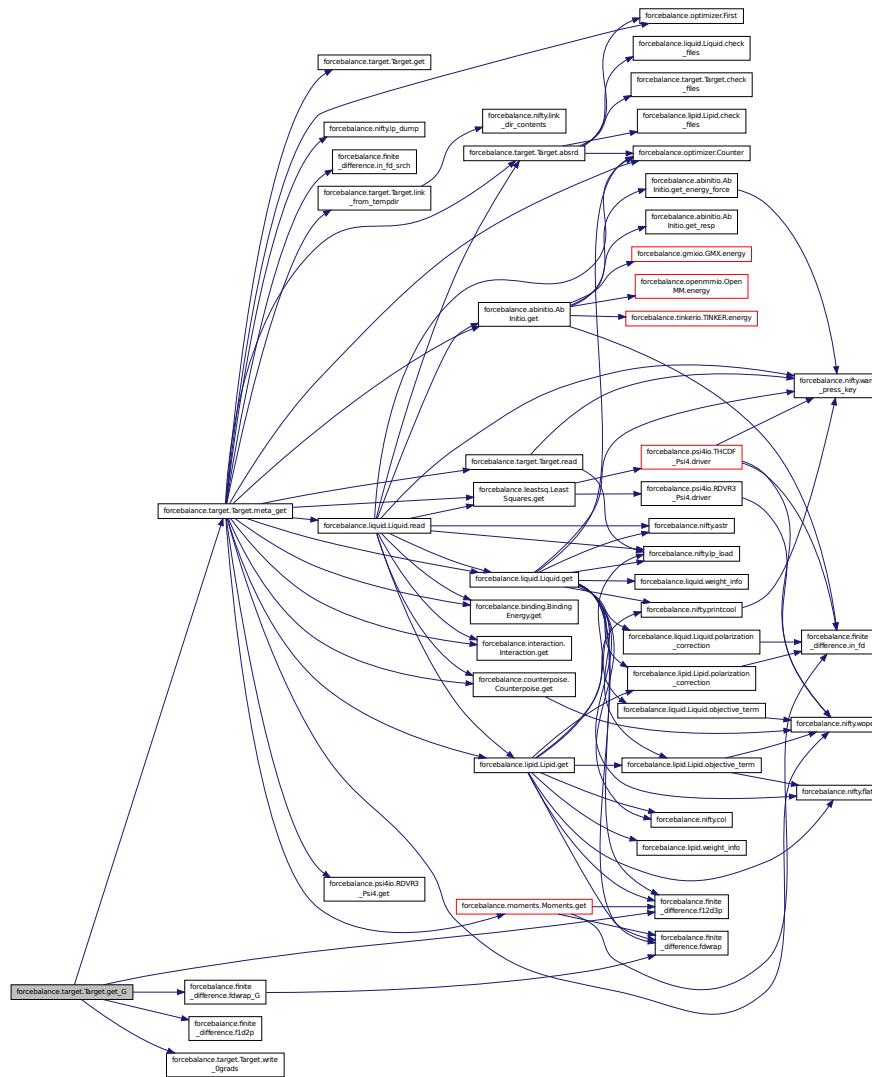
```
def forcebalance.target.Target.get_G ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



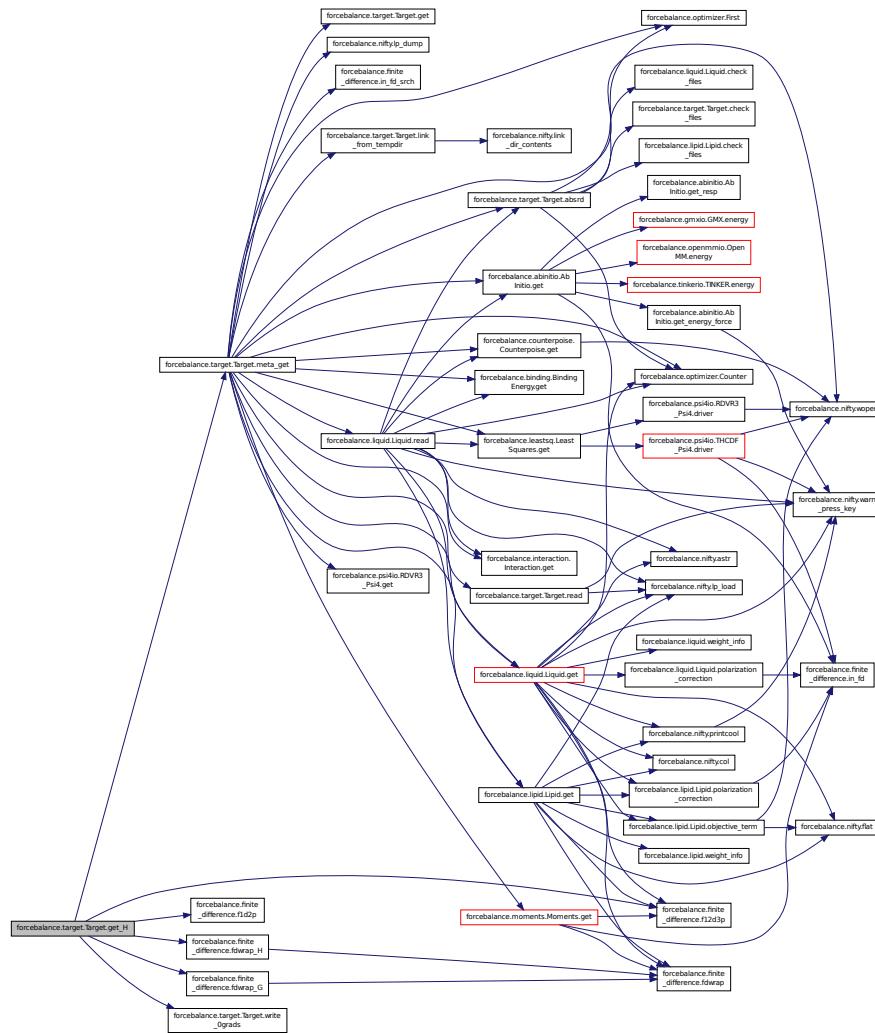
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the fd2_pids and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

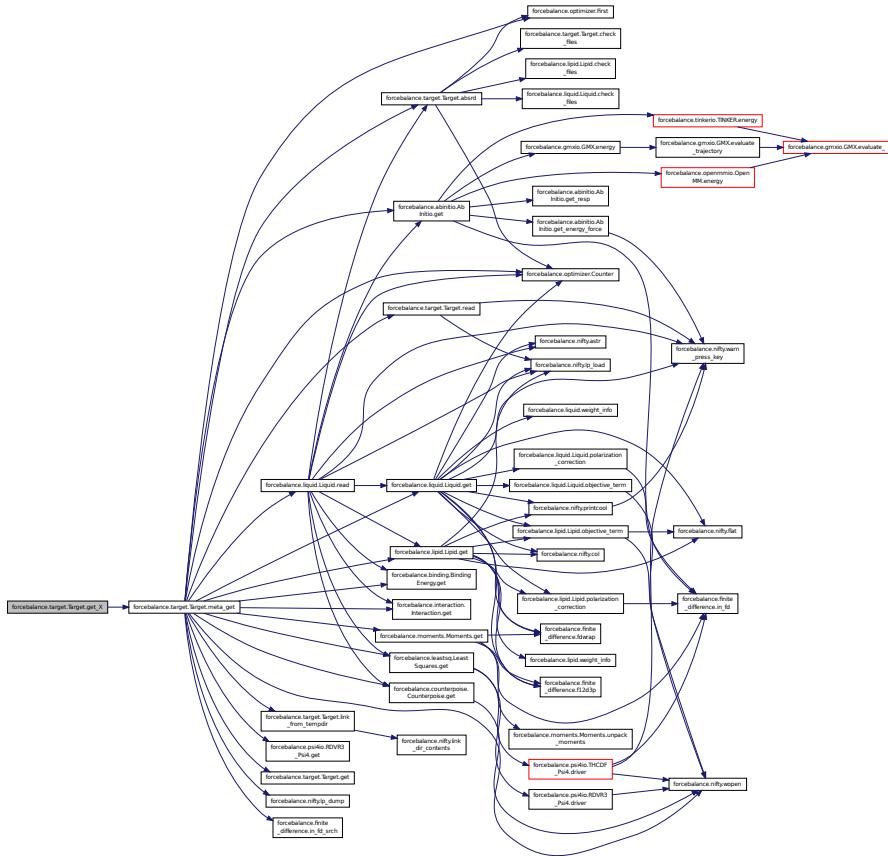
Here is the call graph for this function:



def forcebalance.target.Target.get.X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

Here is the call graph for this function:



def forcebalance.vibration.Vibration.indicate (*self*) [inherited] Print qualitative indicator.

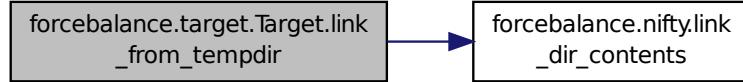
Definition at line 110 of file vibration.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir(self, absdestdir) [inherited] Definition at line 315 of file target.py.

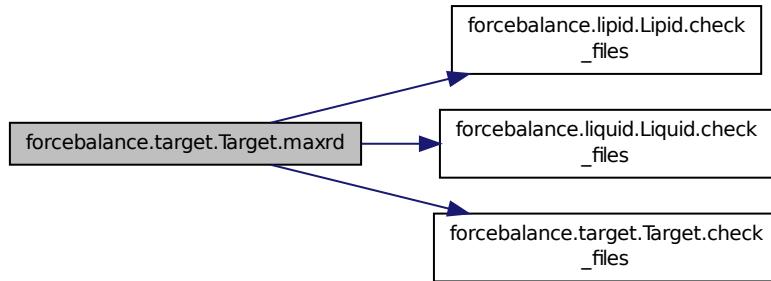
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

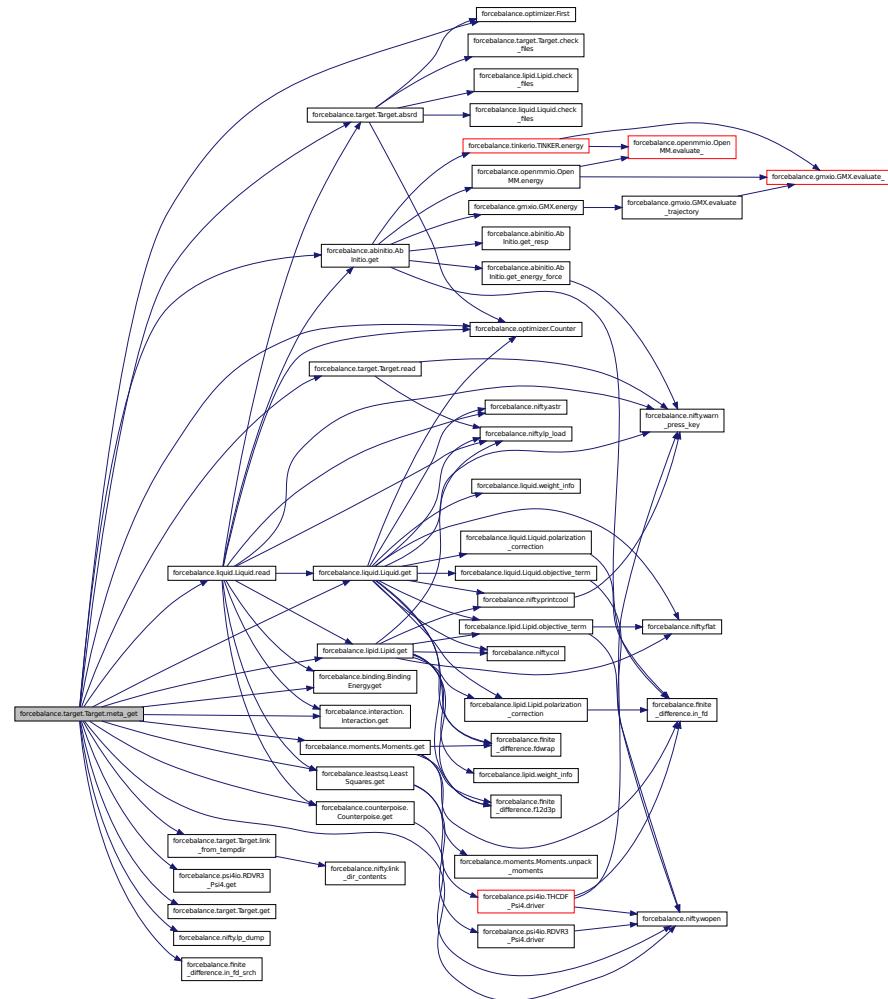


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

Here is the call graph for this function:

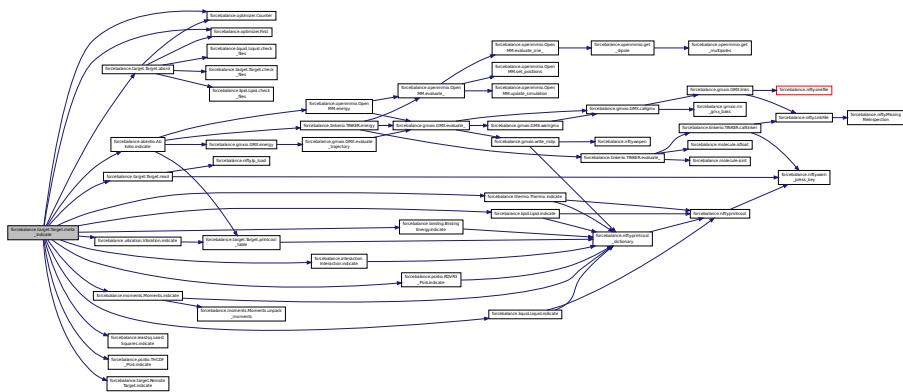


def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.

Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

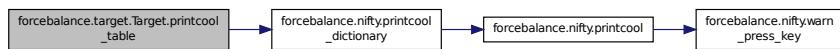
The input should be something like:

Parameters

<i>data</i>	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
<i>headings</i>	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
<i>banner</i>	Optional heading line, which will be printed at the top in the title.
<i>footnote</i>	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

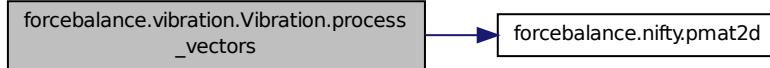
Here is the call graph for this function:



def forcebalance.vibration.Vibration.process_vectors (self, vecs, verbose = False, check = False)
[inherited] Return a set of normal and mass-weighted eigenvectors such that their outer product is the identity.

Definition at line 127 of file vibration.py.

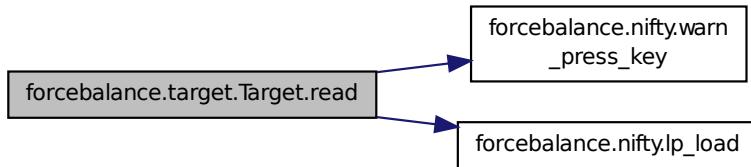
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.vibration.Vibration.read_reference_data (self) [inherited] Read the reference vibrational data from a file.

Definition at line 69 of file vibration.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

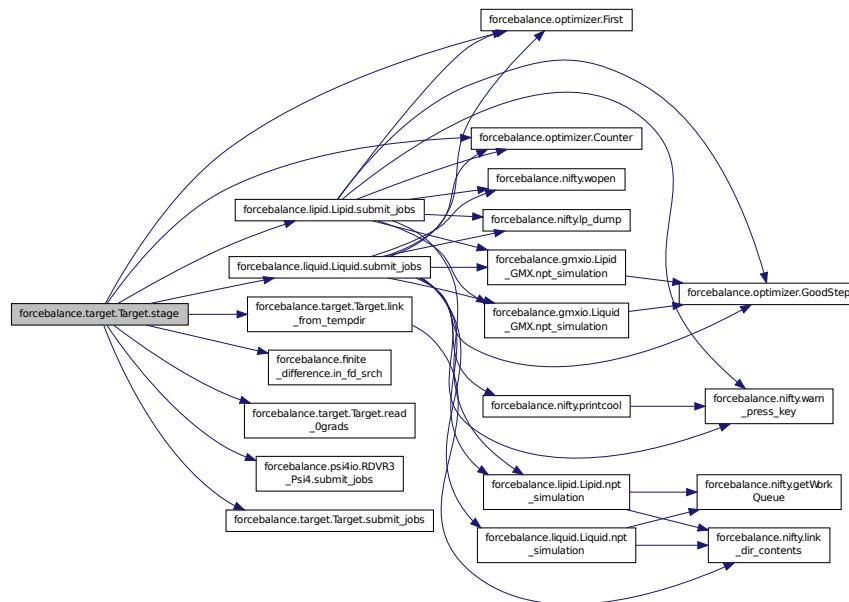
def forcebalance.BaseClass.set_option (self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

```
def forcebalance.target.Target.stage( self, mvals, AGrad = False, AHess = False, customdir = None )  
[inherited] Stages the directory for the target, and then launches Work Queue processes if any.
```

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



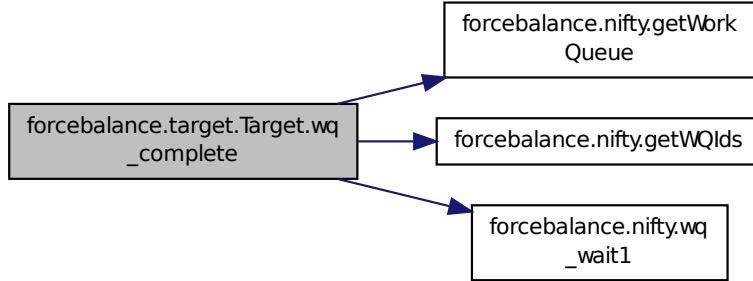
```
def forcebalance.target.Target.submit_jobs( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.vibration.Vibration.vibration_driver( self ) [inherited] Definition at line 118 of file vibration.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.75.4 Member Data Documentation

forcebalance.vibration.Vibration.c2r [inherited] Definition at line 178 of file vibration.py.

forcebalance.vibration.Vibration.calc_eigvals [inherited] Definition at line 198 of file vibration.py.

forcebalance.vibration.Vibration.engine [inherited] Read in the reference data.

Build keyword dictionaries to pass to engine. Create engine object.

Definition at line 63 of file vibration.py.

forcebalance.gmxio.Vibration_GMX.engine Default file names for coordinates and key file.

Definition at line 1497 of file gmxio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.vibration.Vibration.na [inherited] Number of atoms.

Definition at line 71 of file vibration.py.

forcebalance.vibration.Vibration.objective [inherited] Definition at line 199 of file vibration.py.

forcebalance.vibration.Vibration.overlaps [inherited] Definition at line 183 of file vibration.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.vibration.Vibration.reassign [inherited] Definition at line 165 of file vibration.py.

forcebalance.vibration.Vibration.ref_eigvals [inherited] Definition at line 72 of file vibration.py.

forcebalance.vibration.Vibration.ref_eigvecs [inherited] Definition at line 73 of file vibration.py.

forcebalance.vibration.Vibration.ref_eigvecs_nrm_mw [inherited] Definition at line 155 of file vibration.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.vibration.Vibration.vfnm [inherited] The vdata.txt file that contains the vibrations.

Definition at line 56 of file vibration.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

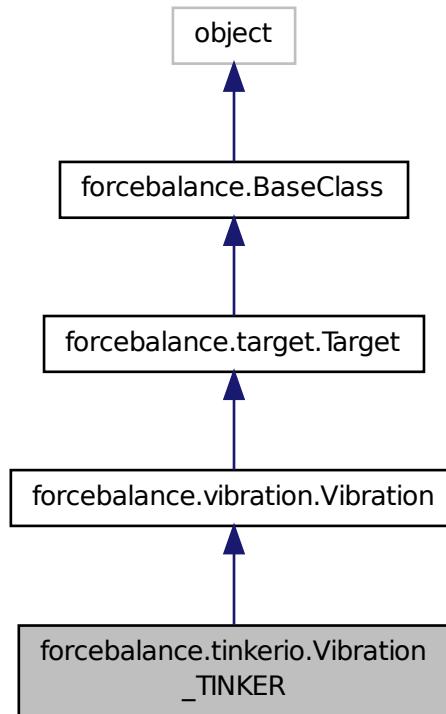
The documentation for this class was generated from the following file:

- [gmxio.py](#)

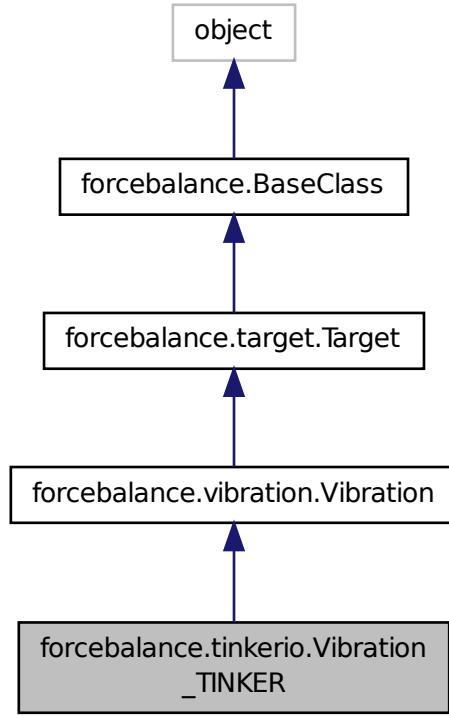
8.76 forcebalance.tinkerio.Vibration_TINKER Class Reference

Vibrational frequency matching using [TINKER](#).

Inheritance diagram for forcebalance.tinkerio.Vibration_TINKER:



Collaboration diagram for forcebalance.tinkerio.Vibration_TINKER:



Public Member Functions

- def `__init__`
- def `read_reference_data`

Read the reference vibrational data from a file.
- def `indicate`

Print qualitative indicator.
- def `vibration_driver`
- def `process_vectors`

Return a set of normal and mass-weighted eigenvectors such that their outer product is the identity.
- def `get`

Evaluate objective function.
- def `get_X`

Computes the objective function contribution without any parametric derivatives.
- def `read_Ograds`

Read a file from the target directory containing names of parameters that don't contribute to the gradient.
- def `write_Ograds`

Write a file to the target directory containing names of parameters that don't contribute to the gradient.
- def `get_G`

- def `get_H`
Computes the objective function contribution and its gradient.
- def `link_from_tempdir`
Computes the objective function contribution and its gradient / Hessian.
- def `refresh_temp_directory`
Back up the temporary directory if desired, delete it and then create a new one.
- def `check_files`
Check this directory for the presence of readable files when the 'read' option is set.
- def `read`
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.
- def `absrd`
Supply the correct directory specified by user's "read" option.
- def `maxrd`
Supply the latest existing temp-directory containing valid data.
- def `meta_indicate`
Wrap around the indicate function, so it can print to screen and also to a file.
- def `meta_get`
Wrapper around the get function.
- def `submit_jobs`
- def `stage`
Stages the directory for the target, and then launches Work Queue processes if any.
- def `wq_complete`
This method determines whether the Work Queue tasks for the current target have completed.
- def `printcool_table`
Print target information in an organized table format.
- def `__setattr__`
- def `set_option`

Public Attributes

- `engine_`
Default file names for coordinates and key file.
- `vfnm`
The vdata.txt file that contains the vibrations.
- `engine`
Read in the reference data.
- `na`
Number of atoms.
- `ref_eigvals`
- `ref_eigvecs`
- `ref_eigvecs_nrm_mw`
- `reassign`
- `c2r`
- `overlaps`
- `calc_eigvals`
- `objective`
- `rd`
Root directory of the whole project.

- **pgrad**
Iteration where we turn on zero-gradient skipping.
- **tempbase**
Relative directory of target.
- **tempdir**
 $\text{self.tempdir} = \text{os.path.join('temp', self.name)}$ *The directory in which the simulation is running - this can be updated.*
- **FF**
Need the forcefield (here for now)
- **xct**
Counts how often the objective function was computed.
- **gct**
Counts how often the gradient was computed.
- **hct**
Counts how often the Hessian was computed.
- **read_indicate**
Whether to read indicate.log from file when restarting an aborted run.
- **write_indicate**
Whether to write indicate.log at every iteration (true for all but remote.)
- **read_objective**
Whether to read objective.p from file when restarting an aborted run.
- **write_objective**
Whether to write objective.p at every iteration (true for all but remote.)
- **verbose_options**
- **PrintOptionDict**

8.76.1 Detailed Description

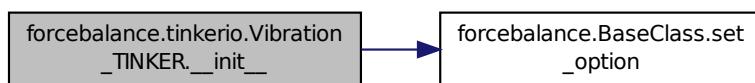
Vibrational frequency matching using [TINKER](#).

Definition at line 1108 of file tinkerio.py.

8.76.2 Constructor & Destructor Documentation

def forcebalance.tinkerio.Vibration_TINKER.__init__ (*self, options, tgt_opts, forcefield*) Definition at line 1109 of file tinkerio.py.

Here is the call graph for this function:



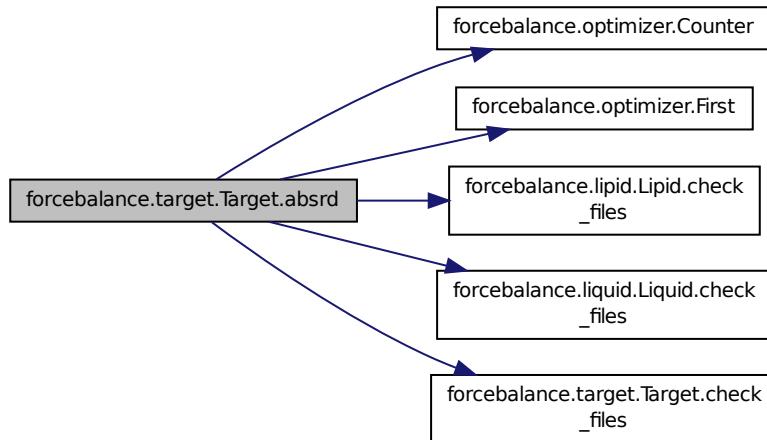
8.76.3 Member Function Documentation

def forcebalance.BaseClass.__setattr__ (*self, key, value*) [inherited] Definition at line 28 of file __init__.py.

```
def forcebalance.target.Target.absrd ( self, inum = None ) [inherited] Supply the correct directory specified by user's "read" option.
```

Definition at line 393 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.check_files ( self, there ) [inherited] Check this directory for the presence of readable files when the 'read' option is set.
```

Definition at line 364 of file target.py.

```
def forcebalance.vibration.Vibration.get ( self, mvals, AGrad=False, AHess=False ) [inherited]  
Evaluate objective function.
```

Definition at line 151 of file vibration.py.

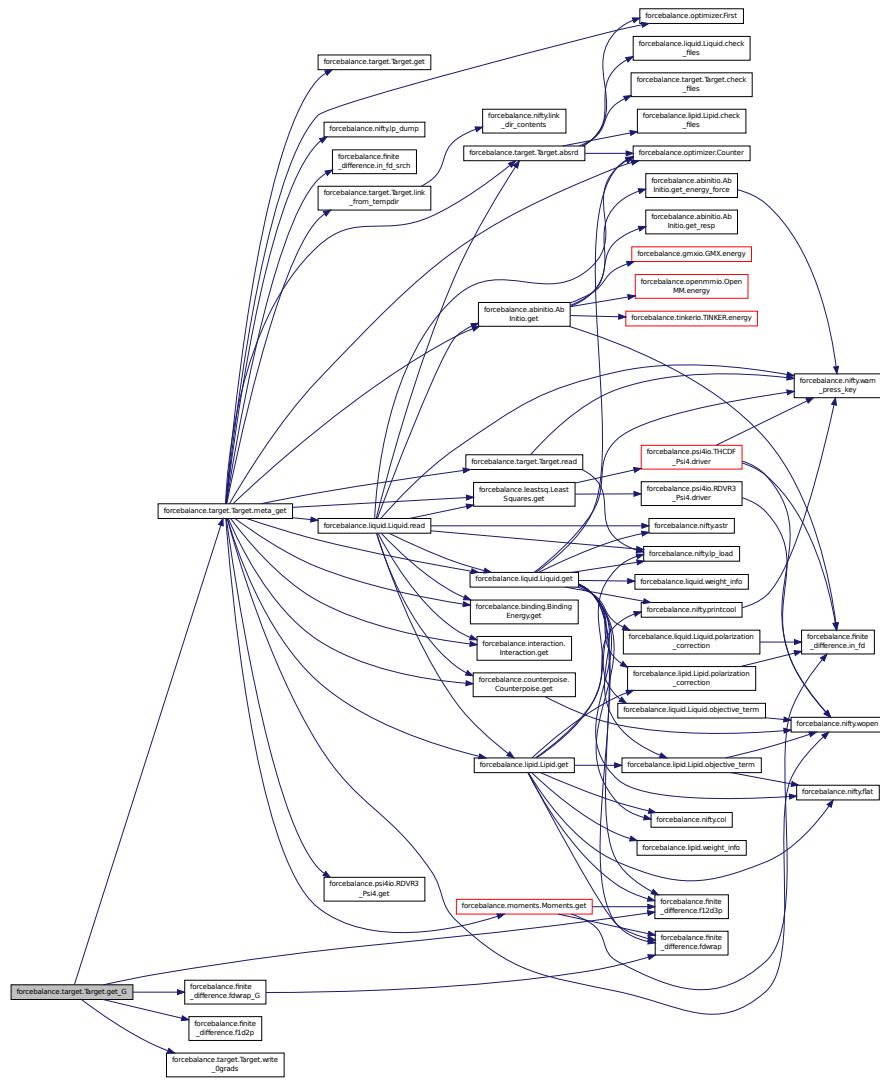
```
def forcebalance.target.Target.get_G ( self, mvals = None ) [inherited] Computes the objective function contribution and its gradient.
```

First the low-level 'get' method is called with the analytic gradient switch turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on. Alternately we can compute the gradient elements and diagonal Hessian elements at the same time using central difference if 'fdhessdiag' is turned on.

In this function we also record which parameters cause a nonzero change in the objective function contribution. Parameters which do not change the objective function will not be differentiated in subsequent calculations. This is recorded in a text file in the targets directory.

Definition at line 272 of file target.py.

Here is the call graph for this function:



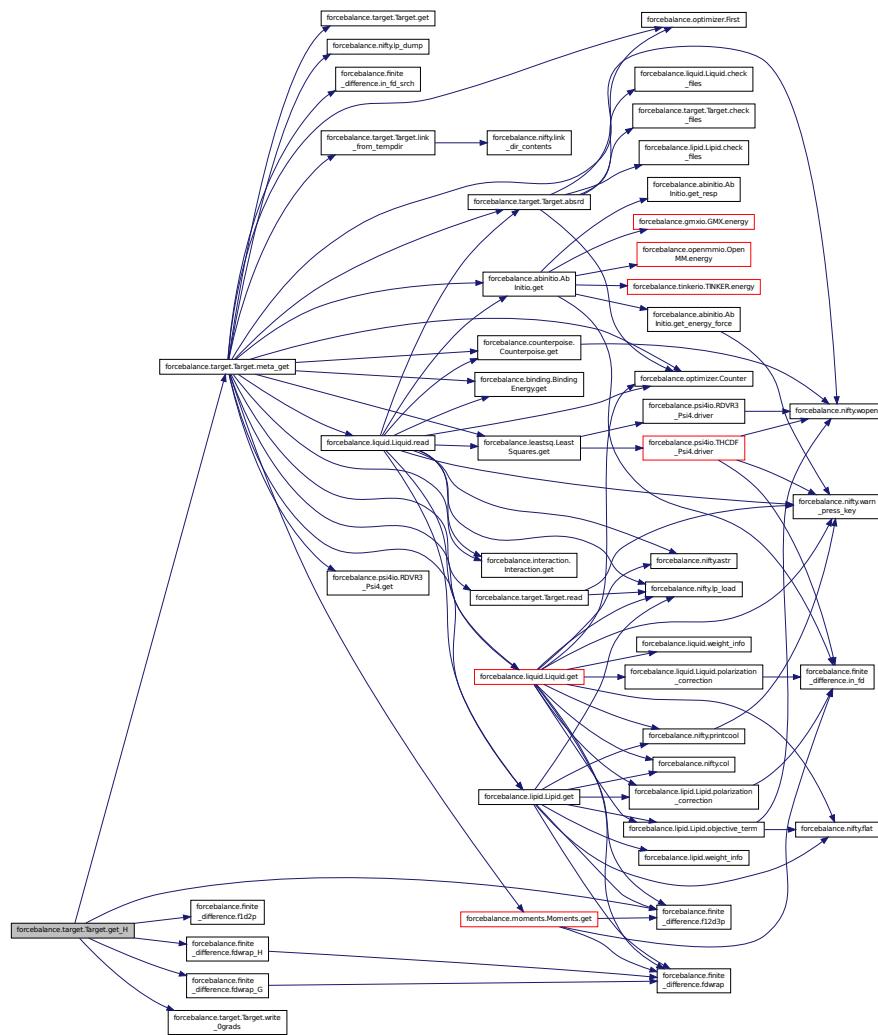
def forcebalance.target.Target.get_H(self, mvals = None) [inherited] Computes the objective function contribution and its gradient / Hessian.

First the low-level 'get' method is called with the analytic gradient and Hessian both turned on. Then we loop through the fd1_pids and compute the corresponding elements of the gradient by finite difference, if the 'fdgrad' switch is turned on.

This is followed by looping through the `fd2.pids` and computing the corresponding Hessian elements by finite difference. Forward finite difference is used throughout for the sake of speed.

Definition at line 296 of file target.py.

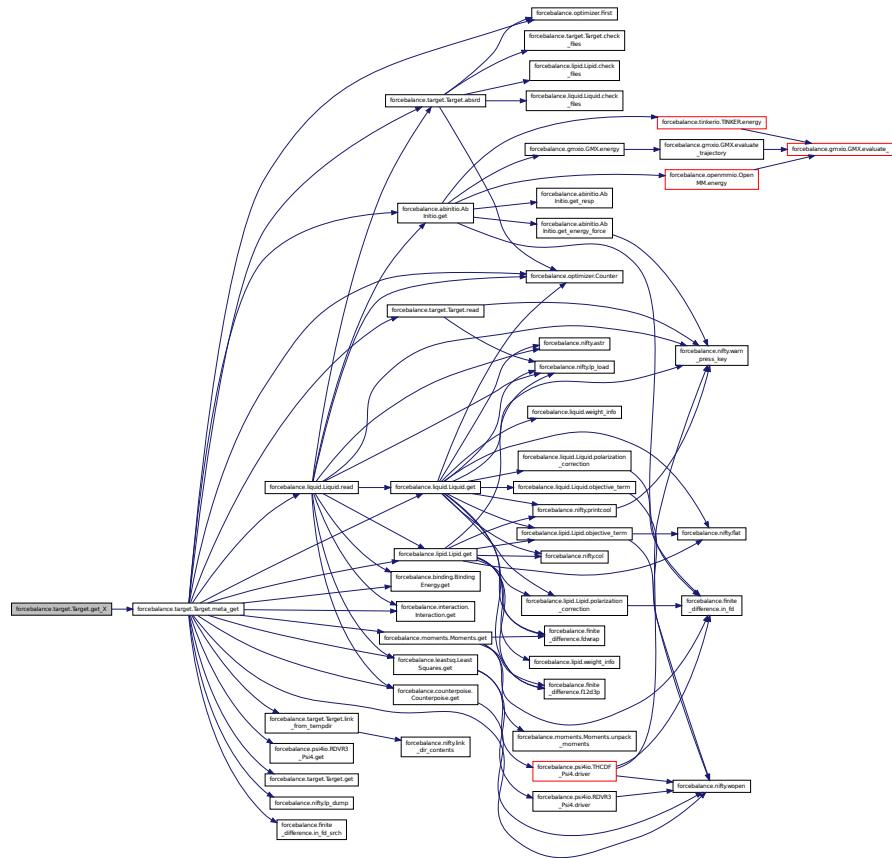
Here is the call graph for this function:



def forcebalance.target.Target.get_X (self, mvals = None) [inherited] Computes the objective function contribution without any parametric derivatives.

Definition at line 184 of file target.py.

Here is the call graph for this function:



def forcebalance.vibration.Vibration.indicate (self) [inherited] Print qualitative indicator.

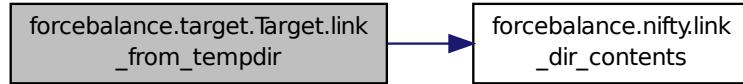
Definition at line 110 of file vibration.py.

Here is the call graph for this function:



def forcebalance.target.Target.link_from_tempdir (self, absdestdir) [inherited] Definition at line 315 of file target.py.

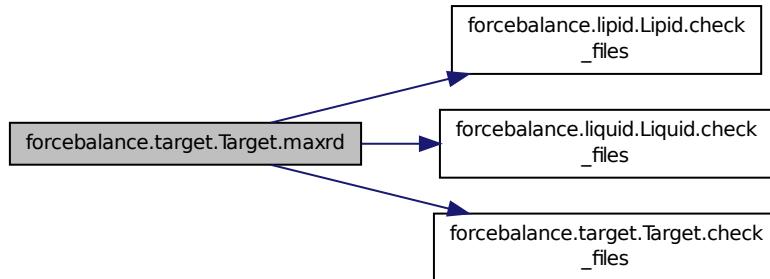
Here is the call graph for this function:



def forcebalance.target.Target.maxrd (self) [inherited] Supply the latest existing temp-directory containing valid data.

Definition at line 447 of file target.py.

Here is the call graph for this function:

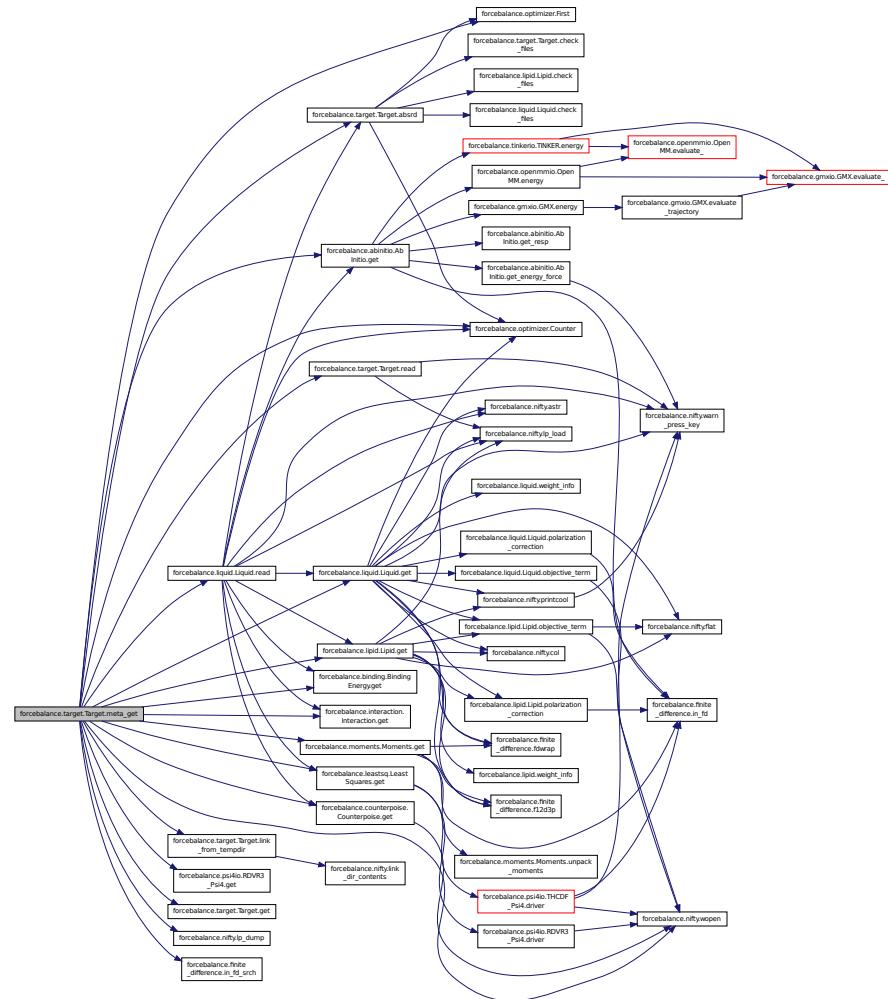


def forcebalance.target.Target.meta_get (self, mvals, AGrad = False, AHess = False, customdir = None) [inherited] Wrapper around the get function.

Create the directory for the target, and then calls 'get'. If we are reading existing data, go into the appropriate read directory and call [read\(\)](#) instead. The 'get' method should not worry about the directory that it's running in.

Definition at line 511 of file target.py.

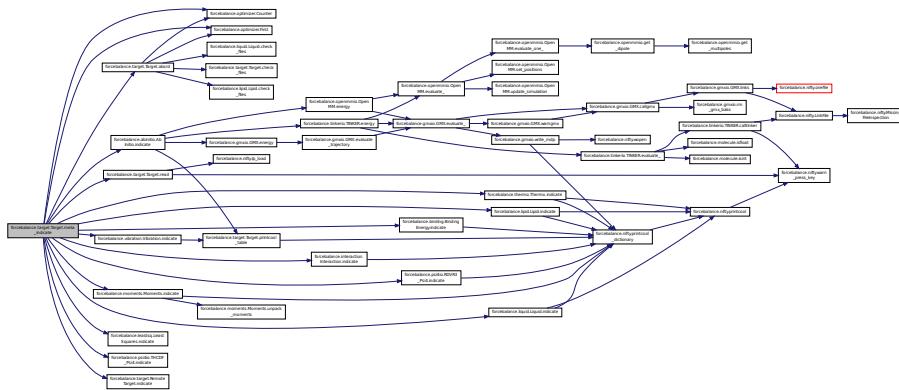
Here is the call graph for this function:



def forcebalance.target.Target.meta_indicate (self) [inherited] Wrap around the indicate function, so it can print to screen and also to a file.

If reading from checkpoint file, don't call the indicate() function, instead just print the file contents to the screen.
Definition at line 469 of file target.py.

Here is the call graph for this function:



```
def forcebalance.target.Target.printcool_table( self, data = OrderedDict([]), headings = [], banner = None, footnote = None, color = 0 ) [inherited] Print target information in an organized table format.
```

Implemented 6/30 because multiple targets are already printing out tabulated information in very similar ways. This method is a simple wrapper around printcool_dictionary.

The input should be something like:

Parameters

data	Column contents in the form of an OrderedDict, with string keys and list vals. The key is printed in the leftmost column and the vals are printed in the other columns. If non-strings are passed, they will be converted to strings (not recommended).
headings	Column headings in the form of a list. It must be equal to the number to the list length for each of the "vals" in OrderedDict, plus one. Use "\n" characters to specify long column names that may take up more than one line.
banner	Optional heading line, which will be printed at the top in the title.
footnote	Optional footnote line, which will be printed at the bottom.

Definition at line 638 of file target.py.

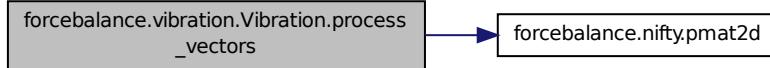
Here is the call graph for this function:



```
def forcebalance.vibration.Vibration.process_vectors( self, vecs, verbose = False, check = False ) [inherited] Return a set of normal and mass-weighted eigenvectors such that their outer product is the identity.
```

Definition at line 127 of file vibration.py.

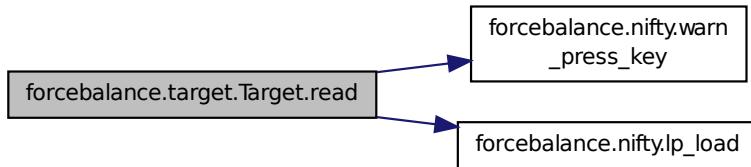
Here is the call graph for this function:



def forcebalance.target.Target.read (self, mvals, AGrad = False, AHess = False) [inherited]
Read data from disk for the initial optimization step if the user has provided the directory to the "read" option.

Definition at line 379 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.read_0grads (self) [inherited] Read a file from the target directory containing names of parameters that don't contribute to the gradient.

Note that we are checking the derivatives of the objective function, and not the derivatives of the quantities that go into building the objective function. However, it is the quantities that we actually differentiate. Since there is a simple chain rule relationship, the parameters that do/don't contribute to the objective function/quantities are the same.

However, property gradients do contribute to objective function Hessian elements, so we cannot use the same mechanism for excluding the calculation of property Hessians. This is mostly fine since we rarely if ever calculate an explicit property Hessian.

Definition at line 207 of file target.py.

def forcebalance.vibration.Vibration.read_reference_data (self) [inherited] Read the reference vibrational data from a file.

Definition at line 69 of file vibration.py.

def forcebalance.target.Target.refresh_temp_directory (self) [inherited] Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 321 of file target.py.

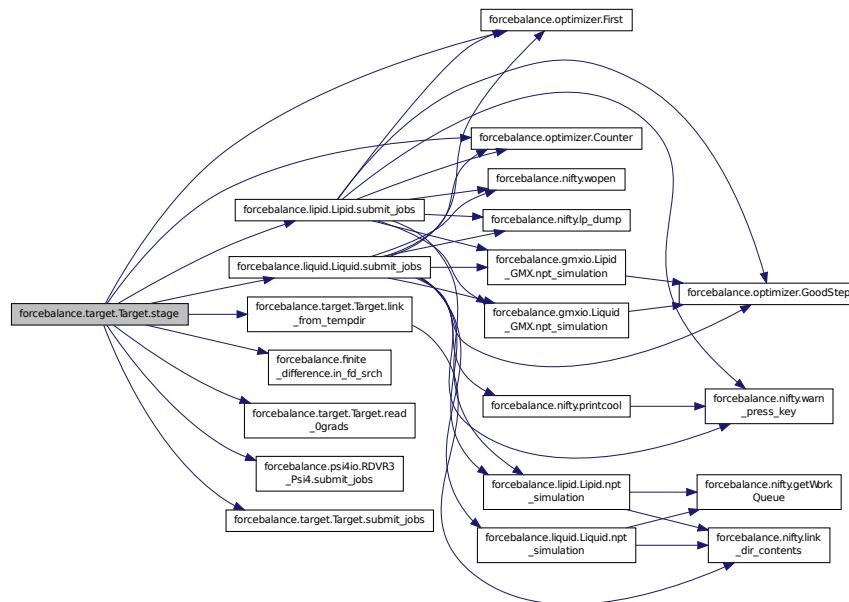
def forcebalance.BaseClass.set_option (self, in_dict, src_key, dest_key = None, val = None, default = None, forceprint = False) [inherited] Definition at line 42 of file __init__.py.

```
def forcebalance.target.Target.stage( self, mvals, AGrad = False, AHess = False, customdir = None )  
[inherited] Stages the directory for the target, and then launches Work Queue processes if any.
```

The 'get' method should not worry about the directory that it's running in.

Definition at line 565 of file target.py.

Here is the call graph for this function:



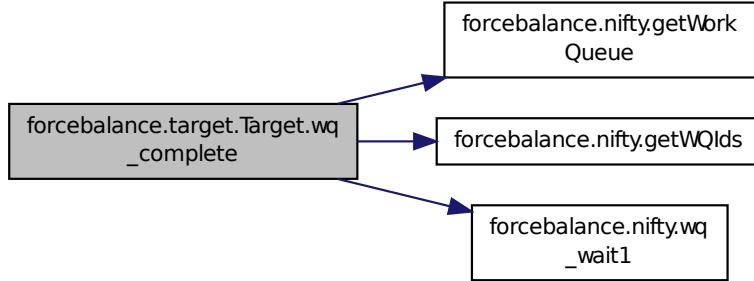
```
def forcebalance.target.Target.submit_jobs( self, mvals, AGrad = False, AHess = False )  
[inherited] Definition at line 555 of file target.py.
```

```
def forcebalance.vibration.Vibration.vibration_driver( self ) [inherited] Definition at line 118 of file vibration.py.
```

```
def forcebalance.target.Target.wq_complete( self ) [inherited] This method determines whether the Work Queue tasks for the current target have completed.
```

Definition at line 602 of file target.py.

Here is the call graph for this function:



def forcebalance.target.Target.write_0grads (self, Ans) [inherited] Write a file to the target directory containing names of parameters that don't contribute to the gradient.

Definition at line 225 of file target.py.

8.76.4 Member Data Documentation

forcebalance.vibration.Vibration.c2r [inherited] Definition at line 178 of file vibration.py.

forcebalance.vibration.Vibration.calc_eigvals [inherited] Definition at line 198 of file vibration.py.

forcebalance.vibration.Vibration.engine [inherited] Read in the reference data.

Build keyword dictionaries to pass to engine. Create engine object.

Definition at line 63 of file vibration.py.

forcebalance.tinkerio.Vibration.TINKER.engine Default file names for coordinates and key file.

Definition at line 1113 of file tinkerio.py.

forcebalance.target.Target.FF [inherited] Need the forcefield (here for now)

Definition at line 160 of file target.py.

forcebalance.target.Target.gct [inherited] Counts how often the gradient was computed.

Definition at line 164 of file target.py.

forcebalance.target.Target.hct [inherited] Counts how often the Hessian was computed.

Definition at line 166 of file target.py.

forcebalance.vibration.Vibration.na [inherited] Number of atoms.

Definition at line 71 of file vibration.py.

forcebalance.vibration.Vibration.objective [inherited] Definition at line 199 of file vibration.py.

forcebalance.vibration.Vibration.overlaps [inherited] Definition at line 183 of file vibration.py.

forcebalance.target.Target.pgrad [inherited] Iteration where we turn on zero-gradient skipping.

Dictionary of whether to call the derivatives.

Definition at line 127 of file target.py.

forcebalance.BaseClass.PrintOptionDict [inherited] Definition at line 44 of file __init__.py.

forcebalance.target.Target.rd [inherited] Root directory of the whole project.

Submit jobs to the Work Queue.

Name of the target Type of target Relative weight of the target Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals How many seconds to sleep (if any) Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Whether to make backup files Directory to read data from.

Definition at line 123 of file target.py.

forcebalance.target.Target.read_indicate [inherited] Whether to read indicate.log from file when restarting an aborted run.

Definition at line 168 of file target.py.

forcebalance.target.Target.read_objective [inherited] Whether to read objective.p from file when restarting an aborted run.

Definition at line 172 of file target.py.

forcebalance.vibration.Vibration.reassign [inherited] Definition at line 165 of file vibration.py.

forcebalance.vibration.Vibration.ref_eigvals [inherited] Definition at line 72 of file vibration.py.

forcebalance.vibration.Vibration.ref_eigvecs [inherited] Definition at line 73 of file vibration.py.

forcebalance.vibration.Vibration.ref_eigvecs_nrm_mw [inherited] Definition at line 155 of file vibration.py.

forcebalance.target.Target.rundir [inherited] self.tempdir = os.path.join('temp',self.name) The directory in which the simulation is running - this can be updated.

Directory of the current iteration; if not None, then the simulation runs under temp/target.name/iteration_number. The 'customdir' is customizable and can go below anything.

Not expecting more than ten thousand iterations Go into the directory where [get\(\)](#) will be executed. Write mathematical parameters to file; will be used to checkpoint calculation. Read in file that specifies which derivatives may be skipped.

Definition at line 158 of file target.py.

forcebalance.target.Target.tempbase [inherited] Relative directory of target.

Temporary (working) directory; it is temp/(target.name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 152 of file target.py.

forcebalance.target.Target.tempdir [inherited] Definition at line 155 of file target.py.

forcebalance.BaseClass.verbose_options [inherited] Definition at line 40 of file __init__.py.

forcebalance.vibration.Vibration.vfnm [inherited] The vdata.txt file that contains the vibrations.

Definition at line 56 of file vibration.py.

forcebalance.target.Target.write_indicate [**inherited**] Whether to write indicate.log at every iteration (true for all but remote.)

Definition at line 170 of file target.py.

forcebalance.target.Target.write_objective [**inherited**] Whether to write objective.p at every iteration (true for all but remote.)

Definition at line 174 of file target.py.

forcebalance.target.Target.xct [**inherited**] Counts how often the objective function was computed.

Definition at line 162 of file target.py.

The documentation for this class was generated from the following file:

- [tinkerio.py](#)

9 File Documentation

9.1 __init__.py File Reference

Classes

- class [forcebalance.BaseClass](#)

Provides some nifty functions that are common to all ForceBalance classes.

- class [forcebalance.BaseReader](#)

The 'reader' class.

Namespaces

- [forcebalance](#)

Variables

- tuple [forcebalance.__version__](#) = pkg_resources.get_distribution("forcebalance")

9.2 abinitio.py File Reference

Classes

- class [forcebalance.abinitio.AblInitio](#)

Subclass of Target for fitting force fields to ab initio data.

Namespaces

- [forcebalance.abinitio](#)

Ab-initio fitting module (energies, forces, resp).

Functions

- def [forcebalance.abinitio.weighted_variance](#)

A more generalized version of build_objective which is callable for derivatives, but the covariance is not there anymore.

- def [forcebalance.abinitio.weighted_variance2](#)

A bit of a hack, since we have to subtract out two mean quantities to get Hessian elements.

- def [forcebalance.abinitio.build_objective](#)

This function builds an objective function (number) from the complicated polytensor and covariance matrices.

Variables

- tuple `forcebalance.abinitio.logger` = getLogger(__name__)

9.3 abinitio_internal.py File Reference

Classes

- class `forcebalance.abinitio_internal.AblInitio_Internal`

Subclass of Target for force and energy matching using an internal implementation.

Namespaces

- `forcebalance.abinitio_internal`
Internal implementation of energy matching (for TIP3P water only)

9.4 amberio.py File Reference

Classes

- class `forcebalance.amberio.Mol2_Reader`
Finite state machine for parsing Mol2 force field file.
- class `forcebalance.amberio.FrcMod_Reader`
Finite state machine for parsing FrcMod force field file.
- class `forcebalance.amberio.AblInitio_AMBER`
Subclass of Target for force and energy matching using AMBER.

Namespaces

- `forcebalance.amberio`
AMBER force field input/output.

Functions

- def `forcebalance.amberio.is_mol2_atom`

Variables

- tuple `forcebalance.amberio.logger` = getLogger(__name__)
- dictionary `forcebalance.amberio.mol2_pdct` = {'COUL': {'Atom': [1], 8: ''}}
- dictionary `forcebalance.amberio.frcmod_pdct`

9.5 api.dox File Reference

9.6 binding.py File Reference

Classes

- class `forcebalance.binding.BindingEnergy`
Improved subclass of Target for fitting force fields to binding energies.

Namespaces

- `forcebalance.binding`
Binding energy fitting module.

Functions

- def `forcebalance.binding.parse_interactions`

Parse through the interactions input file.

Variables

- tuple `forcebalance.binding.logger` = getLogger(__name__)

9.7 chemistry.py File Reference

Namespaces

- `forcebalance.chemistry`

Functions

- def `forcebalance.chemistry.LookupByMass`
- def `forcebalance.chemistry.BondStrengthByLength`

Variables

- tuple `forcebalance.chemistry.BondEnergies` = defaultdict(lambda:defaultdict(dict))
- list `forcebalance.chemistry.Radii`

Covalent radii from Cordero et al.
- tuple `forcebalance.chemistry.PeriodicTable`
- list `forcebalance.chemistry.Elements`
- list `forcebalance.chemistry.BondChars` = ['-','=','3']
- string `forcebalance.chemistry.data_from_web`
- tuple `forcebalance.chemistry.line` = line.expandtabs()
- tuple `forcebalance.chemistry.BE` = float(line.split()[1])
- tuple `forcebalance.chemistry.L` = float(line.split()[2])
- tuple `forcebalance.chemistry.atoms` = re.split('[-=3]', line.split()[0])
- list `forcebalance.chemistry.A` = atoms[0]
- list `forcebalance.chemistry.B` = atoms[1]
- tuple `forcebalance.chemistry.bo` = BondChars.index(re.findall('[-=3]', line.split()[0])[0])

9.8 contact.py File Reference

Namespaces

- `forcebalance.contact`

Functions

- def `forcebalance.contact.atom_distances`

For each frame in xyzlist, compute the (euclidean) distance between pairs of atoms whos indices are given in contacts.

- def `forcebalance.contact.residue_distances`

For each frame in xyzlist, and for each pair of residues in the array contact, compute the distance between the closest pair of atoms such that one of them belongs to each residue.

9.9 counterpoise.py File Reference

Classes

- class `forcebalance.counterpoise.Counterpoise`

Target subclass for matching the counterpoise correction.

Namespaces

- `forcebalance.counterpoise`

Match an empirical potential to the counterpoise correction for basis set superposition error (BSSE).

Variables

- tuple `forcebalance.counterpoise.logger = getLogger(__name__)`

9.10 custom.io.py File Reference

Classes

- class `forcebalance.custom_io.Gen_Reader`

Finite state machine for parsing custom GROMACS force field files.

Namespaces

- `forcebalance.custom_io`

Custom force field parser.

Variables

- list `forcebalance.custom_io.cptypes = [None, 'CPGAUSS', 'CPEXPG', 'CPGEXP']`

Types of counterpoise correction.

- list `forcebalance.custom_io.ndtypes = [None]`

Types of NDDO correction.

- dictionary `forcebalance.custom.io.fdict`

Section -> Interaction type dictionary.

- dictionary `forcebalance.custom.io.pdict`

Interaction type -> Parameter Dictionary.

9.11 engine.py File Reference

Classes

- class `forcebalance.engine.Engine`

Base class for all engines.

Namespaces

- `forcebalance.engine`

Variables

- tuple `forcebalance.engine.logger = getLogger(__name__)`

9.12 finite_difference.py File Reference

Namespaces

- `forcebalance.finite_difference`

Functions

- def `forcebalance.finite_difference.f1d2p`
A two-point finite difference stencil.
- def `forcebalance.finite_difference.f1d5p`
A highly accurate five-point finite difference stencil for computing derivatives of a function.
- def `forcebalance.finite_difference.f1d7p`
A highly accurate seven-point finite difference stencil for computing derivatives of a function.
- def `forcebalance.finite_difference.f12d7p`
- def `forcebalance.finite_difference.f12d3p`
A three-point finite difference stencil.
- def `forcebalance.finite_difference.f2var`
A finite difference stencil for a function of two variables.
- def `forcebalance.finite_difference.in_fd`
Invoking this function from anywhere will tell us whether we're being called by a finite-difference function.
- def `forcebalance.finite_difference.in_fd_src`
Invoking this function from anywhere will tell us whether we're being called by a finite-difference function.
- def `forcebalance.finite_difference.fdwrap`
A function wrapper for finite difference designed for differentiating 'get'-type functions.
- def `forcebalance.finite_difference.fdwrap_G`
A driver to fdwrap for gradients (see documentation for fdwrap) Inputs: tgt = The Target containing the objective function that we want to differentiate mvals0 = The 'central' values of the mathematical parameters - i.e.
- def `forcebalance.finite_difference.fdwrap_H`
A driver to fdwrap for Hessians (see documentation for fdwrap) Inputs: tgt = The Target containing the objective function that we want to differentiate mvals0 = The 'central' values of the mathematical parameters - i.e.

Variables

- tuple `forcebalance.finite_difference.logger` = getLogger(__name__)

9.13 forcefield.py File Reference

Classes

- class `forcebalance.forcefield.BackedUpDict`
- class `forcebalance.forcefield.FF`

Force field class.

Namespaces

- `forcebalance.forcefield`

Force field module.

Functions

- def `forcebalance.forcefield.determine_fftype`
Determine the type of a force field file.
- def `forcebalance.forcefield.rs_override`
This function takes in a dictionary (`rsfactors`) and a string (`termtype`).

Variables

- tuple `forcebalance.forcefield.logger` = getLogger(`_name_`)
- dictionary `forcebalance.forcefield.FF_Extensions`
- dictionary `forcebalance.forcefield.FF_IOModules`

9.14 gmxio.py File Reference

Classes

- class `forcebalance.gmxio.ITP_Reader`
Finite state machine for parsing GROMACS force field files.
- class `forcebalance.gmxio.GMX`
Derived from Engine object for carrying out general purpose GROMACS calculations.
- class `forcebalance.gmxio.Liquid_GMX`
- class `forcebalance.gmxio.Lipid_GMX`
- class `forcebalance.gmxio.AbInitio_GMX`
Subclass of AbInitio for force and energy matching using GROMACS.
- class `forcebalance.gmxio.BindingEnergy_GMX`
Binding energy matching using Gromacs.
- class `forcebalance.gmxio.Interaction_GMX`
Interaction energy matching using GROMACS.
- class `forcebalance.gmxio.Moments_GMX`
Multipole moment matching using GROMACS.
- class `forcebalance.gmxio.Vibration_GMX`
Vibrational frequency matching using GROMACS.
- class `forcebalance.gmxio.Thermo_GMX`
Thermodynamical property matching using GROMACS.

Namespaces

- `forcebalance.gmxio`
GROMACS input/output.

Functions

- def `forcebalance.gmxio.write_mdp`
Create or edit a Gromacs MDP file.
- def `forcebalance.gmxio.write_ndx`
Create or edit a Gromacs ndx file.
- def `forcebalance.gmxio.parse_atomtype_line`
Parses the 'atomtype' line.
- def `forcebalance.gmxio.rm_gmx_baks`

Variables

- tuple `forcebalance.gmxio.logger` = getLogger(`_name_`)
- list `forcebalance.gmxio.nftypes` = [None, 'VDW', 'VDW_BHAM']
VdW interaction function types.
- list `forcebalance.gmxio.pftypes` = [None, 'VPAIR', 'VPAIR_BHAM']
Pairwise interaction function types.
- list `forcebalance.gmxio.bftypes` = [None, 'BONDS', 'G96BONDS', 'MORSE']
Bonded interaction function types.
- list `forcebalance.gmxio.aftypes`
Angle interaction function types.
- list `forcebalance.gmxio.dftypes` = [None, 'PDIHS', 'IDIHS', 'RBDIHS', 'PIMPDIHS', 'FOURDIHS', None, None, 'TABDIHS', 'PDIHMULS']
Dihedral interaction function types.
- dictionary `forcebalance.gmxio.fdict`
Section -> Interaction type dictionary.
- dictionary `forcebalance.gmxio.pdict`
Interaction type -> Parameter Dictionary.

9.15 interaction.py File Reference

Classes

- class `forcebalance.interaction.Interaction`
Subclass of Target for fitting force fields to interaction energies.

Namespaces

- `forcebalance.interaction`
Interaction energy fitting module.

Variables

- tuple `forcebalance.interaction.logger` = getLogger(`_name_`)

9.16 leastsq.py File Reference

Classes

- class `forcebalance.leastsq.LeastSquares`
Subclass of Target for general least squares fitting.

Namespaces

- `forcebalance.leastsq`
- `forcebalance.abinitio`
Ab-initio fitting module (energies, forces, resp).

Functions

- def `forcebalance.leastsq.CheckBasis`
- def `forcebalance.leastsq.LastMvals`

Variables

- tuple `forcebalance.leastsq.logger` = getLogger(`_name_`)
- `forcebalance.leastsq.CHECK_BASIS` = False
- `forcebalance.leastsq.LAST_MVALS` = None

9.17 lipid.py File Reference

Classes

- class `forcebalance.lipid.Lipid`

Subclass of Target for lipid property matching.

Namespaces

- `forcebalance.lipid`

Matching of lipid bulk properties.

Functions

- def `forcebalance.lipid.weight_info`

Variables

- tuple `forcebalance.lipid.logger` = getLogger(`_name_`)

9.18 liquid.py File Reference

Classes

- class `forcebalance.liquid.Liquid`

Subclass of Target for liquid property matching.

Namespaces

- `forcebalance.liquid`

Matching of liquid bulk properties.

Functions

- def `forcebalance.liquid.weight_info`

Variables

- tuple `forcebalance.liquid.logger` = getLogger(`_name_`)

9.19 Mol2.py File Reference

Classes

- class `forcebalance.Mol2.mol2_atom`

This is to manage mol2 atomic lines on the form: 1 C1 5.4790 42.2880 49.5910 C.ar 1 <1> 0.0424.

- class `forcebalance.Mol2.mol2_bond`

This is to manage mol2 bond lines on the form: 1 1 2 ar.

- class `forcebalance.Mol2.mol2`

This is to manage one mol2 series of lines on the form:

- class `forcebalance.Mol2.mol2_set`

Namespaces

- `forcebalance.Mol2`

Variables

- tuple `forcebalance.Mol2.data = mol2_set(sys.argv[1], subset=["RNase.xray.inh8.1QHC"])`

9.20 mol2io.py File Reference

Classes

- class `forcebalance.mol2io.Mol2_Reader`

Finite state machine for parsing Mol2 force field file.

Namespaces

- `forcebalance.mol2io`
Mol2 I/O.

Variables

- dictionary `forcebalance.mol2io.mol2_pdct = {'COUL': {'Atom': [1], 6: ''}}`

9.21 molecule.py File Reference

Classes

- class `forcebalance.molecule.MyG`
- class `forcebalance.molecule.MolfileTimestep`
Wrapper for the timestep C structure used in molfile plugins.
- class `forcebalance.molecule.Molecule`
Lee-Ping's general file format conversion class.

Namespaces

- `forcebalance.molecule`

Functions

- def `forcebalance.molecule.getElement`
- def `forcebalance.molecule.elem_from_atomname`
Given an atom name, attempt to get the element in most cases.
- def `forcebalance.molecule.nodematch`
- def `forcebalance.molecule.isint`
ONLY matches integers! If you have a decimal point? None shall pass!
- def `forcebalance.molecule.isfloat`
Matches ANY number; it can be a decimal, scientific notation, integer, or what have you.
- def `forcebalance.molecule.CubicLattice`
This function takes in three lattice lengths and three lattice angles, and tries to return a complete box specification.

- def `forcebalance.molecule.BuildLatticeFromLengthsAngles`
This function takes in three lattice lengths and three lattice angles, and tries to return a complete box specification.
- def `forcebalance.molecule.BuildLatticeFromVectors`
This function takes in three lattice vectors and tries to return a complete box specification.
- def `forcebalance.molecule.format_xyz_coord`
Print a line consisting of (element, x, y, z) in accordance with .xyz file format.
- def `forcebalance.molecule.format_gro_coord`
Print a line in accordance with .gro file format, with six decimal points of precision.
- def `forcebalance.molecule.format_xyzgen_coord`
Print a line consisting of (element, p, q, r, s, t, ...) where (p, q, r) are arbitrary atom-wise data (this might happen, for instance, with atomic charges)
- def `forcebalance.molecule.format_gro_box`
Print a line corresponding to the box vector in accordance with .gro file format.
- def `forcebalance.molecule.is_gro_coord`
Determines whether a line contains GROMACS data or not.
- def `forcebalance.molecule.is_charmm_coord`
Determines whether a line contains CHARMM data or not.
- def `forcebalance.molecule.is_gro_box`
Determines whether a line contains a GROMACS box vector or not.
- def `forcebalance.molecule.add_strip_to_mat`
- def `forcebalance.molecule.pvec`
- def `forcebalance.molecule.grouper`
Groups a big long iterable into groups of ten or what have you.
- def `forcebalance.molecule.even_list`
Creates a list of number sequences divided as evenly as possible.
- def `forcebalance.molecule.both`
- def `forcebalance.molecule.diff`
- def `forcebalance.molecule.either`
- def `forcebalance.molecule.EulerMatrix`
Constructs an Euler matrix from three Euler angles.
- def `forcebalance.molecule.ComputeOverlap`
Computes an 'overlap' between two molecules based on some fictitious density.
- def `forcebalance.molecule.AlignToDensity`
Computes a "overlap density" from two frames.
- def `forcebalance.molecule.AlignToMoments`
Pre-aligns molecules to 'moment of inertia'.
- def `forcebalance.molecule.get_rotate_translate`
- def `forcebalance.molecule.cartesian_product2`
Form a Cartesian product of two NumPy arrays.
- def `forcebalance.molecule.main`

Variables

- tuple `forcebalance.molecule.FrameVariableNames`
- tuple `forcebalance.molecule.AtomVariableNames` = set(['elem', 'partial_charge', 'atomname', 'atomtype', 'tinker-suf', 'resid', 'resname', 'qcsuf', 'qm_ghost', 'chain', 'altloc', 'icode'])
- tuple `forcebalance.molecule.MetaVariableNames` = set(['fnm', 'ftype', 'qcrems', 'qctemplate', 'qcerr', 'charge', 'mult', 'bonds'])

- tuple `forcebalance.molecule.QuantumVariableNames` = set(['qcrems', 'qctemplate', 'charge', 'mult', 'qcsuf', 'qm-ghost'])
- `forcebalance.molecule.AllVariableNames` = QuantumVariableNames|AtomVariableNames|MetaVariableNames|FrameVariableNames
- list `forcebalance.molecule.Radii`
- list `forcebalance.molecule.Elements`
- tuple `forcebalance.molecule.PeriodicTable`
- float `forcebalance.molecule.bohrang` = 0.529177249
One bohr equals this many angstroms.
- tuple `forcebalance.molecule.splitter` = re.compile(r'(\s+|\S+)')
- tuple `forcebalance.molecule.Box` = namedtuple('Box',[‘a’;‘b’;‘c’;‘alpha’;‘beta’;‘gamma’;‘A’;‘B’;‘C’;‘V’])
- int `forcebalance.molecule.radian` = 180
- int `forcebalance.molecule.have_contact` = 0

9.22 moments.py File Reference

Classes

- class `forcebalance.moments.Moments`

Subclass of Target for fitting force fields to multipole moments (from experiment or theory).

Namespaces

- `forcebalance.moments`

Multipole moment fitting module.

Variables

- tuple `forcebalance.moments.logger` = getLogger(__name__)

9.23 nifty.py File Reference

Classes

- class `forcebalance.nifty.Pickler_LP`

A subclass of the python Pickler that implements pickling of _ElementTree types.

- class `forcebalance.nifty.Unpickler_LP`

A subclass of the python Unpickler that implements unpickling of _ElementTree types.

- class `forcebalance.nifty.LineChunker`

Namespaces

- `forcebalance.nifty`

Nifty functions, intended to be imported by any module within ForceBalance.

Functions

- def `forcebalance.nifty.pvec1d`

Printout of a 1-D vector.

- def `forcebalance.nifty.astr`

Write an array to a string so we can use it to key a dictionary.

- def `forcebalance.nifty.pmat2d`

- def `forcebalance.nifty.grouper`
Printout of a 2-D matrix.
- def `forcebalance.nifty.encode`
Get the representative integer value from an array.
- def `forcebalance.nifty.segments`
Cool-looking printout for slick formatting of output.
- def `forcebalance.nifty.commadash`
See documentation for printcool; this is a nice way to print out keys/values in a dictionary.
- def `forcebalance.nifty.uncommadash`
ONLY matches integers! If you have a decimal point? None shall pass!
- def `forcebalance.nifty.isfloat`
Matches ANY number; it can be a decimal, scientific notation, what have you CAUTION - this will also match an integer.
- def `forcebalance.nifty.isdecimal`
Matches things with a decimal only; see isint and isfloat.
- def `forcebalance.nifty.floatoran`
Returns a big number if we encounter NaN.
- def `forcebalance.nifty.col`
Given any list, array, or matrix, return a 1-column matrix.
- def `forcebalance.nifty.row`
Given any list, array, or matrix, return a 1-row matrix.
- def `forcebalance.nifty.flat`
Given any list, array, or matrix, return a single-index array.
- def `forcebalance.nifty.monotonic`
Invert a matrix using singular value decomposition.
- def `forcebalance.nifty.get_least_squares`
Compute the (cross) statistical inefficiency of (two) timeseries.
- def `forcebalance.nifty.statisticalInefficiency`
Use this instead of pickle.dump for pickling anything that contains _ElementTree types.
- def `forcebalance.nifty.lp_dump`
Use this instead of pickle.load for unpickling anything that contains _ElementTree types.
- def `forcebalance.nifty.lp_load`
Submit a job to the Work Queue.
- def `forcebalance.nifty.queue_up_src_dest`
Submit a job to the Work Queue.
- def `forcebalance.nifty.wq_wait1`

This function waits ten seconds to see if a task in the Work Queue has finished.

- def `forcebalance.nifty.wq_wait`

This function waits until the work queue is completely empty.
- def `forcebalance.nifty.click`

Stopwatch function for timing.
- def `forcebalance.nifty.bak`
- def `forcebalance.nifty.onefile`
- def `forcebalance.nifty.GoInto`
- def `forcebalance.nifty.allsplit`
- def `forcebalance.nifty.Leave`
- def `forcebalance.nifty.MissingFileInspection`
- def `forcebalance.nifty.wopen`

If trying to write to a symbolic link, remove it first.
- def `forcebalance.nifty.LinkFile`
- def `forcebalance.nifty.CopyFile`
- def `forcebalance.nifty.link_dir_contents`
- def `forcebalance.nifty.remove_if_exists`

Remove the file if it exists (doesn't return an error).
- def `forcebalance.nifty.which`
- def `forcebalance.nifty.warn_press_key`
- def `forcebalance.nifty.warn_once`

Prints a warning but will only do so once in a given run.
- def `forcebalance.nifty.concurrent_map`

Similar to the builtin function map().

Variables

- tuple `forcebalance.nifty.logger` = getLogger(__name__)
- float `forcebalance.nifty.kb` = 0.0083144100163

Boltzmann constant.
- float `forcebalance.nifty.eqcgmx` = 2625.5002

Q-Chem to GMX unit conversion for energy.
- float `forcebalance.nifty.fqcgmx` = -49621.9

Q-Chem to GMX unit conversion for force.
- float `forcebalance.nifty.bohrang` = 0.529177249

One bohr equals this many angstroms.
- string `forcebalance.nifty.XMLFILE` = 'x'

Pickle uses 'flags' to pickle and unpickle different variable types.
- `forcebalance.nifty.WORK_QUEUE` = None
- tuple `forcebalance.nifty.WQIDS` = defaultdict(list)
- list `forcebalance.nifty.specific_lst`
- tuple `forcebalance.nifty.specific_dct` = dict(list(itertools.chain(*[[j,i[1]] for j in i[0]] for i in specific_lst)))

9.24 objective.py File Reference

Classes

- class `forcebalance.objective.Objective`

Objective function.
- class `forcebalance.objective.Penalty`

Penalty functions for regularizing the force field optimizer.

Namespaces

- `forcebalance.objective`

ForceBalance objective function.

Variables

- tuple `forcebalance.objective.logger` = getLogger(`__name__`)
- dictionary `forcebalance.objective.Implemented_Targets`

The table of implemented Targets.

- list `forcebalance.objective.Letters` = ['X','G','H']

This is the canonical lettering that corresponds to : objective function, gradient, Hessian.

9.25 openmmio.py File Reference

Classes

- class `forcebalance.openmmio.OpenMM_Reader`
Class for parsing OpenMM force field files.
- class `forcebalance.openmmio.OpenMM`
Derived from Engine object for carrying out general purpose OpenMM calculations.
- class `forcebalance.openmmio.Liquid_OpenMM`
Condensed phase property matching using OpenMM.
- class `forcebalance.openmmio.AbInitio_OpenMM`
Force and energy matching using OpenMM.
- class `forcebalance.openmmio.BindingEnergy_OpenMM`
Binding energy matching using OpenMM.
- class `forcebalance.openmmio.Interaction_OpenMM`
Interaction matching using OpenMM.
- class `forcebalance.openmmio.Moments_OpenMM`
Multipole moment matching using OpenMM.

Namespaces

- `forcebalance.openmmio`
OpenMM input/output.

Functions

- def `forcebalance.openmmio.energy_components`
- def `forcebalance.openmmio.get_multipoles`
Return the current multipole moments in Debye and Buckingham units.
- def `forcebalance.openmmio.get_dipole`
Return the current dipole moment in Debye.
- def `forcebalance.openmmio.PrepareVirtualSites`
Prepare a list of function wrappers and vsite parameters from the system.
- def `forcebalance.openmmio.ResetVirtualSites.fast`
Given a set of OpenMM-compatible positions and a System object, compute the correct virtual site positions according to the System.
- def `forcebalance.openmmio.ResetVirtualSites`

Given a set of OpenMM-compatible positions and a System object, compute the correct virtual site positions according to the System.

- def `forcebalance.openmmio.GetVirtualSiteParameters`
Return an array of all virtual site parameters in the system.
- def `forcebalance.openmmio.CopyAmoebaBondParameters`
- def `forcebalance.openmmio.CopyAmoebaOutOfPlaneBendParameters`
- def `forcebalance.openmmio.CopyAmoebaAngleParameters`
- def `forcebalance.openmmio.CopyAmoebaInPlaneAngleParameters`
- def `forcebalance.openmmio.CopyAmoebaVdwParameters`
- def `forcebalance.openmmio.CopyAmoebaMultipoleParameters`
- def `forcebalance.openmmio.CopyHarmonicBondParameters`
- def `forcebalance.openmmio.CopyHarmonicAngleParameters`
- def `forcebalance.openmmio.CopyPeriodicTorsionParameters`
- def `forcebalance.openmmio.CopyNonbondedParameters`
- def `forcebalance.openmmio.do_nothing`
- def `forcebalance.openmmio.CopySystemParameters`
Copy parameters from one system (i.e.
- def `forcebalance.openmmio.UpdateSimulationParameters`
- def `forcebalance.openmmio.SetAmoebaVirtualExclusions`
- def `forcebalance.openmmio.MTSVVVRIntegrator`
Create a multiple timestep velocity verlet with velocity randomization (VVVR) integrator.

Variables

- tuple `forcebalance.openmmio.logger` = getLogger(__name__)
- dictionary `forcebalance.openmmio.suffix_dict`
- string `forcebalance.openmmio.pdict` = "XML_Override"
pdict is a useless variable if the force field is XML.

9.26 optimizer.py File Reference

Classes

- class `forcebalance.optimizer.Optimizer`
Optimizer class.

Namespaces

- `forcebalance.optimizer`
Optimization algorithms.

Functions

- def `forcebalance.optimizer.Counter`
- def `forcebalance.optimizer.First`
- def `forcebalance.optimizer.GoodStep`

Variables

- tuple `forcebalance.optimizer.logger` = getLogger(__name__)
- int `forcebalance.optimizer.ITERATION` = 0
- int `forcebalance.optimizer.GOODSTEP` = 0
- int `forcebalance.optimizer.ITERINIT` = 0

9.27 output.py File Reference

Classes

- class `forcebalance.output.ForceBalanceLogger`

This logger starts out with a default handler that writes to stdout addHandler removes this default the first time another handler is added.
- class `forcebalance.output.RawStreamHandler`

Exactly like output.StreamHandler except it does no extra formatting before sending logging messages to the stream.
- class `forcebalance.output.RawFileHandler`

Exactly like output.FileHandler except it does no extra formatting before sending logging messages to the file.
- class `forcebalance.output.CleanStreamHandler`

Similar to RawStreamHandler except it does not write terminal escape codes.
- class `forcebalance.output.CleanFileHandler`

File handler that does not write terminal escape codes and carriage returns to files.
- class `forcebalance.output.ModLogger`

Namespaces

- `forcebalance.output`

9.28 parser.py File Reference

Namespaces

- `forcebalance.parser`

Input file parser for ForceBalance jobs.

Functions

- def `forcebalance.parser.read_mvals`
- def `forcebalance.parser.read_pvals`
- def `forcebalance.parser.read_priors`
- def `forcebalance.parser.read_internals`
- def `forcebalance.parser.printsection`

Print out a section of the input file in a parser-compliant and readable format.
- def `forcebalance.parser.parse_inputs`

Parse through the input file and read all user-supplied options.

Variables

- tuple `forcebalance.parser.logger` = getLogger(__name__)
- dictionary `forcebalance.parser.gen_opts_types`

Default general options.
- dictionary `forcebalance.parser.tgt_opts_types`

Default fitting target options.
- tuple `forcebalance.parser.all_opts_names` = list(itertools.chain(*[i.keys() for i in gen_opts_types.values()]))
- list `forcebalance.parser.iocc` = []

Check for uniqueness of option names.
- dictionary `forcebalance.parser.gen_opts_defaults` = {}

Default general options - basically a collapsed version of gen_opts_types.
- dictionary `forcebalance.parser.subdict` = {}

- dictionary `forcebalance.parser.tgt_opts_defaults = {}`
Default target options - basically a collapsed version of tgt_opts_types.
- dictionary `forcebalance.parser.bkwd`
Option maps for maintaining backward compatibility.
- list `forcebalance.parser.mainsections = ["SIMULATION","TARGET","OPTIONS","END","NONE"]`
Listing of sections in the input file.
- dictionary `forcebalance.parser.ParsTab`
ParsTab that refers to subsection parsers.

9.29 psi4io.py File Reference

Classes

- class `forcebalance.psi4io.GBS_Reader`
Interaction type -> Parameter Dictionary.
- class `forcebalance.psi4io.THCDF_Psi4`
- class `forcebalance.psi4io.Grid_Reader`
Finite state machine for parsing DVR grid files.
- class `forcebalance.psi4io.RDVR3_Psi4`
Subclass of Target for R-DVR3 grid fitting.

Namespaces

- `forcebalance.psi4io`
PSI4 force field input/output.

Variables

- tuple `forcebalance.psi4io.logger = getLogger(__name__)`

9.30 PT.py File Reference

Namespaces

- `forcebalance.PT`

Variables

- dictionary `forcebalance.PT.PeriodicTable`
- list `forcebalance.PT.Elements`

9.31 qchemio.py File Reference

Classes

- class `forcebalance.qchemio.QCIn_Reader`
Finite state machine for parsing Q-Chem input files.

Namespaces

- `forcebalance.qchemio`
Q-Chem input file parser.

Functions

- def `forcebalance.qchemio.QChem_Dielectric_Energy`

Variables

- tuple `forcebalance.qchemio.logger` = getLogger(__name__)
- list `forcebalance.qchemio.ndtypes` = [None]
Types of counterpoise correction cptypes = [None, 'BASS', 'BASSP'] Types of NDDO correction.
- dictionary `forcebalance.qchemio.pdict`
Section -> Interaction type dictionary.

9.32 quantity.py File Reference

Classes

- class `forcebalance.quantity.Quantity`
Base class for thermodynamical quantity used for fitting.
- class `forcebalance.quantity.Quantity_Density`
- class `forcebalance.quantity.Quantity_H_vap`

Namespaces

- `forcebalance.quantity`

Functions

- def `forcebalance.quantity.mean_stderr`
Return mean and standard deviation of a time series ts.
- def `forcebalance.quantity.energy_derivatives`
Compute the first derivatives of a set of snapshot energies with respect to the force field parameters.

Variables

- tuple `forcebalance.quantity.logger` = getLogger(__name__)

9.33 target.py File Reference

Classes

- class `forcebalance.target.Target`
Base class for all fitting targets.
- class `forcebalance.target.RemoteTarget`

Namespaces

- `forcebalance.target`

Variables

- tuple `forcebalance.target.logger` = getLogger(__name__)

9.34 thermo.py File Reference

Classes

- class `forcebalance.thermo.Thermo`
A target for fitting general experimental data sets.
- class `forcebalance.thermo.Point`

Namespaces

- `forcebalance.thermo`

Variables

- tuple `forcebalance.thermo.logger` = getLogger(`_name_`)

9.35 tinkerio.py File Reference

Classes

- class `forcebalance.tinkerio.Tinker_Reader`
Finite state machine for parsing `TINKER` force field files.
- class `forcebalance.tinkerio.TINKER`
Engine for carrying out general purpose `TINKER` calculations.
- class `forcebalance.tinkerio.Liquid_TINKER`
Condensed phase property matching using `TINKER`.
- class `forcebalance.tinkerio.AbInitio_TINKER`
Subclass of Target for force and energy matching using `TINKER`.
- class `forcebalance.tinkerio.BindingEnergy_TINKER`
Binding energy matching using `TINKER`.
- class `forcebalance.tinkerio.Interaction_TINKER`
Subclass of Target for interaction matching using `TINKER`.
- class `forcebalance.tinkerio.Moments_TINKER`
Subclass of Target for multipole moment matching using `TINKER`.
- class `forcebalance.tinkerio.Vibration_TINKER`
Vibrational frequency matching using `TINKER`.

Namespaces

- `forcebalance.tinkerio`
`TINKER` input/output.

Functions

- def `forcebalance.tinkerio.write_key`
Create or edit a `TINKER` .key file.

Variables

- list `forcebalance.tinkerio.allp`
- list `forcebalance.tinkerio.eckeys`
- tuple `forcebalance.tinkerio.logger` = getLogger(`_name_`)
- dictionary `forcebalance.tinkerio.pdict`

9.36 vibration.py File Reference

Classes

- class `forcebalance.vibration.Vibration`

Subclass of Target for fitting force fields to vibrational spectra (from experiment or theory).

Namespaces

- `forcebalance.vibration`

Vibrational mode fitting module.

Functions

- def `forcebalance.vibration.count_assignment`

Variables

- tuple `forcebalance.vibration.logger` = getLogger(`_name_`)

Index

`_add_`
 `forcebalance::molecule::Molecule`, 543
`_delitem_`
 `forcebalance::molecule::Molecule`, 543
`_enter_`
 `forcebalance::nifty::LineChunker`, 409
`_eq_`
 `forcebalance::forcefield::FF`, 296
 `forcebalance::molecule::MyG`, 621
`_exit_`
 `forcebalance::nifty::LineChunker`, 409
`_getattr_`
 `forcebalance::molecule::Molecule`, 543
`_getitem_`
 `forcebalance::molecule::Molecule`, 543
`_hash_`
 `forcebalance::molecule::MyG`, 621
`_iadd_`
 `forcebalance::molecule::Molecule`, 544
`_init_`
 `forcebalance::abinitio::AbInitio`, 79
 `forcebalance::abinitio_internal::AbInitio_Internal`, 146
 `forcebalance::amberio::AbInitio_AMBER`, 102
 `forcebalance::amberio::FrcMod_Reader`, 309
 `forcebalance::amberio::Mol2_Reader`, 537
 `forcebalance::BaseClass`, 209
 `forcebalance::BaseReader`, 211
 `forcebalance::binding::BindingEnergy`, 215
 `forcebalance::counterpoise::Counterpoise`, 277
 `forcebalance::custom_io::Gen_Reader`, 315
 `forcebalance::engine::Engine`, 292
 `forcebalance::forcefield::BackedUpDict`, 207
 `forcebalance::forcefield::FF`, 295
 `forcebalance::gmxio::AbInitio_GMX`, 124
 `forcebalance::gmxio::BindingEnergy_GMX`, 230
 `forcebalance::gmxio::GMX`, 319
 `forcebalance::gmxio::Interaction_GMX`, 348
 `forcebalance::gmxio::ITP_Reader`, 392
 `forcebalance::gmxio::Lipid_GMX`, 433
 `forcebalance::gmxio::Liquid_GMX`, 468
 `forcebalance::gmxio::Moments_GMX`, 578
 `forcebalance::gmxio::Thermo_GMX`, 751
 `forcebalance::gmxio::Vibration_GMX`, 795
 `forcebalance::interaction::Interaction`, 333
 `forcebalance::leastsq::LeastSquares`, 397
 `forcebalance::lipid::Lipid`, 414
 `forcebalance::liquid::Liquid`, 450
 `forcebalance::Mol2::mol2`, 524
 `forcebalance::Mol2::mol2_atom`, 528
 `forcebalance::Mol2::mol2_bond`, 531
 `forcebalance::Mol2::mol2_set`, 538

`forcebalance::mol2io::Mol2_Reader`, 534
`forcebalance::molecule::Molecule`, 543
`forcebalance::molecule::MyG`, 621
`forcebalance::moments::Moments`, 563
`forcebalance::nifty::LineChunker`, 409
`forcebalance::nifty::Pickler_LP`, 657
`forcebalance::nifty::Unpickler_LP`, 777
`forcebalance::objective::Objective`, 624
`forcebalance::objective::Penalty`, 654
`forcebalance::openmmio::AbInitio_OpenMM`, 168
`forcebalance::openmmio::BindingEnergy_OpenMM`, 245
`forcebalance::openmmio::Interaction_OpenMM`, 363
`forcebalance::openmmio::Liquid_OpenMM`, 488
`forcebalance::openmmio::Moments_OpenMM`, 593
`forcebalance::openmmio::OpenMM`, 629
`forcebalance::openmmio::OpenMM_Reader`, 638
`forcebalance::optimizer::Optimizer`, 642
`forcebalance::output::CleanStreamHandler`, 273
`forcebalance::output::ForceBalanceLogger`, 307
`forcebalance::output::RawStreamHandler`, 670
`forcebalance::psi4io::GBS_Reader`, 312
`forcebalance::psi4io::Grid_Reader`, 329
`forcebalance::psi4io::RDVR3_Psi4`, 674
`forcebalance::psi4io::THCDF_Psi4`, 718
`forcebalance::qcchemio::QCIn_Reader`, 661
`forcebalance::quantity::Quantity`, 664
`forcebalance::quantity::Quantity_Density`, 666
`forcebalance::quantity::Quantity_H_vap`, 668
`forcebalance::target::RemoteTarget`, 690
`forcebalance::target::Target`, 704
`forcebalance::thermo::Point`, 659
`forcebalance::thermo::Thermo`, 735
`forcebalance::tinkerio::AbInitio_TINKER`, 190
`forcebalance::tinkerio::BindingEnergy_TINKER`, 260
`forcebalance::tinkerio::Interaction_TINKER`, 378
`forcebalance::tinkerio::Liquid_TINKER`, 507
`forcebalance::tinkerio::Moments_TINKER`, 608
`forcebalance::tinkerio::TINKER`, 767
`forcebalance::tinkerio::Tinker_Reader`, 775
`forcebalance::tinkerio::Vibration_TINKER`, 810
`forcebalance::vibration::Vibration`, 781

`_init_.py`, 822
`_iter_`
 `forcebalance::molecule::Molecule`, 544
`_len_`
 `forcebalance::molecule::Molecule`, 544
`_missing_`
 `forcebalance::forcefield::BackedUpDict`, 207
`_repr_`
 `forcebalance::Mol2::mol2`, 524

forcebalance::Mol2::mol2_atom, 528
 forcebalance::Mol2::mol2_bond, 531
 __setattr__
 forcebalance::abinitio::AbInitio, 79
 forcebalance::abinitio_internal::AbInitio_Internal, 146
 forcebalance::amberio::AbInitio_AMBER, 102
 forcebalance::BaseClass, 209
 forcebalance::binding::BindingEnergy, 215
 forcebalance::counterpoise::Counterpoise, 277
 forcebalance::engine::Engine, 292
 forcebalance::forcefield::FF, 296
 forcebalance::gmxio::AbInitio_GMX, 124
 forcebalance::gmxio::BindingEnergy_GMX, 230
 forcebalance::gmxio::GMX, 319
 forcebalance::gmxio::Interaction_GMX, 349
 forcebalance::gmxio::Lipid_GMX, 433
 forcebalance::gmxio::Liquid_GMX, 468
 forcebalance::gmxio::Moments_GMX, 578
 forcebalance::gmxio::Thermo_GMX, 751
 forcebalance::gmxio::Vibration_GMX, 795
 forcebalance::interaction::Interaction, 333
 forcebalance::leastsq::LeastSquares, 397
 forcebalance::lipid::Lipid, 415
 forcebalance::liquid::Liquid, 450
 forcebalance::molecule::Molecule, 544
 forcebalance::moments::Moments, 563
 forcebalance::objective::Objective, 624
 forcebalance::openmmio::AbInitio_OpenMM, 168
 forcebalance::openmmio::BindingEnergy_OpenMM,
 245
 forcebalance::openmmio::Interaction_OpenMM, 364
 forcebalance::openmmio::Liquid_OpenMM, 488
 forcebalance::openmmio::Moments_OpenMM, 593
 forcebalance::openmmio::OpenMM, 629
 forcebalance::optimizer::Optimizer, 642
 forcebalance::psi4io::RDVR3_Psi4, 674
 forcebalance::psi4io::THCDF_Psi4, 718
 forcebalance::target::RemoteTarget, 690
 forcebalance::target::Target, 704
 forcebalance::thermo::Thermo, 735
 forcebalance::tinkerio::AbInitio_TINKER, 190
 forcebalance::tinkerio::BindingEnergy_TINKER, 260
 forcebalance::tinkerio::Interaction_TINKER, 379
 forcebalance::tinkerio::Liquid_TINKER, 507
 forcebalance::tinkerio::Moments_TINKER, 608
 forcebalance::tinkerio::TINKER, 767
 forcebalance::tinkerio::Vibration_TINKER, 810
 forcebalance::vibration::Vibration, 781
 __str__
 forcebalance::quantity::Quantity, 664
 forcebalance::quantity::Quantity_Density, 666
 forcebalance::quantity::Quantity_H_vap, 668
 forcebalance::thermo::Point, 659
 __version__
 forcebalance, 15

A

forcebalance::chemistry, 20
 forcebalance::openmmio::OpenMM, 635
 forcebalance::tinkerio::TINKER, 772

a

forcebalance::objective::Penalty, 656

AMOEBA

forcebalance::openmmio::OpenMM, 635

AStr

forcebalance::molecule::MyG, 621

abinitio.py, 822

abinitio_internal.py, 823

abskey

forcebalance::tinkerio::TINKER, 772

absrd

forcebalance::abinitio::AbInitio, 79
 forcebalance::abinitio_internal::AbInitio_Internal, 146
 forcebalance::amberio::AbInitio_AMBER, 102
 forcebalance::binding::BindingEnergy, 215
 forcebalance::counterpoise::Counterpoise, 277
 forcebalance::gmxio::AbInitio_GMX, 124
 forcebalance::gmxio::BindingEnergy_GMX, 230
 forcebalance::gmxio::Interaction_GMX, 349
 forcebalance::gmxio::Lipid_GMX, 433
 forcebalance::gmxio::Liquid_GMX, 468
 forcebalance::gmxio::Moments_GMX, 578
 forcebalance::gmxio::Thermo_GMX, 751
 forcebalance::gmxio::Vibration_GMX, 795
 forcebalance::interaction::Interaction, 333
 forcebalance::leastsq::LeastSquares, 397
 forcebalance::lipid::Lipid, 415
 forcebalance::liquid::Liquid, 450
 forcebalance::moments::Moments, 563
 forcebalance::openmmio::AbInitio_OpenMM, 168
 forcebalance::openmmio::BindingEnergy_OpenMM,
 245
 forcebalance::openmmio::Interaction_OpenMM, 364
 forcebalance::openmmio::Liquid_OpenMM, 488
 forcebalance::openmmio::Moments_OpenMM, 593
 forcebalance::psi4io::RDVR3_Psi4, 674
 forcebalance::psi4io::THCDF_Psi4, 718
 forcebalance::target::RemoteTarget, 690
 forcebalance::target::Target, 704
 forcebalance::thermo::Thermo, 735
 forcebalance::tinkerio::AbInitio_TINKER, 190
 forcebalance::tinkerio::BindingEnergy_TINKER, 260
 forcebalance::tinkerio::Interaction_TINKER, 379
 forcebalance::tinkerio::Liquid_TINKER, 507
 forcebalance::tinkerio::Moments_TINKER, 608
 forcebalance::tinkerio::Vibration_TINKER, 810
 forcebalance::vibration::Vibration, 781

add_quantum

```

    forcebalance::molecule::Molecule, 544
add_strip_to_mat
    forcebalance::molecule, 38
add_virtual_site
    forcebalance::molecule::Molecule, 544
addHandler
    forcebalance::output::ForceBalanceLogger, 307
addff
    forcebalance::forcefield::FF, 296
addff_txt
    forcebalance::forcefield::FF, 297
addff_xml
    forcebalance::forcefield::FF, 298
adict
    forcebalance::amberio::FrcMod_Reader, 310
    forcebalance::amberio::Mol2_Reader, 537
    forcebalance::BaseReader, 212
    forcebalance::custom_io::Gen_Reader, 316
    forcebalance::gmxio::ITP_Reader, 393
    forcebalance::mol2io::Mol2_Reader, 534
    forcebalance::openmmio::OpenMM_Reader, 639
    forcebalance::psi4io::GBS_Reader, 313
    forcebalance::psi4io::Grid_Reader, 329
    forcebalance::qchemio::QCIn_Reader, 662
    forcebalance::tinkerio::Tinker_Reader, 776
adjh
    forcebalance::optimizer::Optimizer, 642
aftypes
    forcebalance::gmxio, 32
align
    forcebalance::molecule::Molecule, 544
align_by_moments
    forcebalance::molecule::Molecule, 545
align_center
    forcebalance::molecule::Molecule, 545
AlignToDensity
    forcebalance::molecule, 38
AlignToMoments
    forcebalance::molecule, 38
Alive
    forcebalance::molecule::MyG, 622
all_at_once
    forcebalance::amberio::AbInitio_AMBER, 114
all_opts_names
    forcebalance::parser, 66
all_pairwise_rmsd
    forcebalance::molecule::Molecule, 545
AllResults
    forcebalance::gmxio::Liquid_GMX, 481
    forcebalance::liquid::Liquid, 462
    forcebalance::openmmio::Liquid_OpenMM, 500
    forcebalance::tinkerio::Liquid_TINKER, 520
AllVariableNames
    forcebalance::molecule, 42
allp
    forcebalance::tinkerio, 73
allsplit
    forcebalance::nifty, 47
amberio.py, 823
amom
    forcebalance::psi4io::GBS_Reader, 313
Anneal
    forcebalance::optimizer::Optimizer, 642
api.dox, 823
append
    forcebalance::molecule::Molecule, 546
assign_field
    forcebalance::forcefield::FF, 299
assign_p0
    forcebalance::forcefield::FF, 299
astr
    forcebalance::nifty, 47
atom
    forcebalance::amberio::FrcMod_Reader, 310
    forcebalance::amberio::Mol2_Reader, 537
    forcebalance::mol2io::Mol2_Reader, 534
    forcebalance::qchemio::QCIn_Reader, 662
    forcebalance::tinkerio::Tinker_Reader, 776
atom_distances
    forcebalance::contact, 21
atom_id
    forcebalance::Mol2::mol2_atom, 530
atom_name
    forcebalance::Mol2::mol2_atom, 530
atom_select
    forcebalance::molecule::Molecule, 546
atom_stack
    forcebalance::molecule::Molecule, 546
atom_type
    forcebalance::Mol2::mol2_atom, 530
AtomLists
    forcebalance::abinitio::AbInitio, 92
    forcebalance::abinitio_internal::AbInitio_Internal, 158
    forcebalance::amberio::AbInitio_AMBER, 114
    forcebalance::gmxio::AbInitio_GMX, 136
    forcebalance::gmxio::GMX, 325
    forcebalance::openmmio::AbInitio_OpenMM, 180
    forcebalance::openmmio::OpenMM, 635
    forcebalance::tinkerio::AbInitio_TINKER, 202
    forcebalance::tinkerio::TINKER, 772
AtomMask
    forcebalance::abinitio::AbInitio, 92
    forcebalance::abinitio_internal::AbInitio_Internal, 158
    forcebalance::amberio::AbInitio_AMBER, 114
    forcebalance::gmxio::AbInitio_GMX, 136
    forcebalance::gmxio::GMX, 325
    forcebalance::openmmio::AbInitio_OpenMM, 180
    forcebalance::openmmio::OpenMM, 635

```

forcebalance::tinkerio::AbInitio_TINKER, 202
 forcebalance::tinkerio::TINKER, 772
AtomTypes
 forcebalance::amberio::FrcMod_Reader, 310
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 212
 forcebalance::custom.io::Gen_Reader, 316
 forcebalance::gmxio::ITP_Reader, 393
 forcebalance::mol2io::Mol2_Reader, 535
 forcebalance::openmmio::OpenMM_Reader, 639
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
 forcebalance::qchemio::QCIn_Reader, 662
 forcebalance::tinkerio::Tinker_Reader, 776
AtomVariableNames
 forcebalance::molecule, 42
atomnames
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::forcefield::FF, 304
 forcebalance::gmxio::ITP_Reader, 393
atoms
 forcebalance::chemistry, 20
 forcebalance::Mol2::mol2, 527
atomtype_to_mass
 forcebalance::gmxio::ITP_Reader, 393
atomtypes
 forcebalance::gmxio::ITP_Reader, 393
B
 forcebalance::chemistry, 20
 forcebalance::openmmio::OpenMM, 635
 forcebalance::tinkerio::TINKER, 772
b
 forcebalance::objective::Penalty, 656
BE
 forcebalance::chemistry, 20
BFGS
 forcebalance::optimizer::Optimizer, 643
backup_dict
 forcebalance::forcefield::BackedUpDict, 207
bak
 forcebalance::nifty, 47
bakdir
 forcebalance::optimizer::Optimizer, 651
BasinHopping
 forcebalance::optimizer::Optimizer, 643
basis_number
 forcebalance::psi4io::GBS_Reader, 313
bftypes
 forcebalance::gmxio, 32
bhyp
 forcebalance::optimizer::Optimizer, 651
bidirect
 forcebalance::psi4io::RDVR3_Psi4, 685
binding.py, 823
bkwd
 forcebalance::parser, 66
bo
 forcebalance::chemistry, 20
bohrang
 forcebalance::molecule, 42
 forcebalance::nifty, 56
boltz_wts
 forcebalance::abinitio::AbInitio, 92
 forcebalance::abinitio.internal::AbInitio_Internal, 158
 forcebalance::amberio::AbInitio_AMBER, 114
 forcebalance::gmxio::AbInitio_GMX, 136
 forcebalance::openmmio::AbInitio_OpenMM, 180
 forcebalance::tinkerio::AbInitio_TINKER, 202
bond_id
 forcebalance::Mol2::mol2_bond, 532
bond_type
 forcebalance::Mol2::mol2_bond, 532
BondChars
 forcebalance::chemistry, 20
BondEnergies
 forcebalance::chemistry, 20
BondStrengthByLength
 forcebalance::chemistry, 20
bonds
 forcebalance::Mol2::mol2, 527
both
 forcebalance::molecule, 39
Box
 forcebalance::molecule, 42
boxes
 forcebalance::molecule::Molecule, 558
buf
 forcebalance::nifty::LineChunker, 410
build_invdist
 forcebalance::abinitio::AbInitio, 80
 forcebalance::abinitio.internal::AbInitio_Internal, 146
 forcebalance::amberio::AbInitio_AMBER, 102
 forcebalance::gmxio::AbInitio_GMX, 124
 forcebalance::openmmio::AbInitio_OpenMM, 168
 forcebalance::tinkerio::AbInitio_TINKER, 190
build_objective
 forcebalance::abinitio, 16
build_pid
 forcebalance::amberio::FrcMod_Reader, 309
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 211
 forcebalance::custom.io::Gen_Reader, 315
 forcebalance::gmxio::ITP_Reader, 392
 forcebalance::mol2io::Mol2_Reader, 534
 forcebalance::openmmio::OpenMM_Reader, 638
 forcebalance::psi4io::GBS_Reader, 312
 forcebalance::psi4io::Grid_Reader, 329

forcebalance::qchemio::QCIn_Reader, 661
 forcebalance::tinkerio::Tinker_Reader, 775
build_topology
 forcebalance::molecule::Molecule, 546
BuildLatticeFromLengthsAngles
 forcebalance::molecule, 39
BuildLatticeFromVectors
 forcebalance::molecule, 39
built_bonds
 forcebalance::molecule::Molecule, 558

c2r
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
CHECK_BASIS
 forcebalance::leastsq, 34
calc_eigvals
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
calc_moments
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::moments::Moments, 573
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::tinkerio::Moments_TINKER, 618
calc_scd
 forcebalance::gmxio::GMX, 319
callback
 forcebalance::nifty::LineChunker, 410
callderivs
 forcebalance::psi4io::RDVR3_Psi4, 685
callgmx
 forcebalance::gmxio::GMX, 319
calltinker
 forcebalance::tinkerio::TINKER, 767
cartesian_product2
 forcebalance::molecule, 39
center_of_mass
 forcebalance::molecule::Molecule, 546
charge
 forcebalance::Mol2::mol2_atom, 530
charge_type
 forcebalance::Mol2::mol2, 527
check_files
 forcebalance::abinitio::AbInitio, 80
 forcebalance::abinitio_internal::AbInitio_Internal, 146
 forcebalance::amberio::AbInitio_AMBER, 102
 forcebalance::binding::BindingEnergy, 216
 forcebalance::counterpoise::Counterpoise, 278
 forcebalance::gmxio::AbInitio_GMX, 124
 forcebalance::gmxio::BindingEnergy_GMX, 231
 forcebalance::gmxio::Interaction_GMX, 349
 forcebalance::gmxio::Lipid_GMX, 433

 forcebalance::gmxio::Liquid_GMX, 468
 forcebalance::gmxio::Moments_GMX, 579
 forcebalance::gmxio::Thermo_GMX, 752
 forcebalance::gmxio::Vibration_GMX, 796
 forcebalance::interaction::Interaction, 334
 forcebalance::leastsq::LeastSquares, 397
 forcebalance::lipid::Lipid, 415
 forcebalance::liquid::Liquid, 450
 forcebalance::moments::Moments, 564
 forcebalance::openmmio::AbInitio_OpenMM, 168
 forcebalance::openmmio::BindingEnergy_OpenMM,
 246
 forcebalance::openmmio::Interaction_OpenMM, 364
 forcebalance::openmmio::Liquid_OpenMM, 488
 forcebalance::openmmio::Moments_OpenMM, 594
 forcebalance::psi4io::RDVR3_Psi4, 675
 forcebalance::psi4io::THCDF_Psi4, 719
 forcebalance::target::RemoteTarget, 690
 forcebalance::target::Target, 705
 forcebalance::thermo::Thermo, 736
 forcebalance::tinkerio::AbInitio_TINKER, 190
 forcebalance::tinkerio::BindingEnergy_TINKER, 261
 forcebalance::tinkerio::Interaction_TINKER, 379
 forcebalance::tinkerio::Liquid_TINKER, 507
 forcebalance::tinkerio::Moments_TINKER, 609
 forcebalance::tinkerio::Vibration_TINKER, 811
 forcebalance::vibration::Vibration, 781
CheckBasis
 forcebalance::leastsq, 34
chemistry.py, 824
chk
 forcebalance::optimizer::Optimizer, 651
click
 forcebalance::nifty, 47
close
 forcebalance::nifty::LineChunker, 409
cnum
 forcebalance::qchemio::QCIn_Reader, 662
col
 forcebalance::nifty, 47
commadash
 forcebalance::nifty, 47
comments
 forcebalance::Mol2::mol2, 527
 forcebalance::Mol2::mol2_set, 538
comms
 forcebalance::molecule::Molecule, 558
compounds
 forcebalance::Mol2::mol2_set, 538
compute
 forcebalance::objective::Penalty, 654
compute_mass
 forcebalance::openmmio::OpenMM, 629
compute_netforce_torque

forcebalance::abinitio::AbInitio, 80
 forcebalance::abinitio_internal::AbInitio_Internal, 146
 forcebalance::amberio::AbInitio_AMBER, 102
 forcebalance::gmxio::AbInitio_GMX, 124
 forcebalance::openmmio::AbInitio_OpenMM, 168
 forcebalance::tinkerio::AbInitio_TINKER, 190
 compute_volume
 forcebalance::openmmio::OpenMM, 629
 ComputeOverlap
 forcebalance::molecule, 39
 concurrent_map
 forcebalance::nifty, 47
 ConjugateGradient
 forcebalance::optimizer::Optimizer, 643
 contact.py, 824
 contraction_number
 forcebalance::psi4io::GBS_Reader, 313
 coords
 forcebalance::abinitio_internal::AbInitio_Internal, 158
 forcebalance::amberio::AbInitio_AMBER, 114
 CopyAmoebaAngleParameters
 forcebalance::openmmio, 59
 CopyAmoebaBondParameters
 forcebalance::openmmio, 59
 CopyAmoebaInPlaneAngleParameters
 forcebalance::openmmio, 59
 CopyAmoebaMultipoleParameters
 forcebalance::openmmio, 59
 CopyAmoebaOutOfPlaneBendParameters
 forcebalance::openmmio, 59
 CopyAmoebaVdwParameters
 forcebalance::openmmio, 59
 CopyFile
 forcebalance::nifty, 47
 CopyHarmonicAngleParameters
 forcebalance::openmmio, 59
 CopyHarmonicBondParameters
 forcebalance::openmmio, 60
 CopyNonbondedParameters
 forcebalance::openmmio, 60
 CopyPeriodicTorsionParameters
 forcebalance::openmmio, 60
 CopySystemParameters
 forcebalance::openmmio, 60
 count_assignment
 forcebalance::vibration, 74
 Counter
 forcebalance::optimizer, 62
 counterpoise.py, 825
 cpqm
 forcebalance::counterpoise::Counterpoise, 289
 cotypes
 forcebalance::custom_io, 23
 create_mvals
 forcebalance::forcefield::FF, 299
 create_pvals
 forcebalance::forcefield::FF, 300
 create_simulation
 forcebalance::openmmio::OpenMM, 629
 createWorkQueue
 forcebalance::nifty, 48
 CubicLattice
 forcebalance::molecule, 39
 custom_io.py, 825

D

forcebalance::leastsq::LeastSquares, 407
 forcebalance::psi4io::THCDF_Psi4, 730
 DATfnm
 forcebalance::psi4io::THCDF_Psi4, 730
 DF_Energy
 forcebalance::psi4io::THCDF_Psi4, 730
 Data
 forcebalance::molecule::Molecule, 558
 data
 forcebalance::Mol2, 36
 forcebalance::thermo::Point, 659
 data_from_web
 forcebalance::chemistry, 20
 defaultHandler
 forcebalance::output::ForceBalanceLogger, 307
 denoms
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Thermo_GMX, 762
 forcebalance::moments::Moments, 573
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::thermo::Thermo, 745
 forcebalance::tinkerio::Moments_TINKER, 618
 destroy
 forcebalance::psi4io::GBS_Reader, 313
 destroyWorkQueue
 forcebalance::nifty, 48
 determine_fftype
 forcebalance::forcefield, 28
 dftypes
 forcebalance::gmxio, 32
 diff
 forcebalance::molecule, 39
 dihe
 forcebalance::amberio::FrcMod_Reader, 310
 divisor
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::tinkerio::Interaction_TINKER, 388
 do_nothing
 forcebalance::openmmio, 60
 do_self_pol

forcebalance::gmxio::Lipid_GMX, 444
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::lipid::Lipid, 426
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
double
 forcebalance::gmxio::GMX, 326
driver
 forcebalance::psi4io::RDVR3_Psi4, 675
 forcebalance::psi4io::THCDF_Psi4, 719
dx
 forcebalance::optimizer::Optimizer, 652
DynDict
 forcebalance::tinkerio::Liquid_TINKER, 520
DynDict_New
 forcebalance::tinkerio::Liquid_TINKER, 520
e
 forcebalance::molecule::MyG, 621
e_err
 forcebalance::abinitio::AbInitio, 92
 forcebalance::abinitio_internal::AbInitio_Internal, 158
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 136
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::AbInitio_OpenMM, 180
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::tinkerio::AbInitio_TINKER, 202
 forcebalance::tinkerio::Interaction_TINKER, 388
e_err_pct
 forcebalance::abinitio::AbInitio, 92
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 136
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::AbInitio_OpenMM, 180
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::tinkerio::AbInitio_TINKER, 202
 forcebalance::tinkerio::Interaction_TINKER, 388
e_ref
 forcebalance::abinitio::AbInitio, 92
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 136
 forcebalance::openmmio::AbInitio_OpenMM, 180
 forcebalance::tinkerio::AbInitio_TINKER, 202
eckeys
 forcebalance::tinkerio, 73
edit_qcrems
 forcebalance::molecule::Molecule, 546
ef

forcebalance::molecule::MyG, 621
either
 forcebalance::molecule, 39
elem_from_atomname
 forcebalance::molecule, 39
element
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
Elements
 forcebalance::chemistry, 20
 forcebalance::molecule, 42
 forcebalance::psi4io::THCDF_Psi4, 730
 forcebalance::PT, 68
elements
 forcebalance::psi4io::RDVR3_Psi4, 685
emd0
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
emit
 forcebalance::output::CleanFileHandler, 272
 forcebalance::output::CleanStreamHandler, 274
 forcebalance::output::RawFileHandler, 669
 forcebalance::output::RawStreamHandler, 671
emm
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::tinkerio::Interaction_TINKER, 388
encode
 forcebalance::nifty, 48
energy
 forcebalance::gmxio::GMX, 320
 forcebalance::openmmio::OpenMM, 629
 forcebalance::tinkerio::TINKER, 767
energy_all
 forcebalance::abinitio::AbInitio, 80
 forcebalance::abinitio_internal::AbInitio_Internal, 146
 forcebalance::amberio::AbInitio_AMBER, 102
 forcebalance::gmxio::AbInitio_GMX, 125
 forcebalance::openmmio::AbInitio_OpenMM, 169
 forcebalance::tinkerio::AbInitio_TINKER, 191
energy_components
 forcebalance::openmmio, 60
energy_derivatives
 forcebalance::quantity, 70
energy_dipole
 forcebalance::gmxio::GMX, 320
 forcebalance::openmmio::OpenMM, 630
 forcebalance::tinkerio::TINKER, 768
energy_force

forcebalance::gmxio::GMX, 320
 forcebalance::openmmio::OpenMM, 630
 forcebalance::tinkerio::TINKER, 768
energy_force_all
 forcebalance::abinitio::AbInitio, 80
 forcebalance::abinitio_internal::AbInitio_Internal, 147
 forcebalance::amberio::AbInitio_AMBER, 102
 forcebalance::gmxio::AbInitio_GMX, 125
 forcebalance::openmmio::AbInitio_OpenMM, 169
 forcebalance::tinkerio::AbInitio_TINKER, 191
energy_force_driver_all
 forcebalance::abinitio_internal::AbInitio_Internal, 147
 forcebalance::amberio::AbInitio_AMBER, 102
energy_force_driver_all_external
 forcebalance::amberio::AbInitio_AMBER, 103
energy_force_one
 forcebalance::abinitio::AbInitio, 80
 forcebalance::abinitio_internal::AbInitio_Internal, 147
 forcebalance::amberio::AbInitio_AMBER, 103
 forcebalance::gmxio::AbInitio_GMX, 125
 forcebalance::gmxio::GMX, 320
 forcebalance::openmmio::AbInitio_OpenMM, 169
 forcebalance::openmmio::OpenMM, 630
 forcebalance::tinkerio::AbInitio_TINKER, 191
 forcebalance::tinkerio::TINKER, 768
energy_force_transform
 forcebalance::abinitio::AbInitio, 80
 forcebalance::abinitio_internal::AbInitio_Internal, 147
 forcebalance::amberio::AbInitio_AMBER, 103
 forcebalance::gmxio::AbInitio_GMX, 125
 forcebalance::openmmio::AbInitio_OpenMM, 169
 forcebalance::tinkerio::AbInitio_TINKER, 191
energy_force_transform_one
 forcebalance::abinitio::AbInitio, 81
 forcebalance::abinitio_internal::AbInitio_Internal, 147
 forcebalance::amberio::AbInitio_AMBER, 103
 forcebalance::gmxio::AbInitio_GMX, 125
 forcebalance::openmmio::AbInitio_OpenMM, 169
 forcebalance::tinkerio::AbInitio_TINKER, 191
energy_one
 forcebalance::abinitio::AbInitio, 81
 forcebalance::abinitio_internal::AbInitio_Internal, 148
 forcebalance::amberio::AbInitio_AMBER, 104
 forcebalance::gmxio::AbInitio_GMX, 126
 forcebalance::gmxio::GMX, 321
 forcebalance::openmmio::AbInitio_OpenMM, 170
 forcebalance::openmmio::OpenMM, 631
 forcebalance::tinkerio::AbInitio_TINKER, 192
energy_part
 forcebalance::binding::BindingEnergy, 225
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::openmmio::BindingEnergy_OpenMM,
 255
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
energy_rmsd
 forcebalance::gmxio::GMX, 321
 forcebalance::openmmio::OpenMM, 631
 forcebalance::tinkerio::TINKER, 769
energy_termnames
 forcebalance::gmxio::GMX, 321
engine
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::interaction::Interaction, 343
 forcebalance::moments::Moments, 573
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::tinkerio::AbInitio_TINKER, 203
 forcebalance::tinkerio::Interaction_TINKER, 388
 forcebalance::tinkerio::Moments_TINKER, 618
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
engine.py, 825
engine
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::gmxio::Lipid_GMX, 444
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Thermo_GMX, 762
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::openmmio::BindingEnergy_OpenMM,
 255
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::tinkerio::AbInitio_TINKER, 203
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
 forcebalance::tinkerio::Interaction_TINKER, 388
 forcebalance::tinkerio::Liquid_TINKER, 520
 forcebalance::tinkerio::Moments_TINKER, 618
 forcebalance::tinkerio::Vibration_TINKER, 820
engines
 forcebalance::binding::BindingEnergy, 225
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::openmmio::BindingEnergy_OpenMM,
 255
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
engname
 forcebalance::gmxio::Lipid_GMX, 444

forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::gmxio::Thermo_GMX, 762
 forcebalance::lipid::Lipid, 426
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::quantity::Quantity, 664
 forcebalance::quantity::Quantity_Density, 666
 forcebalance::quantity::Quantity_H_vap, 668
 forcebalance::tinkerio::Liquid_TINKER, 520
eqcgmx
 forcebalance::nifty, 56
eqm
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::tinkerio::AbInitio_TINKER, 203
 forcebalance::tinkerio::Interaction_TINKER, 388
error
 forcebalance::output::ModLogger, 523
esp_err
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
espval
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
espxyz
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
EulerMatrix
 forcebalance::molecule, 40
evaluate_
 forcebalance::gmxio::GMX, 321
 forcebalance::openmmio::OpenMM, 631
 forcebalance::tinkerio::TINKER, 769
evaluate_one_
 forcebalance::openmmio::OpenMM, 632
evaluate_snapshot

forcebalance::gmxio::GMX, 322
evaluate_trajectory
 forcebalance::gmxio::GMX, 322
even_list
 forcebalance::molecule, 40
excision
 forcebalance::forcefield::FF, 304
 forcebalance::optimizer::Optimizer, 652
extra_output
 forcebalance::gmxio::Lipid_GMX, 444
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::lipid::Lipid, 426
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
extract
 forcebalance::quantity::Quantity, 664
 forcebalance::quantity::Quantity_Density, 666
 forcebalance::quantity::Quantity_H_vap, 668
extract_int
 forcebalance::nifty, 48
f12d3p
 forcebalance::finite_difference, 25
f12d7p
 forcebalance::finite_difference, 25
f1d2p
 forcebalance::finite_difference, 25
f1d5p
 forcebalance::finite_difference, 25
f1d7p
 forcebalance::finite_difference, 25
f2var
 forcebalance::finite_difference, 25
f_err
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
f_err_pct
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
f_ref
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181

forcebalance::tinkerio::AbInitio_TINKER, 203
FDCheckG
 forcebalance::optimizer::Optimizer, 644
FDCheckH
 forcebalance::optimizer::Optimizer, 644
FF
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::binding::BindingEnergy, 225
 forcebalance::counterpoise::Counterpoise, 289
 forcebalance::engine::Engine, 292
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::gmxio::GMX, 326
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::gmxio::Lipid_GMX, 444
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Thermo_GMX, 762
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::interaction::Interaction, 343
 forcebalance::leastsq::LeastSquares, 407
 forcebalance::lipid::Lipid, 426
 forcebalance::liquid::Liquid, 462
 forcebalance::moments::Moments, 573
 forcebalance::objective::Objective, 625
 forcebalance::objective::Penalty, 656
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::openmmio::BindingEnergy_OpenMM, 255
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::openmmio::OpenMM, 635
 forcebalance::optimizer::Optimizer, 652
 forcebalance::psi4io::RDVR3_Psi4, 685
 forcebalance::psi4io::THCDF_Psi4, 730
 forcebalance::target::RemoteTarget, 699
 forcebalance::target::Target, 714
 forcebalance::thermo::Thermo, 745
 forcebalance::tinkerio::AbInitio_TINKER, 203
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
 forcebalance::tinkerio::Interaction_TINKER, 388
 forcebalance::tinkerio::Liquid_TINKER, 520
 forcebalance::tinkerio::Moments_TINKER, 618
 forcebalance::tinkerio::TINKER, 772
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
FF_Extensions
 forcebalance::forcefield, 29
FF_IOModules
 forcebalance::forcefield, 29
FFAtomTypes

forcebalance::forcefield::FF, 304
FFMolecules
 forcebalance::forcefield::FF, 304
FUSE
 forcebalance::objective::Penalty, 654
FUSE_BARRIER
 forcebalance::objective::Penalty, 655
FUSE_L0
 forcebalance::objective::Penalty, 655
factor
 forcebalance::psi4io::RDVR3_Psi4, 685
fadd
 forcebalance::objective::Penalty, 656
failmsg
 forcebalance::optimizer::Optimizer, 652
fdict
 forcebalance::custom_io, 23
 forcebalance::gmxio, 32
fdwrap
 forcebalance::finite_difference, 25
fdwrap_G
 forcebalance::finite_difference, 26
fdwrap_H
 forcebalance::finite_difference, 26
feed
 forcebalance::amberio::FrcMod_Reader, 309
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 211
 forcebalance::custom_io::Gen_Reader, 315
 forcebalance::gmxio::ITP_Reader, 393
 forcebalance::mol2io::Mol2_Reader, 534
 forcebalance::openmmio::OpenMM_Reader, 638
 forcebalance::psi4io::GBS_Reader, 312
 forcebalance::psi4io::Grid_Reader, 329
 forcebalance::qchemio::QCIn_Reader, 661
 forcebalance::tinkerio::Tinker_Reader, 775
ffdata
 forcebalance::forcefield::FF, 304
ffdata_isxml
 forcebalance::forcefield::FF, 304
ffxml
 forcebalance::openmmio::OpenMM, 635
find_angles
 forcebalance::molecule::Molecule, 546
find_dihedrals
 forcebalance::molecule::Molecule, 547
find_spacings
 forcebalance::forcefield::FF, 300
finite_difference.py, 826
First
 forcebalance::optimizer, 62
fitatoms
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159

forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
 flat
 forcebalance::nifty, 48
 floatornan
 forcebalance::nifty, 48
 fmul
 forcebalance::objective::Penalty, 656
 force
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
 force_map
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
 forcebalance, 14
 ._version..., 15
 forcebalance.abinitio, 16
 forcebalance.abinitio.AbInitio, 75
 forcebalance.abinitio_internal, 16
 forcebalance.abinitio_internal.AbInitio_Internal, 140
 forcebalance.amberio, 17
 forcebalance.amberio.AbInitio_AMBER, 96
 forcebalance.amberio.FrcMod_Reader, 307
 forcebalance.amberio.Mol2_Reader, 535
 forcebalance.BaseClass, 207
 forcebalance.BaseReader, 209
 forcebalance.binding, 18
 forcebalance.binding.BindingEnergy, 212
 forcebalance.chemistry, 19
 forcebalance.contact, 21
 forcebalance.counterpoise, 22
 forcebalance.counterpoise.Counterpoise, 274
 forcebalance.custom_io, 23
 forcebalance.custom_io.Gen_Reader, 314
 forcebalance.engine, 24
 forcebalance.engine.Engine, 290
 forcebalance.finite_difference, 24
 forcebalance.forcefield, 27
 forcebalance.forcefield.BackedUpDict, 206
 forcebalance.forcefield.FF, 293
 forcebalance.gmxio, 29
 forcebalance.gmxio.AbInitio_GMX, 118
 forcebalance.gmxio.BindingEnergy_GMX, 226
 forcebalance.gmxio.GMX, 316
 forcebalance.gmxio.ITP_Reader, 390
 forcebalance.gmxio.Interaction_GMX, 345
 forcebalance.gmxio.Lipid_GMX, 429
 forcebalance.gmxio.Liquid_GMX, 464
 forcebalance.gmxio.Moments_GMX, 574
 forcebalance.gmxio.Thermo_GMX, 747
 forcebalance.gmxio.Vibration_GMX, 792
 forcebalance.interaction, 33
 forcebalance.interaction.Interaction, 330
 forcebalance.leastsq, 34
 forcebalance.leastsq.LeastSquares, 394
 forcebalance.lipid, 34
 forcebalance.lipid.Lipid, 410
 forcebalance.liquid, 35
 forcebalance.liquid.Liquid, 447
 forcebalance.Mol2, 36
 forcebalance.Mol2.mol2, 523
 forcebalance.Mol2.mol2_atom, 527
 forcebalance.Mol2.mol2_bond, 530
 forcebalance.Mol2.mol2_set, 538
 forcebalance.mol2io, 36
 forcebalance.mol2io.Mol2_Reader, 533
 forcebalance.molecule, 37
 forcebalance.molecule.Molecule, 539
 forcebalance.molecule.MolfileTimestep, 559
 forcebalance.molecule.MyG, 620
 forcebalance.moments, 44
 forcebalance.moments.Moments, 560
 forcebalance.nifty, 44
 forcebalance.nifty.LineChunker, 408
 forcebalance.nifty.Pickler_LP, 656
 forcebalance.nifty.Unpickler_LP, 776
 forcebalance.objective, 57
 forcebalance.objective.Objective, 622
 forcebalance.objective.Penalty, 653
 forcebalance.openmmio, 58
 forcebalance.openmmio.AbInitio_OpenMM, 162
 forcebalance.openmmio.BindingEnergy_OpenMM, 241
 forcebalance.openmmio.Interaction_OpenMM, 360
 forcebalance.openmmio.Liquid_OpenMM, 483
 forcebalance.openmmio.Moments_OpenMM, 589
 forcebalance.openmmio.OpenMM, 626
 forcebalance.openmmio.OpenMM_Reader, 637
 forcebalance.optimizer, 62
 forcebalance.optimizer.Optimizer, 639
 forcebalance.output, 63
 forcebalance.output.CleanFileHandler, 271
 forcebalance.output.CleanStreamHandler, 273
 forcebalance.output.ForceBalanceLogger, 306
 forcebalance.output.ModLogger, 522
 forcebalance.output.RawFileHandler, 669
 forcebalance.output.RawStreamHandler, 670
 forcebalance.PT, 68
 forcebalance.parser, 63

forcebalance.psi4io, 67
 forcebalance.psi4io.GBS_Reader, 310
 forcebalance.psi4io.Grid_Reader, 327
 forcebalance.psi4io.RDVR3_Psi4, 671
 forcebalance.psi4io.THCDF_Psi4, 715
 forcebalance.qchemio, 68
 forcebalance.qchemio.QCIn_Reader, 659
 forcebalance.quantity, 70
 forcebalance.quantity.Quantity, 662
 forcebalance.quantity.Quantity_Density, 665
 forcebalance.quantity.Quantity_H_vap, 667
 forcebalance.target, 71
 forcebalance.target.RemoteTarget, 687
 forcebalance.target.Target, 700
 forcebalance.thermo, 71
 forcebalance.thermo.Point, 658
 forcebalance.thermo.Thermo, 732
 forcebalance.tinkerio, 71
 forcebalance.tinkerio.ABInitio_TINKER, 184
 forcebalance.tinkerio.BindingEnergy_TINKER, 256
 forcebalance.tinkerio.Interaction_TINKER, 375
 forcebalance.tinkerio.Liquid_TINKER, 502
 forcebalance.tinkerio.Moments_TINKER, 604
 forcebalance.tinkerio.TINKER, 764
 forcebalance.tinkerio.Tinker_Reader, 773
 forcebalance.tinkerio.Vibration_TINKER, 807
 forcebalance.vibration, 74
 forcebalance.vibration.Vibration, 777
 forcebalance::BaseClass
 __init__, 209
 __setattr__, 209
 PrintOptionDict, 209
 set_option, 209
 verbose_options, 209
 forcebalance::BaseReader
 __init__, 211
 adict, 212
 AtomTypes, 212
 build_pid, 211
 feed, 211
 itype, 212
 In, 212
 molatom, 212
 Molecules, 212
 pdict, 212
 Split, 211
 suffix, 212
 Whites, 211
 forcebalance::Mol2
 data, 36
 forcebalance::Mol2::mol2
 __init__, 524
 __repr__, 524
 atoms, 527
 bonds, 527
 charge_type, 527
 comments, 527
 get_atom, 524
 get_bonded_atoms, 525
 mol_name, 527
 mol_type, 527
 num_atoms, 527
 num_bonds, 527
 num_feat, 527
 num_sets, 527
 num_subst, 527
 out, 525
 parse, 525
 set_charge_type, 526
 set_donor_acceptor_atoms, 526
 set_mol_name, 526
 set_mol_type, 527
 set_num_atoms, 527
 set_num_bonds, 527
 set_num_feat, 527
 set_num_sets, 527
 set_num_subst, 527
 forcebalance::Mol2::mol2_atom
 __init__, 528
 __repr__, 528
 atom_id, 530
 atom_name, 530
 atom_type, 530
 charge, 530
 parse, 528
 set_atom_id, 529
 set_atom_name, 529
 set_atom_type, 529
 set_charge, 529
 set_crds, 530
 set_status_bit, 530
 set_subst_id, 530
 set_subst_name, 530
 status_bit, 530
 subst_id, 530
 subst_name, 530
 x, 530
 y, 530
 z, 530
 forcebalance::Mol2::mol2_bond
 __init__, 531
 __repr__, 531
 bond_id, 532
 bond_type, 532
 origin_atom_id, 532
 parse, 531
 set_bond_id, 532
 set_bond_type, 532

```

set_origin_atom_id, 532
set_status_bit, 532
set_target_atom_id, 532
status_bit, 532
target_atom_id, 532
forcebalance::Mol2::mol2_set
    __init__, 538
    comments, 538
    compounds, 538
    num_compounds, 538
    parse, 538
forcebalance::PT
    Elements, 68
    PeriodicTable, 68
forcebalance::abinitio
    build_objective, 16
    logger, 16
    weighted_variance, 16
    weighted_variance2, 16
forcebalance::abinitio::AbInitio
    __init__, 79
    __setattr__, 79
    absrd, 79
    AtomLists, 92
    AtomMask, 92
    boltz_wts, 92
    build_invdist, 80
    check_files, 80
    compute_netforce_torque, 80
    e_err, 92
    e_err_pct, 92
    e_ref, 92
    emd0, 93
    energy_all, 80
    energy_force_all, 80
    energy_force_one, 80
    energy_force_transform, 80
    energy_force_transform_one, 81
    energy_one, 81
    engine, 93
    eqm, 93
    esp_err, 93
    espval, 93
    espxyz, 93
    f_err, 93
    f_err_pct, 93
    f_ref, 93
    FF, 93
    fitatoms, 93
    force, 93
    force_map, 93
    fqm, 93
    fref, 93
    gct, 93
    get, 81
    get_G, 83
    get_H, 84
    get_X, 85
    get_energy_force, 82
    get_resp, 85
    hct, 93
    indicate, 86
    invdists, 93
    link_from_tempdir, 86
    maxrd, 87
    meta_get, 87
    meta_indicate, 88
    mol, 93
    nesp, 94
    new_vsites, 94
    nf_err, 94
    nf_err_pct, 94
    nf_ref, 94
    nftqm, 94
    nnf, 94
    nparticles, 94
    ns, 94
    ntq, 94
    objective, 94
    pgrad, 94
    PrintOptionDict, 94
    printcool_table, 89
    qfnm, 94
    qmatoms, 94
    qmboltz_wts, 94
    rd, 94
    read, 89
    read_0grads, 90
    read_indicate, 95
    read_objective, 95
    read_reference_data, 90
    refresh_temp_directory, 91
    respterm, 95
    rundir, 95
    save_vmvalls, 95
    set_option, 91
    stage, 91
    submit_jobs, 91
    tempbase, 95
    tempdir, 95
    tq_err, 95
    tq_err_pct, 95
    tq_ref, 95
    use_nft, 95
    verbose_options, 95
    w_energy, 95
    w_force, 95
    w_netforce, 96

```

w_resp, 96
 w_torque, 96
 whamboltz, 96
 wq_complete, 92
 write_0grads, 92
 write_indicate, 96
 write_objective, 96
 xct, 96
forcebalance::abinitio_internal::AbInitio_Internal
 __init__, 146
 __setattr__, 146
 absrd, 146
 AtomLists, 158
 AtomMask, 158
 boltz_wts, 158
 build_invdist, 146
 check_files, 146
 compute_netforce_torque, 146
 coords, 158
 e_err, 158
 e_err_pct, 159
 e_ref, 159
 emd0, 159
 energy_all, 146
 energy_force_all, 147
 energy_force_driver_all, 147
 energy_force_one, 147
 energy_force_transform, 147
 energy_force_transform_one, 147
 energy_one, 148
 engine, 159
 eqm, 159
 esp_err, 159
 espval, 159
 espxyz, 159
 f_err, 159
 f_err_pct, 159
 f_ref, 159
 FF, 159
 fitatoms, 159
 force, 159
 force_map, 159
 fqm, 159
 fref, 159
 gct, 159
 get, 148
 get_G, 149
 get_H, 150
 get_X, 151
 get_energy_force, 148
 get_resp, 151
 hct, 160
 indicate, 152
 invdists, 160
 link_from_tempdir, 152
 maxrd, 153
 meta_get, 153
 meta_indicate, 154
 mol, 160
 nesp, 160
 new_vsites, 160
 nf_err, 160
 nf_err_pct, 160
 nf_ref, 160
 nftqm, 160
 nmf, 160
 nparticles, 160
 ns, 160
 ntq, 160
 objective, 160
 pgrad, 160
 PrintOptionDict, 160
 printcool_table, 155
 qfnm, 160
 qmatoms, 160
 qmboltz_wts, 160
 rd, 161
 read, 155
 read_0grads, 156
 read_indicate, 161
 read_objective, 161
 read_reference_data, 156
 refresh_temp_directory, 157
 respterm, 161
 rundir, 161
 save_vmvalls, 161
 set_option, 157
 stage, 157
 submit_jobs, 157
 tempbase, 161
 tempdir, 161
 tq_err, 161
 tq_err_pct, 161
 tq_ref, 161
 use_nft, 161
 verbose_options, 161
 w_energy, 161
 w_force, 162
 w_netforce, 162
 w_resp, 162
 w_torque, 162
 whamboltz, 162
 wq_complete, 158
 write_0grads, 158
 write_indicate, 162
 write_objective, 162
 xct, 162
forcebalance::amberio

```

frcmod_pdct, 18
is_mol2_atom, 18
logger, 18
mol2_pdct, 18
forcebalance::amberio::AbInitio_AMBER
    __init__, 102
    __setattr__, 102
    absrd, 102
    all_at_once, 114
    AtomLists, 114
    AtomMask, 114
    boltz_wts, 114
    build_invdist, 102
    check_files, 102
    compute_netforce_torque, 102
    coords, 114
    e_err, 115
    e_err_pct, 115
    e_ref, 115
    emd0, 115
    energy_all, 102
    energy_force_all, 102
    energy_force_driver_all, 102
    energy_force_one, 103
    energy_force_transform, 103
    energy_force_transform_one, 103
    energy_one, 104
    engine, 115
    eqm, 115
    esp_err, 115
    espval, 115
    espxyz, 115
    f_err, 115
    f_err_pct, 115
    f_ref, 115
    FF, 115
    fitatoms, 115
    force, 115
    force_map, 115
    fqm, 115
    fref, 115
    gct, 116
    get, 104
    get_G, 105
    get_H, 106
    get_X, 107
    get_energy_force, 104
    get_resp, 107
    hct, 116
    indicate, 108
    invdists, 116
    link_from_tempdir, 108
    maxrd, 109
    meta_get, 109
    meta_indicate, 110
    mol, 116
    nesp, 116
    new_vsites, 116
    nf_err, 116
    nf_err_pct, 116
    nf_ref, 116
    nftqm, 116
    nnf, 116
    nparticles, 116
    ns, 116
    ntq, 116
    objective, 116
    pgrad, 116
    prepare_temp_directory, 111
    PrintOptionDict, 116
    printcool_table, 111
    qfnm, 116
    qmatoms, 116
    qmboltz_wts, 117
    rd, 117
    read, 111
    read_0grads, 112
    read_indicate, 117
    read_objective, 117
    read_reference_data, 112
    refresh_temp_directory, 113
    respterm, 117
    rundir, 117
    save_vmvalls, 117
    set_option, 113
    stage, 113
    submit_jobs, 114
    tempbase, 117
    tempdir, 117
    tq_err, 117
    tq_err_pct, 117
    tq_ref, 117
    use_nft, 117
    verbose_options, 118
    w_energy, 118
    w_force, 118
    w_netforce, 118
    w_resp, 118
    w_torque, 118
    whamboltz, 118
    wq_complete, 114
    write_0grads, 114
    write_indicate, 118
    write_objective, 118
    xct, 118
forcebalance::amberio::FrcMod_Reader
    __init__, 309
    adict, 310

```

atom, 310
 AtomTypes, 310
 build_pid, 309
 dihe, 310
 feed, 309
 itype, 310
 In, 310
 molatom, 310
 Molecules, 310
 pdict, 310
 Split, 309
 suffix, 310
 Whites, 310
forcebalance::amberio::Mol2_Reader
 __init__, 537
 adict, 537
 atom, 537
 AtomTypes, 537
 atomnames, 537
 build_pid, 537
 feed, 537
 itype, 537
 In, 537
 mol, 537
 molatom, 537
 Molecules, 537
 pdict, 537
 section, 538
 Split, 537
 suffix, 538
 Whites, 537
forcebalance::binding
 logger, 19
 parse_interactions, 19
forcebalance::binding::BindingEnergy
 __init__, 215
 __setattr__, 215
 absrd, 215
 check_files, 216
 energy_part, 225
 engines, 225
 FF, 225
 gct, 225
 get, 216
 get_G, 216
 get_H, 217
 get_X, 218
 hct, 225
 indicate, 219
 inter_opts, 225
 link_from_tempdir, 219
 maxrd, 220
 meta_get, 220
 meta_indicate, 221
 objective, 225
 pgrad, 225
 PrintDict, 225
 PrintOptionDict, 225
 printcool_table, 222
 RMSDDict, 225
 rd, 225
 read, 222
 read_0grads, 223
 read_indicate, 225
 read_objective, 225
 refresh_temp_directory, 223
 rmsd_part, 225
 rundir, 226
 set_option, 223
 stage, 223
 submit_jobs, 224
 system_driver, 224
 tempbase, 226
 tempdir, 226
 verbose_options, 226
 wq_complete, 224
 write_0grads, 224
 write_indicate, 226
 write_objective, 226
 xct, 226
forcebalance::chemistry
 A, 20
 atoms, 20
 B, 20
 BE, 20
 bo, 20
 BondChars, 20
 BondEnergies, 20
 BondStrengthByLength, 20
 data_from_web, 20
 Elements, 20
 L, 20
 line, 20
 LookupByMass, 20
 PeriodicTable, 20
 Radii, 21
forcebalance::contact
 atom_distances, 21
 residue_distances, 22
forcebalance::counterpoise
 logger, 22
forcebalance::counterpoise::Counterpoise
 __init__, 277
 __setattr__, 277
 absrd, 277
 check_files, 278
 cpqm, 289
 FF, 289

```

gct, 289
get, 278
get_G, 279
get_H, 280
get_X, 281
hct, 289
link_from_tempdir, 282
load_cp, 282
loadxyz, 282
maxrd, 284
meta_get, 284
meta_indicate, 285
na, 289
ns, 289
pgrad, 289
PrintOptionDict, 289
printcool_table, 286
rd, 289
read, 286
read_0grads, 287
read_indicate, 289
read_objective, 289
refresh_temp_directory, 287
rundir, 289
set_option, 287
stage, 287
submit_jobs, 288
tempbase, 289
tempdir, 290
verbose_options, 290
wq_complete, 288
write_0grads, 288
write_indicate, 290
write_objective, 290
xct, 290
xyzs, 290
forcebalance::custom_io
    cotypes, 23
    fdict, 23
    ndtypes, 23
    pdict, 23
forcebalance::custom_io::Gen_Reader
    __init__, 315
    adict, 316
    AtomTypes, 316
    build_pid, 315
    feed, 315
    itype, 316
    In, 316
    molatom, 316
    Molecules, 316
    pdict, 316
    sec, 316
    Split, 316
suffix, 316
Whites, 316
forcebalance::engine
    logger, 24
forcebalance::engine::Engine
    __init__, 292
    __setattr__, 292
    FF, 292
    name, 292
    prepare, 292
    PrintOptionDict, 292
    readsrc, 292
    root, 292
    set_option, 292
    setopts, 292
    srkdir, 292
    target, 292
    tempdir, 292
    verbose, 292
    verbose_options, 292
forcebalance::finite_difference
    f12d3p, 25
    f12d7p, 25
    f1d2p, 25
    f1d5p, 25
    f1d7p, 25
    f2var, 25
    fdwrap, 25
    fdwrap_G, 26
    fdwrap_H, 26
    in_fd, 26
    in_fd_srch, 27
    logger, 27
forcebalance::forcefield
    determine_fftype, 28
    FF_Extensions, 29
    FF_IOModules, 29
    logger, 29
    rs_override, 28
forcebalance::forcefield::BackedUpDict
    __init__, 207
    __missing__, 207
    backup_dict, 207
forcebalance::forcefield::FF
    __eq__, 296
    __init__, 295
    __setattr__, 296
    addff, 296
    addff_txt, 297
    addff_xml, 298
    assign_field, 299
    assign_p0, 299
    atomnames, 304
    create_mvals, 299

```

```

create_pvls, 300
excision, 304
FFAtomTypes, 304
FFMolecules, 304
ffdata, 304
ffdata_isxml, 304
find_spacings, 300
linedestroy_save, 304
linedestroy_this, 304
list_map, 301
make, 301
make_redirect, 302
map, 304
mktransmat, 302
np, 304
openmmxml, 304
patoms, 304
pfields, 305
plist, 305
print_map, 302
PrintOptionDict, 305
prmdestroy_save, 305
prmdestroy_this, 305
pvls0, 305
qid, 305
qid2, 305
qmap, 305
Readers, 305
redirect, 305
rs, 305
rsmake, 303
set_option, 303
sprint_map, 303
tinkerprm, 305
tm, 305
tml, 305
verbose_options, 305
forcebalance::gmxio
    aftytypes, 32
    bftytypes, 32
    dftytypes, 32
    fdict, 32
    logger, 33
    nftytypes, 33
    parse_atomtype_line, 31
    pdict, 33
    pftypes, 33
    rm_gmx_baks, 31
    write_mdp, 31
    write_ndx, 32
forcebalance::gmxio::AbInitio_GMX
    __init__, 124
    __setattr__, 124
    absrd, 124
    AtomLists, 136
    AtomMask, 136
    boltz_wts, 136
    build_invdist, 124
    check_files, 124
    compute_netforce_torque, 124
    e_err, 136
    e_err_pct, 136
    e_ref, 136
    emd0, 137
    energy_all, 125
    energy_force_all, 125
    energy_force_one, 125
    energy_force_transform, 125
    energy_force_transform_one, 125
    energy_one, 126
    engine, 137
    engine_, 137
    eqm, 137
    esp_err, 137
    espval, 137
    espxyz, 137
    f_err, 137
    f_err_pct, 137
    f_ref, 137
    FF, 137
    fitatoms, 137
    force, 137
    force_map, 137
    fqm, 137
    fref, 137
    gct, 137
    get, 126
    get_G, 127
    get_H, 128
    get_X, 129
    get_energy_force, 126
    get_resp, 129
    hct, 137
    indicate, 130
    invdists, 138
    link_from_tempdir, 130
    maxrd, 131
    meta_get, 131
    meta_indicate, 132
    mol, 138
    nesp, 138
    new_vsites, 138
    nf_err, 138
    nf_err_pct, 138
    nf_ref, 138
    nftqm, 138
    nnf, 138
    nparticles, 138

```

ns, 138
 ntq, 138
 objective, 138
 pgrad, 138
 PrintOptionDict, 138
 printcool_table, 133
 qfnm, 138
 qatoms, 138
 qmboltz_wts, 138
 rd, 138
 read, 133
 read_0grads, 134
 read_indicate, 139
 read_objective, 139
 read_reference_data, 134
 refresh_temp_directory, 135
 respterm, 139
 rundir, 139
 save_vmvalls, 139
 set_option, 135
 stage, 135
 submit_jobs, 135
 tempbase, 139
 tempdir, 139
 tq_err, 139
 tq_err_pct, 139
 tq_ref, 139
 use_nft, 139
 verbose_options, 139
 w_energy, 139
 w_force, 139
 w_netforce, 140
 w_resp, 140
 w_torque, 140
 whamboltz, 140
 wq_complete, 136
 write_0grads, 136
 write_indicate, 140
 write_objective, 140
 xct, 140
 forcebalance::gmxio::BindingEnergy_GMX
 __init__, 230
 __setattr__, 230
 absrd, 230
 check_files, 231
 energy_part, 240
 engine_, 240
 engines, 240
 FF, 240
 gct, 240
 get, 231
 get_G, 231
 get_H, 232
 get_X, 233
 hct, 240
 indicate, 234
 inter_opts, 240
 link_from_tempdir, 234
 maxrd, 235
 meta_get, 235
 meta_indicate, 236
 objective, 240
 pgrad, 240
 PrintDict, 240
 PrintOptionDict, 240
 printcool_table, 237
 RMSDDict, 241
 rd, 240
 read, 237
 read_0grads, 238
 read_indicate, 240
 read_objective, 240
 refresh_temp_directory, 238
 rmsd_part, 240
 rundir, 241
 set_option, 238
 stage, 238
 submit_jobs, 239
 system_driver, 239
 tempbase, 241
 tempdir, 241
 verbose_options, 241
 wq_complete, 239
 write_0grads, 239
 write_indicate, 241
 write_objective, 241
 xct, 241
 forcebalance::gmxio::GMX
 __init__, 319
 __setattr__, 319
 AtomLists, 325
 AtomMask, 325
 calc_scd, 319
 callgmx, 319
 double, 326
 energy, 320
 energy_dipole, 320
 energy_force, 320
 energy_force_one, 320
 energy_one, 321
 energy_rmsd, 321
 energy_ternnames, 321
 evaluate_, 321
 evaluate_snapshot, 322
 evaluate_trajectory, 322
 FF, 326
 generate_vsites_positions, 322
 gmx_defs, 326

gmxpath, 326
 gmxsuffix, 326
 interaction_energy, 322
 links, 323
 md, 323
 mdene, 326
 mdp, 326
 mdtraj, 326
 mol, 326
 molecular_dynamics, 323
 multipole_moments, 324
 n_snaps, 324
 name, 326
 normal_modes, 324
 optimize, 324
 pbc, 326
 prepare, 325
 PrintOptionDict, 326
 readsrc, 325
 root, 326
 scd_persnap, 325
 set_option, 325
 setopts, 325
 srkdir, 326
 target, 326
 tempdir, 326
 top, 326
 valkwrd, 326
 verbose, 327
 verbose_options, 327
 warnmgmx, 325
forcebalance::gmxio::ITP_Reader
 __init__, 392
 adict, 393
 AtomTypes, 393
 atomnames, 393
 atomtype_to_mass, 393
 atomtypes, 393
 build_pid, 392
 feed, 393
 itype, 393
 In, 393
 mol, 393
 molatom, 393
 Molecules, 393
 nbtype, 393
 pdict, 394
 sec, 394
 Split, 393
 suffix, 394
 Whites, 393
forcebalance::gmxio::Interaction_GMX
 __init__, 348
 __setattr__, 349
 absrd, 349
 check_files, 349
 divisor, 358
 e_err, 358
 e_err_pct, 358
 emm, 358
 engine, 358
 engine_, 358
 eqm, 358
 FF, 358
 gct, 358
 get, 349
 get_G, 349
 get_H, 350
 get_X, 351
 hct, 358
 indicate, 352
 label, 358
 link_from_tempdir, 352
 maxrd, 353
 meta_get, 353
 meta_indicate, 354
 mol, 358
 ns, 358
 objective, 358
 pgrad, 358
 prefactor, 358
 PrintOptionDict, 358
 printcool_table, 355
 qfnm, 358
 rd, 359
 read, 355
 read_0grads, 356
 read_indicate, 359
 read_objective, 359
 read_reference_data, 356
 refresh_temp_directory, 356
 rundir, 359
 select1, 359
 select2, 359
 set_option, 356
 stage, 356
 submit_jobs, 357
 tempbase, 359
 tempdir, 359
 verbose_options, 359
 weight, 359
 wq_complete, 357
 write_0grads, 357
 write_indicate, 359
 write_objective, 359
 xct, 360
forcebalance::gmxio::Lipid_GMX
 __init__, 433

__setattr__, 433
 absrd, 433
 check_files, 433
 do_self_pol, 444
 engine_, 444
 engname, 444
 extra_output, 444
 FF, 444
 gas_engine, 444
 gct, 444
 get, 433
 get_G, 434
 get_H, 435
 get_X, 436
 Gp, 444
 hct, 444
 indicate, 437
 Labels, 444
 last_traj, 444
 LfDict, 445
 LfDict_New, 445
 link_from_tempdir, 437
 lipid_mol, 445
 MBarEnergy, 445
 maxrd, 438
 meta_get, 438
 meta_indicate, 439
 npt_simulation, 440
 nptfiles, 445
 nptpx, 445
 Objective, 445
 objective_term, 440
 pgrad, 445
 PhasePoints, 445
 polarization_correction, 440
 Pp, 445
 prepare_temp_directory, 441
 PrintOptionDict, 445
 printcool_table, 441
 rd, 445
 read, 441
 read_0grads, 442
 read_data, 442
 read_indicate, 445
 read_objective, 445
 RefData, 445
 refresh_temp_directory, 442
 rundir, 445
 SavedMVal, 445
 SavedTraj, 446
 scripts, 446
 set_option, 442
 stage, 442
 submit_jobs, 443
 tempbase, 446
 tempdir, 446
 verbose_options, 446
 w_al, 446
 w_alpha, 446
 w_cp, 446
 w_eps0, 446
 w_kappa, 446
 w_rho, 446
 w_scd, 446
 Wp, 446
 wq_complete, 443
 write_0grads, 444
 write_indicate, 446
 write_objective, 446
 xct, 446
 Xp, 446
 forcebalance::gmxi::Liquid_GMX
 __init__, 468
 __setattr__, 468
 absrd, 468
 AllResults, 481
 check_files, 468
 do_self_pol, 481
 engine_, 481
 engname, 481
 extra_output, 481
 FF, 481
 gas_engine, 481
 gas_engine_args, 481
 gas_mol, 481
 gct, 481
 get, 468
 get_G, 470
 get_H, 471
 get_X, 472
 Gp, 481
 hct, 481
 indicate, 473
 Labels, 481
 last_traj, 481
 LfDict, 481
 LfDict_New, 481
 link_from_tempdir, 473
 liquid_mol, 481
 MBarEnergy, 481
 maxrd, 474
 meta_get, 474
 meta_indicate, 475
 npt_simulation, 476
 nptfiles, 481
 nptpx, 481
 Objective, 481
 objective_term, 476

pgrad, 482
 PhasePoints, 482
 polarization_correction, 476
 Pp, 482
 prepare_temp_directory, 477
 PrintOptionDict, 482
 printcool_table, 477
 rd, 482
 read, 477
 read_0grads, 478
 read_data, 478
 read_indicate, 482
 read_objective, 482
 RefData, 482
 refresh_temp_directory, 478
 rundir, 482
 SavedTraj, 482
 scripts, 482
 set_option, 478
 stage, 478
 submit_jobs, 479
 tempbase, 482
 tempdir, 482
 verbose_options, 482
 w_alpha, 482
 w_cp, 483
 w_eps0, 483
 w_hvap, 483
 w_kappa, 483
 w_rho, 483
 Wp, 483
 wq_complete, 480
 write_0grads, 480
 write_indicate, 483
 write_objective, 483
 xct, 483
 Xp, 483
 forcebalance::gmxio::Moments_GMX
 __init__, 578
 __setattr__, 578
 absrd, 578
 calc_moments, 588
 check_files, 579
 denoms, 588
 engine, 588
 engine_, 588
 FF, 588
 gct, 588
 get, 579
 get_G, 579
 get_H, 580
 get_X, 581
 hct, 588
 indicate, 582
 link_from_tempdir, 582
 maxrd, 583
 meta_get, 583
 meta_indicate, 584
 mfnm, 588
 na, 588
 objective, 588
 pgrad, 588
 PrintOptionDict, 588
 printcool_table, 585
 rd, 588
 read, 585
 read_0grads, 586
 read_indicate, 588
 read_objective, 588
 read_reference_data, 586
 ref_eigvals, 589
 ref_eigvecs, 589
 ref_moments, 589
 refresh_temp_directory, 586
 rundir, 589
 set_option, 586
 stage, 586
 submit_jobs, 587
 tempbase, 589
 tempdir, 589
 unpack_moments, 587
 verbose_options, 589
 wq_complete, 587
 write_0grads, 587
 write_indicate, 589
 write_objective, 589
 xct, 589
 forcebalance::gmxio::Thermo_GMX
 __init__, 751
 __setattr__, 751
 absrd, 751
 check_files, 752
 denoms, 762
 engine_, 762
 engname, 762
 FF, 762
 gct, 763
 get, 752
 get_G, 753
 get_H, 754
 get_X, 755
 Gp, 763
 hct, 763
 indicate, 756
 link_from_tempdir, 756
 maxrd, 757
 mdpx, 763
 meta_get, 757

meta_indicate, 758
 Objective, 763
 objective_term, 759
 pgrad, 763
 points, 763
 Pp, 763
 PrintOptionDict, 763
 printcool_table, 759
 rd, 763
 read, 760
 read_0grads, 760
 read_indicate, 763
 read_objective, 763
 refresh_temp_directory, 760
 retrieve, 760
 rundir, 763
 scripts, 763
 set_option, 761
 simpfx, 764
 stage, 761
 submit_jobs, 761
 tempbase, 764
 tempdir, 764
 verbose_options, 764
 weights, 764
 Wp, 764
 wq_complete, 762
 write_0grads, 762
 write_indicate, 764
 write_objective, 764
 xct, 764
 Xp, 764
forcebalance::gmgio::Vibration_GMX
 __init__, 795
 __setattr__, 795
 absrd, 795
 c2r, 805
 calc_eigvals, 805
 check_files, 796
 engine, 805
 engine., 805
 FF, 805
 gct, 805
 get, 796
 get_G, 796
 get_H, 797
 get_X, 798
 hct, 805
 indicate, 799
 link_from_tempdir, 799
 maxrd, 800
 meta_get, 800
 meta_indicate, 801
 na, 805
 objective, 805
 overlaps, 805
 pgrad, 805
 PrintOptionDict, 806
 printcool_table, 802
 process_vectors, 802
 rd, 806
 read, 803
 read_0grads, 803
 read_indicate, 806
 read_objective, 806
 read_reference_data, 803
 reassign, 806
 ref_eigvals, 806
 ref_eigvecs, 806
 ref_eigvecs_nrm_mw, 806
 refresh_temp_directory, 803
 rundir, 806
 set_option, 803
 stage, 803
 submit_jobs, 804
 tempbase, 806
 tempdir, 806
 verbose_options, 806
 vfnm, 806
 vibration_driver, 804
 wq_complete, 804
 write_0grads, 805
 write_indicate, 806
 write_objective, 807
 xct, 807
forcebalance::interaction
 logger, 34
forcebalance::interaction::Interaction
 __init__, 333
 __setattr__, 333
 absrd, 333
 check_files, 334
 divisor, 343
 e_err, 343
 e_err_pct, 343
 emm, 343
 engine, 343
 eqm, 343
 FF, 343
 gct, 343
 get, 334
 get_G, 334
 get_H, 335
 get_X, 336
 hct, 343
 indicate, 337
 label, 343
 link_from_tempdir, 337

maxrd, 338
 meta_get, 338
 meta_indicate, 339
 mol, 343
 ns, 343
 objective, 343
 pgrad, 343
 prefactor, 343
 PrintOptionDict, 343
 printcool_table, 340
 qfnm, 343
 rd, 343
 read, 340
 read_0grads, 341
 read_indicate, 344
 read_objective, 344
 read_reference_data, 341
 refresh_temp_directory, 341
 rundir, 344
 select1, 344
 select2, 344
 set_option, 341
 stage, 341
 submit_jobs, 342
 tempbase, 344
 tempdir, 344
 verbose_options, 344
 weight, 344
 wq_complete, 342
 write_0grads, 342
 write_indicate, 344
 write_objective, 344
 xct, 344
 forcebalance::leastsq
 CHECK_BASIS, 34
 CheckBasis, 34
 LAST_MVALS, 34
 LastMvals, 34
 logger, 34
 forcebalance::leastsq::LeastSquares
 __init__, 397
 __setattr__, 397
 absrd, 397
 check_files, 397
 D, 407
 FF, 407
 gct, 407
 get, 397
 get_G, 398
 get_H, 399
 get_X, 400
 hct, 407
 indicate, 401
 link_from_tempdir, 401
 MAQ, 407
 maxrd, 401
 meta_get, 402
 meta_indicate, 403
 objective, 407
 pgrad, 407
 PrintOptionDict, 407
 printcool_table, 404
 rd, 407
 read, 404
 read_0grads, 405
 read_indicate, 407
 read_objective, 407
 refresh_temp_directory, 405
 rundir, 407
 set_option, 405
 stage, 405
 submit_jobs, 406
 tempbase, 407
 tempdir, 408
 verbose_options, 408
 wq_complete, 406
 write_0grads, 406
 write_indicate, 408
 write_objective, 408
 xct, 408
 forcebalance::lipid
 logger, 35
 weight_info, 35
 forcebalance::lipid::Lipid
 __init__, 414
 __setattr__, 415
 absrd, 415
 check_files, 415
 do_self_pol, 426
 engname, 426
 extra_output, 426
 FF, 426
 gas_engine, 426
 gct, 426
 get, 415
 get_G, 416
 get_H, 417
 get_X, 418
 Gp, 426
 hct, 426
 indicate, 419
 Labels, 426
 last_traj, 426
 link_from_tempdir, 419
 lipid_mol, 426
 MBarEnergy, 427
 maxrd, 420
 meta_get, 420

meta_indicate, 421
 npt_simulation, 422
 Objective, 427
 objective_term, 422
 pgrad, 427
 PhasePoints, 427
 polarization_correction, 422
 Pp, 427
 prepare_temp_directory, 423
 PrintOptionDict, 427
 printcool_table, 423
 rd, 427
 read, 423
 read_0grads, 424
 read_data, 424
 read_indicate, 427
 read_objective, 427
 RefData, 427
 refresh_temp_directory, 424
 rundir, 427
 SavedMVal, 427
 SavedTraj, 427
 set_option, 424
 stage, 424
 submit_jobs, 425
 tempbase, 427
 tempdir, 427
 verbose_options, 428
 w_al, 428
 w_alpha, 428
 w_cp, 428
 w_eps0, 428
 w_kappa, 428
 w_rho, 428
 w_scd, 428
 Wp, 428
 wq_complete, 425
 write_0grads, 426
 write_indicate, 428
 write_objective, 428
 xct, 428
 Xp, 428
 forcebalance::liquid
 logger, 35
 weight_info, 35
 forcebalance::liquid::Liquid
 __init__, 450
 __setattr__, 450
 absrd, 450
 AllResults, 462
 check_files, 450
 do_self_pol, 462
 engname, 462
 extra_output, 462
 FF, 462
 gas_engine, 462
 gas_mol, 462
 gct, 462
 get, 450
 get_G, 451
 get_H, 452
 get_X, 453
 Gp, 462
 hct, 462
 indicate, 454
 Labels, 462
 last_traj, 462
 link_from_tempdir, 454
 liquid_mol, 462
 MBarEnergy, 462
 maxrd, 455
 meta_get, 455
 meta_indicate, 456
 npt_simulation, 457
 Objective, 462
 objective_term, 457
 pgrad, 462
 PhasePoints, 462
 polarization_correction, 457
 Pp, 462
 prepare_temp_directory, 458
 PrintOptionDict, 462
 printcool_table, 458
 rd, 462
 read, 458
 read_0grads, 459
 read_data, 459
 read_indicate, 463
 read_objective, 463
 RefData, 463
 refresh_temp_directory, 459
 rundir, 463
 SavedTraj, 463
 set_option, 459
 stage, 459
 submit_jobs, 460
 tempbase, 463
 tempdir, 463
 verbose_options, 463
 w_alpha, 463
 w_cp, 463
 w_eps0, 463
 w_hvap, 463
 w_kappa, 463
 w_rho, 463
 Wp, 463
 wq_complete, 461
 write_0grads, 461

```

write_indicate, 464
write_objective, 464
xct, 464
Xp, 464
forcebalance::mol2io
    mol2_pdict, 36
forcebalance::mol2io::Mol2_Reader
    __init__, 534
    adict, 534
    atom, 534
    AtomTypes, 535
    build_pid, 534
    feed, 534
    itype, 535
    In, 535
    molatom, 535
    Molecules, 535
    pdict, 535
    Split, 534
    suffix, 535
    Whites, 534
forcebalance::molecule
    add_strip_to_mat, 38
    AlignToDensity, 38
    AlignToMoments, 38
    AllVariableNames, 42
    AtomVariableNames, 42
    bohrang, 42
    both, 39
    Box, 42
    BuildLatticeFromLengthsAngles, 39
    BuildLatticeFromVectors, 39
    cartesian_product2, 39
    ComputeOverlap, 39
    CubicLattice, 39
    diff, 39
    either, 39
    elem_from_atomname, 39
    Elements, 42
    EulerMatrix, 40
    even_list, 40
    format_gro_box, 40
    format_gro_coord, 40
    format_xyz_coord, 40
    format_xyzgen_coord, 40
    FrameVariableNames, 42
    get_rotate_translate, 40
    getElement, 40
    grouper, 40
    have_contact, 43
    is_charmm_coord, 40
    is_gro_box, 41
    is_gro_coord, 41
    isfloat, 42
    isint, 42
    main, 42
    MetaVariableNames, 43
    nodematch, 42
    PeriodicTable, 43
    pvec, 42
    QuantumVariableNames, 43
    radian, 43
    Radii, 43
    splitter, 43
forcebalance::molecule::Molecule
    __add__, 543
    __delitem__, 543
    __getattr__, 543
    __getitem__, 543
    __iadd__, 544
    __init__, 543
    __iter__, 544
    __len__, 544
    __setattr__, 544
    add_quantum, 544
    add_virtual_site, 544
    align, 544
    align_by_moments, 545
    align_center, 545
    all_pairwise_rmsd, 545
    append, 546
    atom_select, 546
    atom_stack, 546
    boxes, 558
    build_topology, 546
    built_bonds, 558
    center_of_mass, 546
    comms, 558
    Data, 558
    edit_qcrems, 546
    find_angles, 546
    find_dihedrals, 547
    foul, 558
    Funnel, 558
    load_frames, 547
    measure_dihedrals, 547
    molecules, 558
    openmm_boxes, 547
    openmm_positions, 547
    pathwise_rmsd, 547
    positive_resid, 558
    radius_of_gyration, 548
    Read_Tab, 559
    read_arc, 548
    read_charmm, 549
    read_com, 549
    read_dcd, 550
    read_gro, 550

```

read_mdcrd, 550
 read_mol2, 551
 read_pdb, 551
 read_qcesp, 551
 read_qcin, 551
 read_qcout, 552
 read_qdata, 552
 read_xyz, 552
 read_xyz0, 553
 ref_rmsd, 553
 repair, 553
 replace_peratom, 554
 replace_peratom_conditional, 554
 require, 554
 require_boxes, 554
 require_resid, 554
 require_resname, 554
 resid, 559
 resname, 559
 rigid_water, 554
 split, 555
 topology, 559
 write, 555
 Write_Tab, 559
 write_arc, 555
 write_dcd, 555
 write_gro, 555
 write_mdcrd, 556
 write_molproq, 556
 write_pdb, 556
 write_qcin, 557
 write_qdata, 557
 write_xyz, 558
 forcebalance::molecule::MyG
 __eq__, 621
 __hash__, 621
 __init__, 621
 AStr, 621
 Alive, 622
 e, 621
 ef, 621
 L, 622
 x, 622
 forcebalance::moments
 logger, 44
 forcebalance::moments::Moments
 __init__, 563
 __setattr__, 563
 absrd, 563
 calc_moments, 573
 check_files, 564
 denoms, 573
 engine, 573
 FF, 573
 gct, 573
 get, 564
 get_G, 564
 get_H, 565
 get_X, 566
 hct, 573
 indicate, 567
 link_from_tempdir, 567
 maxrd, 568
 meta_get, 568
 meta_indicate, 569
 mfnm, 573
 na, 573
 objective, 573
 pgrad, 573
 PrintOptionDict, 573
 printcool_table, 570
 rd, 573
 read, 570
 read_0grads, 571
 read_indicate, 573
 read_objective, 573
 read_reference_data, 571
 ref_eigvals, 574
 ref_eigvecs, 574
 ref_moments, 574
 refresh_temp_directory, 571
 rundir, 574
 set_option, 571
 stage, 571
 submit_jobs, 572
 tempbase, 574
 tempdir, 574
 unpack_moments, 572
 verbose_options, 574
 wq_complete, 572
 write_0grads, 572
 write_indicate, 574
 write_objective, 574
 xct, 574
 forcebalance::nifty
 allsplit, 47
 astr, 47
 bak, 47
 bohrang, 56
 click, 47
 col, 47
 commadash, 47
 concurrent_map, 47
 CopyFile, 47
 createWorkQueue, 48
 destroyWorkQueue, 48
 encode, 48
 eqcgm, 56

extract_int, 48
 flat, 48
 floatornan, 48
 fqcgmx, 56
 get_least_squares, 49
 getWQIds, 49
 getWorkQueue, 49
 GoInto, 50
 grouper, 50
 invert_svd, 50
 isdecimal, 50
 isfloat, 50
 isint, 50
 kb, 56
 Leave, 51
 link_dir_contents, 51
 LinkFile, 51
 logger, 56
 lp_dump, 51
 lp_load, 51
 MissingFileInspection, 51
 monotonic, 51
 multiD_statisticalInefficiency, 51
 onefile, 52
 orthogonalize, 52
 pmat2d, 52
 printcool, 52
 printcool_dictionary, 53
 pvec1d, 54
 queue_up, 54
 queue_up_src_dest, 54
 remove_if_exists, 54
 row, 54
 segments, 54
 specific_dct, 56
 specific_lst, 56
 statisticalInefficiency, 55
 uncommadash, 55
 WORK_QUEUE, 56
 WQIDS, 57
 warn_once, 55
 warn_press_key, 55
 which, 55
 wopen, 55
 wq_wait, 55
 wq_wait1, 56
 XMLFILE, 57
 forcebalance::nifty::LineChunker
 __enter__, 409
 __exit__, 409
 __init__, 409
 buf, 410
 callback, 410
 close, 409
 nomnom, 410
 push, 410
 forcebalance::nifty::Pickler_LP
 __init__, 657
 forcebalance::nifty::Unpickler_LP
 __init__, 777
 forcebalance::objective
 Implemented_Targets, 57
 Letters, 58
 logger, 58
 forcebalance::objective::Objective
 __init__, 624
 __setattr__, 624
 FF, 625
 Full, 624
 Indicate, 625
 ObjDict, 625
 ObjDict_Last, 625
 Penalty, 625
 PrintOptionDict, 626
 set_option, 625
 Target_Terms, 625
 Targets, 626
 verbose_options, 626
 WTot, 626
 forcebalance::objective::Penalty
 __init__, 654
 a, 656
 b, 656
 compute, 654
 FF, 656
 FUSE, 654
 FUSE_BARRIER, 655
 FUSE_L0, 655
 fadd, 656
 fmul, 656
 HYP, 655
 L2_norm, 655
 Pen_Names, 656
 Pen_Tab, 656
 ptyp, 656
 spacings, 656
 forcebalance::openmmio
 CopyAmoebaAngleParameters, 59
 CopyAmoebaBondParameters, 59
 CopyAmoebaInPlaneAngleParameters, 59
 CopyAmoebaMultipoleParameters, 59
 CopyAmoebaOutOfPlaneBendParameters, 59
 CopyAmoebaVdwParameters, 59
 CopyHarmonicAngleParameters, 59
 CopyHarmonicBondParameters, 60
 CopyNonbondedParameters, 60
 CopyPeriodicTorsionParameters, 60
 CopySystemParameters, 60

do_nothing, 60
 energy_components, 60
 get_dipole, 60
 get_multipoles, 60
 GetVirtualSiteParameters, 60
 logger, 61
 MTSVVVRIntegrator, 60
 pdict, 61
 PrepareVirtualSites, 61
 ResetVirtualSites, 61
 ResetVirtualSites_fast, 61
 SetAmoebaVirtualExclusions, 61
 suffix_dict, 62
 UpdateSimulationParameters, 61
 forcebalance::openmmio::AbInitio_OpenMM
 __init__, 168
 __setattr__, 168
 absrd, 168
 AtomLists, 180
 AtomMask, 180
 boltz_wts, 180
 build_invdist, 168
 check_files, 168
 compute_netforce_torque, 168
 e_err, 180
 e_err_pct, 180
 e_ref, 180
 emd0, 181
 energy_all, 169
 energy_force_all, 169
 energy_force_one, 169
 energy_force_transform, 169
 energy_force_transform_one, 169
 energy_one, 170
 engine, 181
 engine_, 181
 eqm, 181
 esp_err, 181
 espval, 181
 espxyz, 181
 f_err, 181
 f_err_pct, 181
 f_ref, 181
 FF, 181
 fitatoms, 181
 force, 181
 force_map, 181
 fqm, 181
 fref, 181
 gct, 181
 get, 170
 get_G, 171
 get_H, 172
 get_X, 173
 get_energy_force, 170
 get_resp, 173
 hct, 181
 indicate, 174
 invdists, 182
 link_from_tempdir, 174
 maxrd, 175
 meta_get, 175
 meta_indicate, 176
 mol, 182
 nesp, 182
 new_vsites, 182
 nf_err, 182
 nf_err_pct, 182
 nf_ref, 182
 nftqm, 182
 nnf, 182
 nparticles, 182
 ns, 182
 ntq, 182
 objective, 182
 pgrad, 182
 PrintOptionDict, 182
 printcool_table, 177
 qfnm, 182
 qmatoms, 182
 qmboltz_wts, 182
 rd, 182
 read, 177
 read_0grads, 178
 read_indicate, 183
 read_objective, 183
 read_reference_data, 178
 refresh_temp_directory, 179
 respterm, 183
 rundir, 183
 save_vmvalls, 183
 set_option, 179
 stage, 179
 submit_jobs, 179
 tempbase, 183
 tempdir, 183
 tq_err, 183
 tq_err_pct, 183
 tq_ref, 183
 use_nft, 183
 verbose_options, 183
 w_energy, 183
 w_force, 183
 w_netforce, 184
 w_resp, 184
 w_torque, 184
 whamboltz, 184
 wq_complete, 180

```

write_0grads, 180
write_indicate, 184
write_objective, 184
xct, 184
forcebalance::openmmio::BindingEnergy_OpenMM
    __init__, 245
    __setattr__, 245
    absrd, 245
    check_files, 246
    energy_part, 255
    engine_, 255
    engines, 255
    FF, 255
    gct, 255
    get, 246
    get_G, 246
    get_H, 247
    get_X, 248
    hct, 255
    indicate, 249
    inter_opts, 255
    link_from_tempdir, 249
    maxrd, 250
    meta_get, 250
    meta_indicate, 251
    objective, 255
    pgrad, 255
    PrintDict, 255
    PrintOptionDict, 255
    printcool_table, 252
    RMSDDict, 256
    rd, 255
    read, 252
    read_0grads, 253
    read_indicate, 255
    read_objective, 255
    refresh_temp_directory, 253
    rmsd_part, 255
    rundir, 256
    set_option, 253
    stage, 253
    submit_jobs, 254
    system_driver, 254
    tempbase, 256
    tempdir, 256
    verbose_options, 256
    wq_complete, 254
    write_0grads, 254
    write_indicate, 256
    write_objective, 256
    xct, 256
forcebalance::openmmio::Interaction_OpenMM
    __init__, 363
    __setattr__, 364
absrd, 364
check_files, 364
divisor, 373
e_err, 373
e_err_pct, 373
emm, 373
engine, 373
engine_, 373
eqm, 373
FF, 373
gct, 373
get, 364
get_G, 364
get_H, 365
get_X, 366
hct, 373
indicate, 367
label, 373
link_from_tempdir, 367
maxrd, 368
meta_get, 368
meta_indicate, 369
mol, 373
ns, 373
objective, 373
pgrad, 373
prefactor, 373
PrintOptionDict, 373
printcool_table, 370
qfnm, 373
rd, 374
read, 370
read_0grads, 371
read_indicate, 374
read_objective, 374
read_reference_data, 371
refresh_temp_directory, 371
rundir, 374
select1, 374
select2, 374
set_option, 371
stage, 371
submit_jobs, 372
tempbase, 374
tempdir, 374
verbose_options, 374
weight, 374
wq_complete, 372
write_0grads, 372
write_indicate, 374
write_objective, 374
xct, 375
forcebalance::openmmio::Liquid_OpenMM
    __init__, 488

```

__setattr__, 488
 absrd, 488
 AllResults, 500
 check_files, 488
 do_self_pol, 500
 engine_, 500
 engname, 500
 extra_output, 500
 FF, 500
 gas_engine, 500
 gas_engine_args, 500
 gas_mol, 500
 gct, 500
 get, 488
 get_G, 489
 get_H, 490
 get_X, 491
 Gp, 500
 hct, 500
 indicate, 492
 Labels, 500
 last_traj, 500
 link_from_tempdir, 492
 liquid_mol, 500
 MBarEnergy, 500
 maxrd, 493
 meta_get, 493
 meta_indicate, 494
 npt_simulation, 495
 nptfiles, 500
 nptpx, 500
 Objective, 500
 objective_term, 495
 pgrad, 500
 PhasePoints, 500
 polarization_correction, 495
 Pp, 501
 prepare_temp_directory, 496
 PrintOptionDict, 501
 printcool_table, 496
 rd, 501
 read, 496
 read_0grads, 497
 read_data, 497
 read_indicate, 501
 read_objective, 501
 RefData, 501
 refresh_temp_directory, 497
 rundir, 501
 SavedTraj, 501
 scripts, 501
 set_option, 497
 stage, 497
 submit_jobs, 498
 tempbase, 501
 tempdir, 501
 verbose_options, 501
 w_alpha, 501
 w_cp, 501
 w_eps0, 501
 w_hvap, 501
 w_kappa, 502
 w_rho, 502
 Wp, 502
 wq_complete, 499
 write_0grads, 499
 write_indicate, 502
 write_objective, 502
 xct, 502
 Xp, 502
forcebalance::openmmio::Moments_OpenMM
 __init__, 593
 __setattr__, 593
 absrd, 593
 calc_moments, 603
 check_files, 594
 denoms, 603
 engine, 603
 engine_, 603
 FF, 603
 gct, 603
 get, 594
 get_G, 594
 get_H, 595
 get_X, 596
 hct, 603
 indicate, 597
 link_from_tempdir, 597
 maxrd, 598
 meta_get, 598
 meta_indicate, 599
 mfnm, 603
 na, 603
 objective, 603
 pgrad, 603
 PrintOptionDict, 603
 printcool_table, 600
 rd, 603
 read, 600
 read_0grads, 601
 read_indicate, 603
 read_objective, 603
 read_reference_data, 601
 ref_eigvals, 604
 ref_eigvecs, 604
 ref_moments, 604
 refresh_temp_directory, 601
 rundir, 604

```

set_option, 601
stage, 601
submit_jobs, 602
tempbase, 604
tempdir, 604
unpack_moments, 602
verbose_options, 604
wq_complete, 602
write_0grads, 602
write_indicate, 604
write_objective, 604
xct, 604

forcebalance::openmmio::OpenMM
    __init__, 629
    __setattr__, 629
    A, 635
    AMOEBA, 635
    AtomLists, 635
    AtomMask, 635
    B, 635
    compute_mass, 629
    compute_volume, 629
    create_simulation, 629
    energy, 629
    energy_dipole, 630
    energy_force, 630
    energy_force_one, 630
    energy_one, 631
    energy_rmsd, 631
    evaluate_, 631
    evaluate_one_, 632
    FF, 635
    fFXML, 635
    forcefield, 635
    interaction_energy, 632
    mass, 635
    mmopts, 635
    mod, 635
    mol, 635
    molecular_dynamics, 632
    multipole_moments, 633
    name, 635
    nbcharges, 635
    ndof, 635
    normal_modes, 633
    optimize, 633
    pbc, 635
    pdb, 635
    platform, 635
    platname, 635
    precision, 635
    prepare, 634
    PrintOptionDict, 636
    readsrc, 634

                    root, 636
                    set_option, 634
                    set_positions, 634
                    setopts, 634
                    simkwargs, 636
                    simulation, 636
                    srccdir, 636
                    system, 636
                    target, 636
                    tdiv, 636
                    tempdir, 636
                    update_simulation, 634
                    valkwd, 636
                    verbose, 636
                    verbose_options, 636
                    vsinfo, 636
                    vsprm, 636
                    xyz_omm, 636

forcebalance::openmmio::OpenMM_Reader
    __init__, 638
    adict, 639
    AtomTypes, 639
    build_pid, 638
    feed, 638
    itype, 639
    In, 639
    molatom, 639
    Molecules, 639
    pdict, 639
    Split, 638
    suffix, 639
    Whites, 638

forcebalance::optimizer
    Counter, 62
    First, 62
    GOODSTEP, 63
    GoodStep, 63
    ITERATION, 63
    ITERINIT, 63
    logger, 63

forcebalance::optimizer::Optimizer
    __init__, 642
    __setattr__, 642
    adjh, 642
    Anneal, 642
    BFGS, 643
    bakdir, 651
    BasinHopping, 643
    bhyp, 651
    chk, 651
    ConjugateGradient, 643
    dx, 652
    excision, 652
    FDCheckG, 644

```

```

FDCheckH, 644
FF, 652
failmsg, 652
GeneticAlgorithm, 645
Grad, 652
Gradient, 645
H, 652
h, 652
Hess, 652
Hessian, 645
MainOptimizer, 645
mvals0, 652
mvals_bak, 652
NewtonCG, 646
NewtonRaphson, 646
np, 652
Objective, 652
OptTab, 653
Penalty, 653
Powell, 647
prev_bad, 653
PrintOptionDict, 653
readchk, 647
recover, 647
resdir, 653
Run, 647
save_mvals_to_input, 648
Scan_Values, 648
ScanMVals, 648
ScanPVals, 649
Scipy_BFGS, 649
ScipyOptimizer, 649
set_option, 650
Simplex, 650
SinglePoint, 650
step, 650
TruncatedNewton, 651
uncert, 653
Val, 653
verbose_options, 653
writechk, 651
x_best, 653
x_prev, 653
xk_prev, 653
forcebalance::output::CleanFileHandler
emit, 272
forcebalance::output::CleanStreamHandler
__init__, 273
emit, 274
forcebalance::output::ForceBalanceLogger
__init__, 307
addHandler, 307
defaultHandler, 307
removeHandler, 307
forcebalance::output::ModLogger
error, 523
forcebalance::output::RawFileHandler
emit, 669
forcebalance::output::RawStreamHandler
__init__, 670
emit, 671
forcebalance::parser
all_opts_names, 66
blkwd, 66
gen_opts_defaults, 66
gen_opts_types, 66
iocc, 66
logger, 66
mainsections, 67
ParsTab, 67
parse_inputs, 65
printsection, 65
read_internals, 66
read_mvals, 66
read_priors, 66
read_pvals, 66
subdict, 67
tgt_opts_defaults, 67
tgt_opts_types, 67
forcebalance::psi4io
logger, 68
forcebalance::psi4io::GBS_Reader
__init__, 312
adict, 313
amom, 313
AtomTypes, 313
basis_number, 313
build_pid, 312
contraction_number, 313
destroy, 313
element, 313
feed, 312
isdata, 313
itype, 313
last_amom, 313
In, 313
molatom, 313
Molecules, 313
pdct, 313
Split, 313
suffix, 313
Whites, 313
forcebalance::psi4io::Grid_Reader
__init__, 329
adict, 329
AtomTypes, 329
build_pid, 329
element, 329

```

feed, 329
 isdata, 329
 itype, 329
 In, 329
 molatom, 329
 Molecules, 329
 pdict, 329
 point, 329
 radii, 329
 Split, 329
 suffix, 330
 Whites, 329
forcebalance::psi4io::RDVR3_Psi4
 __init__, 674
 __setattr__, 674
 absrd, 674
 bidirect, 685
 callderivs, 685
 check_files, 675
 driver, 675
 elements, 685
 FF, 685
 factor, 685
 gct, 685
 get, 675
 get.G, 676
 get.H, 677
 get.X, 678
 gradd, 685
 hct, 685
 hdiagd, 685
 indicate, 679
 link_from_tempdir, 679
 maxrd, 680
 meta_get, 680
 meta_indicate, 681
 molecules, 685
 objd, 685
 objective, 685
 objfiles, 685
 objvals, 685
 pgrad, 685
 PrintOptionDict, 685
 printcool_table, 682
 rd, 685
 read, 682
 read_0grads, 683
 read_indicate, 685
 read_objective, 686
 refresh_temp_directory, 683
 rundir, 686
 set_option, 683
 stage, 683
 submit_jobs, 684
 tdir, 686
 tempbase, 686
 tempdir, 686
 verbose_options, 686
 wq_complete, 684
 write_0grads, 684
 write_indicate, 686
 write_objective, 686
 xct, 686
forcebalance::psi4io::THCDF_Psi4
 __init__, 718
 __setattr__, 718
 absrd, 718
 check_files, 719
 D, 730
 DATfnm, 730
 DF_Energy, 730
 driver, 719
 Elements, 730
 FF, 730
 GBSfnm, 730
 gct, 730
 get, 719
 get_G, 721
 get_H, 722
 get_X, 723
 hct, 730
 indicate, 724
 link_from_tempdir, 724
 MAQ, 730
 MP2_Energy, 730
 maxrd, 724
 meta_get, 725
 meta_indicate, 726
 Molecules, 730
 objective, 730
 pgrad, 730
 prepare_temp_directory, 727
 PrintOptionDict, 731
 printcool_table, 727
 rd, 731
 read, 728
 read_0grads, 728
 read_indicate, 731
 read_objective, 731
 refresh_temp_directory, 728
 rundir, 731
 set_option, 728
 stage, 728
 submit_jobs, 729
 tempbase, 731
 tempdir, 731
 throw_outs, 731
 verbose_options, 731

```

wq_complete, 729
write_0grads, 729
write_indicate, 731
write_nested_destroy, 730
write_objective, 731
xct, 731
forcebalance::qchemio
    logger, 69
    ndtypes, 69
    pdict, 69
    QChem_Dielectric_Energy, 69
forcebalance::qchemio::QCIn_Reader
    __init__, 661
    adict, 662
    atom, 662
    AtomTypes, 662
    build_pid, 661
    cnum, 662
    feed, 661
    itype, 662
    In, 662
    molatom, 662
    Molecules, 662
    pdict, 662
    sec, 662
    shell, 662
    snum, 662
    Split, 661
    suffix, 662
    Whites, 661
forcebalance::quantity
    energy_derivatives, 70
    logger, 71
    mean_stderr, 70
forcebalance::quantity::Quantity
    __init__, 664
    __str__, 664
    engname, 664
    extract, 664
    name, 664
    pressure, 664
    temperature, 664
forcebalance::quantity::Quantity_Density
    __init__, 666
    __str__, 666
    engname, 666
    extract, 666
    name, 666
    pressure, 666
    temperature, 666
forcebalance::quantity::Quantity_H_vap
    __init__, 668
    __str__, 668
    engname, 668
extract, 668
name, 668
pressure, 668
temperature, 668
forcebalance::target::RemoteTarget
    __init__, 690
    __setattr__, 690
    absrd, 690
    check_files, 690
    FF, 699
    gct, 699
    get, 690
    get_G, 691
    get_H, 691
    get_X, 692
    hct, 699
    indicate, 693
    link_from_tempdir, 693
    maxrd, 693
    meta_get, 694
    meta_indicate, 695
    pgrad, 699
    PrintOptionDict, 699
    printcool_table, 696
    r_options, 699
    r_tgt_opts, 699
    rd, 699
    read, 696
    read_0grads, 697
    read_indicate, 699
    read_objective, 700
    refresh_temp_directory, 697
    remote_indicate, 700
    rundir, 700
    set_option, 697
    stage, 697
    submit_jobs, 698
    tempbase, 700
    tempdir, 700
    verbose_options, 700
    wq_complete, 698
    write_0grads, 699
    write_indicate, 700
    write_objective, 700
    xct, 700
forcebalance::target::Target
    __init__, 704
    __setattr__, 704
    absrd, 704
    check_files, 705
    FF, 714
    gct, 714

```

get, 705
 get_G, 705
 get_H, 706
 get_X, 707
 hct, 714
 link_from_tempdir, 708
 maxrd, 708
 meta_get, 709
 meta_indicate, 710
 pgrad, 714
 PrintOptionDict, 714
 printcool_table, 711
 rd, 714
 read, 711
 read_0grads, 712
 read_indicate, 714
 read_objective, 714
 refresh_temp_directory, 712
 rundir, 714
 set_option, 712
 stage, 712
 submit_jobs, 713
 tempbase, 714
 tempdir, 714
 verbose_options, 714
 wq_complete, 713
 write_0grads, 713
 write_indicate, 714
 write_objective, 715
 xct, 715
 forcebalance::thermo
 logger, 71
 forcebalance::thermo::Point
 __init__, 659
 __str__, 659
 data, 659
 idnr, 659
 pressure, 659
 ref, 659
 temperature, 659
 forcebalance::thermo::Thermo
 __init__, 735
 __setattr__, 735
 absrd, 735
 check_files, 736
 denoms, 745
 FF, 745
 gct, 745
 get, 736
 get_G, 736
 get_H, 737
 get_X, 738
 Gp, 745
 hct, 746
 indicate, 739
 link_from_tempdir, 739
 maxrd, 740
 meta_get, 740
 meta_indicate, 741
 Objective, 746
 objective_term, 742
 pgrad, 746
 points, 746
 Pp, 746
 PrintOptionDict, 746
 printcool_table, 742
 rd, 746
 read, 743
 read_0grads, 743
 read_indicate, 746
 read_objective, 746
 refresh_temp_directory, 743
 retrieve, 743
 rundir, 746
 set_option, 744
 simpx, 746
 stage, 744
 submit_jobs, 744
 tempbase, 746
 tempdir, 746
 verbose_options, 747
 weights, 747
 Wp, 747
 wq_complete, 745
 write_0grads, 745
 write_indicate, 747
 write_objective, 747
 xct, 747
 Xp, 747
 forcebalance::tinkerio
 alp, 73
 eckeys, 73
 logger, 73
 pdict, 73
 write_key, 72
 forcebalance::tinkerio::AbInitio_TINKER
 __init__, 190
 __setattr__, 190
 absrd, 190
 AtomLists, 202
 AtomMask, 202
 boltz_wts, 202
 build_invdist, 190
 check_files, 190
 compute_netforce_torque, 190
 e_err, 202
 e_err_pct, 202
 e_ref, 202

emd0, 203
 energy_all, 191
 energy_force_all, 191
 energy_force_one, 191
 energy_force_transform, 191
 energy_force_transform_one, 191
 energy_one, 192
 engine, 203
 engine_, 203
 eqm, 203
 esp_err, 203
 espval, 203
 espxyz, 203
 f_err, 203
 f_err_pct, 203
 f_ref, 203
 FF, 203
 fitatoms, 203
 force, 203
 force_map, 203
 fqm, 203
 fref, 203
 gct, 203
 get, 192
 get_G, 193
 get_H, 194
 get_X, 195
 get_energy_force, 192
 get_resp, 195
 hct, 203
 indicate, 196
 invdists, 204
 link_from_tempdir, 196
 maxrd, 197
 meta_get, 197
 meta_indicate, 198
 mol, 204
 nesp, 204
 new_vsites, 204
 nf_err, 204
 nf_err_pct, 204
 nf_ref, 204
 nftqm, 204
 nnf, 204
 nparticles, 204
 ns, 204
 ntq, 204
 objective, 204
 pgrad, 204
 PrintOptionDict, 204
 printcool_table, 199
 qfnm, 204
 qmatoms, 204
 qmboltz_wts, 204
 rd, 204
 read, 199
 read_0grads, 200
 read_indicate, 205
 read_objective, 205
 read_reference_data, 200
 refresh_temp_directory, 201
 respterm, 205
 rundir, 205
 save_vmvalls, 205
 set_option, 201
 stage, 201
 submit_jobs, 201
 tempbase, 205
 tempdir, 205
 tq_err, 205
 tq_err_pct, 205
 tq_ref, 205
 use_nft, 205
 verbose_options, 205
 w_energy, 205
 w_force, 205
 w_netforce, 206
 w_resp, 206
 w_torque, 206
 whamboltz, 206
 wq_complete, 202
 write_0grads, 202
 write_indicate, 206
 write_objective, 206
 xct, 206
forcebalance::tinkerio::BindingEnergy_TINKER
 __init__, 260
 __setattr__, 260
 absrd, 260
 check_files, 261
 energy_part, 270
 engine_, 270
 engines, 270
 FF, 270
 gct, 270
 get, 261
 get_G, 261
 get_H, 262
 get_X, 263
 hct, 270
 indicate, 264
 inter_opts, 270
 link_from_tempdir, 264
 maxrd, 265
 meta_get, 265
 meta_indicate, 266
 objective, 270
 pgrad, 270

PrintDict, 270
 PrintOptionDict, 270
 printcool_table, 267
 RMSDDict, 271
 rd, 270
 read, 267
 read_0grads, 268
 read_indicate, 270
 read_objective, 270
 refresh_temp_directory, 268
 rmsd_part, 270
 rundir, 271
 set_option, 268
 stage, 268
 submit_jobs, 269
 system_driver, 269
 tempbase, 271
 tempdir, 271
 verbose_options, 271
 wq_complete, 269
 write_0grads, 269
 write_indicate, 271
 write_objective, 271
 xct, 271
forcebalance::tinkerio::Interaction_TINKER
 __init__, 378
 __setattr__, 379
 absrd, 379
 check_files, 379
 divisor, 388
 e_err, 388
 e_err_pct, 388
 emm, 388
 engine, 388
 engine_, 388
 eqm, 388
 FF, 388
 gct, 388
 get, 379
 get_G, 379
 get_H, 380
 get_X, 381
 hct, 388
 indicate, 382
 label, 388
 link_from_tempdir, 382
 maxrd, 383
 meta_get, 383
 meta_indicate, 384
 mol, 388
 ns, 388
 objective, 388
 pgrad, 388
 prefactor, 388
 PrintOptionDict, 388
 printcool_table, 385
 qfnm, 388
 rd, 389
 read, 385
 read_0grads, 386
 read_indicate, 389
 read_objective, 389
 read_reference_data, 386
 refresh_temp_directory, 386
 rundir, 389
 select1, 389
 select2, 389
 set_option, 386
 stage, 386
 submit_jobs, 387
 tempbase, 389
 tempdir, 389
 verbose_options, 389
 weight, 389
 wq_complete, 387
 write_0grads, 387
 write_indicate, 389
 write_objective, 389
 xct, 390
forcebalance::tinkerio::Liquid_TINKER
 __init__, 507
 __setattr__, 507
 absrd, 507
 AllResults, 520
 check_files, 507
 do_self_pol, 520
 DynDict, 520
 DynDict_New, 520
 engine_, 520
 engname, 520
 extra_output, 520
 FF, 520
 gas_engine, 520
 gas_engine_args, 520
 gas_mol, 520
 gct, 520
 get, 507
 get_G, 509
 get_H, 510
 get_X, 511
 Gp, 520
 hct, 520
 indicate, 512
 Labels, 520
 last_traj, 520
 link_from_tempdir, 512
 liquid_mol, 520
 MBarEnergy, 520

maxrd, 513
 meta_get, 513
 meta_indicate, 514
 npt_simulation, 515
 nptfiles, 520
 nptpx, 520
 Objective, 520
 objective_term, 515
 pgrad, 521
 PhasePoints, 521
 polarization_correction, 515
 Pp, 521
 prepare_temp_directory, 516
 PrintOptionDict, 521
 printcool_table, 516
 rd, 521
 read, 516
 read_0grads, 517
 read_data, 517
 read_indicate, 521
 read_objective, 521
 RefData, 521
 refresh_temp_directory, 517
 rundir, 521
 SavedTraj, 521
 scripts, 521
 set_option, 517
 stage, 517
 submit_jobs, 518
 tempbase, 521
 tempdir, 521
 verbose_options, 521
 w_alpha, 521
 w_cp, 522
 w_eps0, 522
 w_hvap, 522
 w_kappa, 522
 w_rho, 522
 Wp, 522
 wq_complete, 519
 write_0grads, 519
 write_indicate, 522
 write_objective, 522
 xct, 522
 Xp, 522
 forcebalance::tinkerio::Moments_TINKER
 __init__, 608
 __setattr__, 608
 absrd, 608
 calc_moments, 618
 check_files, 609
 denoms, 618
 engine, 618
 engine_, 618
 FF, 618
 gct, 618
 get, 609
 get_G, 609
 get_H, 610
 get_X, 611
 hct, 618
 indicate, 612
 link_from_tempdir, 612
 maxrd, 613
 meta_get, 613
 meta_indicate, 614
 mfnm, 618
 na, 618
 objective, 618
 pgrad, 618
 PrintOptionDict, 618
 printcool_table, 615
 rd, 618
 read, 615
 read_0grads, 616
 read_indicate, 618
 read_objective, 618
 read_reference_data, 616
 ref_eigvals, 619
 ref_eigvecs, 619
 ref_moments, 619
 refresh_temp_directory, 616
 rundir, 619
 set_option, 616
 stage, 616
 submit_jobs, 617
 tempbase, 619
 tempdir, 619
 unpack_moments, 617
 verbose_options, 619
 wq_complete, 617
 write_0grads, 617
 write_indicate, 619
 write_objective, 619
 xct, 619
 forcebalance::tinkerio::TINKER
 __init__, 767
 __setattr__, 767
 A, 772
 abskey, 772
 AtomLists, 772
 AtomMask, 772
 B, 772
 calltinker, 767
 energy, 767
 energy_dipole, 768
 energy_force, 768
 energy_force_one, 768

```

energy_rmsd, 769
evaluate_, 769
FF, 772
interaction_energy, 769
key, 772
mdtraj, 772
mol, 772
molecular_dynamics, 769
multipole_moments, 770
name, 772
normal_modes, 770
optimize, 771
pbc, 772
prepare, 771
PrintOptionDict, 772
prm, 772
readsrc, 771
rigid, 772
root, 772
set_option, 771
setopts, 771
srcdir, 772
target, 772
tempdir, 772
tinkerpath, 772
valkwrd, 772
verbose, 772
verbose_options, 773
warn_vn, 773
forcebalance::tinkerio::Tinker_Reader
__init__, 775
adict, 776
atom, 776
AtomTypes, 776
build_pid, 775
feed, 775
itype, 776
In, 776
molatom, 776
Molecules, 776
pdict, 776
Split, 775
suffix, 776
Whites, 775
forcebalance::tinkerio::Vibration_TINKER
__init__, 810
__setattr__, 810
absrd, 810
c2r, 820
calc_eigvals, 820
check_files, 811
engine, 820
engine_, 820
FF, 820
gct, 820
get, 811
get_G, 811
get_H, 812
get_X, 813
hct, 820
indicate, 814
link_from_tempdir, 814
maxrd, 815
meta_get, 815
meta_indicate, 816
na, 820
objective, 820
overlaps, 820
pgrad, 820
PrintOptionDict, 821
printcool_table, 817
process_vectors, 817
rd, 821
read, 818
read_Ograds, 818
read_indicate, 821
read_objective, 821
read_reference_data, 818
reassign, 821
ref_eigvals, 821
ref_eigvecs, 821
ref_eigvecs_nrm_mw, 821
refresh_temp_directory, 818
rundir, 821
set_option, 818
stage, 818
submit_jobs, 819
tempbase, 821
tempdir, 821
verbose_options, 821
vfnm, 821
vibration_driver, 819
wq_complete, 819
write_Ograds, 820
write_indicate, 821
write_objective, 822
xct, 822
forcebalance::vibration
count_assignment, 74
logger, 74
forcebalance::vibration::Vibration
__init__, 781
__setattr__, 781
absrd, 781
c2r, 790
calc_eigvals, 790
check_files, 781
engine, 790

```

FF, 790
 gct, 790
 get, 781
 get.G, 781
 get.H, 782
 get.X, 783
 hct, 790
 indicate, 784
 link_from_tempdir, 784
 maxrd, 785
 meta_get, 785
 meta_indicate, 786
 na, 790
 objective, 790
 overlaps, 790
 pgrad, 790
 PrintOptionDict, 790
 printcool_table, 787
 process_vectors, 787
 rd, 791
 read, 788
 read_0grads, 788
 read_indicate, 791
 read_objective, 791
 read_reference_data, 788
 reassign, 791
 ref_eigvals, 791
 ref_eigvecs, 791
 ref_eigvecs_nrm_mw, 791
 refresh_temp_directory, 788
 rundir, 791
 set_option, 788
 stage, 788
 submit_jobs, 789
 tempbase, 791
 tempdir, 791
 verbose_options, 791
 vfnm, 791
 vibration_driver, 789
 wq_complete, 789
 write_0grads, 790
 write_indicate, 791
 write_objective, 791
 xct, 792
forcefield
 forcebalance::openmmio::OpenMM, 635
forcefield.py, 826
format_gro_box
 forcebalance::molecule, 40
format_gro_coord
 forcebalance::molecule, 40
format_xyz_coord
 forcebalance::molecule, 40
format_xyzgen_coord

forcebalance::molecule, 40
fout
 forcebalance::molecule::Molecule, 558
fqcgmx
 forcebalance::nifty, 56
fqm
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
FrameVariableNames
 forcebalance::molecule, 42
frcmod_pdict
 forcebalance::amberio, 18
fref
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 115
 forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::tinkerio::AbInitio_TINKER, 203
Full
 forcebalance::objective::Objective, 624
Funnel
 forcebalance::molecule::Molecule, 558
GBSfnm
 forcebalance::psi4io::THCDF_Psi4, 730
GOODSTEP
 forcebalance::optimizer, 63
gas_engine
 forcebalance::gmxio::Lipid_GMX, 444
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::lipid::Lipid, 426
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
gas_engine_args
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
gas_mol
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
gct
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 159
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::binding::BindingEnergy, 225
 forcebalance::counterpoise::Counterpoise, 289

forcebalance::gmxio::AbInitio_GMX, 137
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::gmxio::Lipid_GMX, 444
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Thermo_GMX, 763
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::interaction::Interaction, 343
 forcebalance::leastsq::LeastSquares, 407
 forcebalance::lipid::Lipid, 426
 forcebalance::liquid::Liquid, 462
 forcebalance::moments::Moments, 573
 forcebalance::openmmio::AbInitio_OpenMM, 181
 forcebalance::openmmio::BindingEnergy_OpenMM, 255
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::psi4io::RDVR3_Psi4, 685
 forcebalance::psi4io::THCDF_Psi4, 730
 forcebalance::target::RemoteTarget, 699
 forcebalance::target::Target, 714
 forcebalance::thermo::Thermo, 745
 forcebalance::tinkerio::AbInitio_TINKER, 203
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
 forcebalance::tinkerio::Interaction_TINKER, 388
 forcebalance::tinkerio::Liquid_TINKER, 520
 forcebalance::tinkerio::Moments_TINKER, 618
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
 gen_opts_defaults
 forcebalance::parser, 66
 gen_opts_types
 forcebalance::parser, 66
 generate_vsites_positions
 forcebalance::gmxio::GMX, 322
 GeneticAlgorithm
 forcebalance::optimizer::Optimizer, 645
 get
 forcebalance::abinitio::AbInitio, 81
 forcebalance::abinitio_internal::AbInitio_Internal, 148
 forcebalance::amberio::AbInitio_AMBER, 104
 forcebalance::binding::BindingEnergy, 216
 forcebalance::counterpoise::Counterpoise, 278
 forcebalance::gmxio::AbInitio_GMX, 126
 forcebalance::gmxio::BindingEnergy_GMX, 231
 forcebalance::gmxio::Interaction_GMX, 349
 forcebalance::gmxio::Lipid_GMX, 433
 forcebalance::gmxio::Liquid_GMX, 468
 forcebalance::gmxio::Moments_GMX, 579
 forcebalance::gmxio::Thermo_GMX, 752
 forcebalance::gmxio::Vibration_GMX, 796
 forcebalance::interaction::Interaction, 334
 forcebalance::leastsq::LeastSquares, 397
 forcebalance::lipid::Lipid, 415
 forcebalance::liquid::Liquid, 450
 forcebalance::moments::Moments, 564
 forcebalance::openmmio::AbInitio_OpenMM, 170
 forcebalance::openmmio::BindingEnergy_OpenMM, 246
 forcebalance::openmmio::Interaction_OpenMM, 364
 forcebalance::openmmio::Liquid_OpenMM, 488
 forcebalance::openmmio::Moments_OpenMM, 594
 forcebalance::psi4io::RDVR3_Psi4, 675
 forcebalance::psi4io::THCDF_Psi4, 719
 forcebalance::target::RemoteTarget, 690
 forcebalance::target::Target, 705
 forcebalance::thermo::Thermo, 736
 forcebalance::tinkerio::AbInitio_TINKER, 192
 forcebalance::tinkerio::BindingEnergy_TINKER, 261
 forcebalance::tinkerio::Interaction_TINKER, 379
 forcebalance::tinkerio::Liquid_TINKER, 507
 forcebalance::tinkerio::Moments_TINKER, 609
 forcebalance::tinkerio::Vibration_TINKER, 811
 forcebalance::vibration::Vibration, 781
 get_G
 forcebalance::abinitio::AbInitio, 83
 forcebalance::abinitio_internal::AbInitio_Internal, 149
 forcebalance::amberio::AbInitio_AMBER, 105
 forcebalance::binding::BindingEnergy, 216
 forcebalance::counterpoise::Counterpoise, 279
 forcebalance::gmxio::AbInitio_GMX, 127
 forcebalance::gmxio::BindingEnergy_GMX, 231
 forcebalance::gmxio::Interaction_GMX, 349
 forcebalance::gmxio::Lipid_GMX, 434
 forcebalance::gmxio::Liquid_GMX, 470
 forcebalance::gmxio::Moments_GMX, 579
 forcebalance::gmxio::Thermo_GMX, 753
 forcebalance::gmxio::Vibration_GMX, 796
 forcebalance::interaction::Interaction, 334
 forcebalance::leastsq::LeastSquares, 398
 forcebalance::lipid::Lipid, 416
 forcebalance::liquid::Liquid, 451
 forcebalance::moments::Moments, 564
 forcebalance::openmmio::AbInitio_OpenMM, 171
 forcebalance::openmmio::BindingEnergy_OpenMM, 246
 forcebalance::openmmio::Interaction_OpenMM, 364
 forcebalance::openmmio::Liquid_OpenMM, 489
 forcebalance::openmmio::Moments_OpenMM, 594
 forcebalance::psi4io::RDVR3_Psi4, 676
 forcebalance::psi4io::THCDF_Psi4, 721
 forcebalance::target::RemoteTarget, 691
 forcebalance::target::Target, 705
 forcebalance::thermo::Thermo, 736
 forcebalance::tinkerio::AbInitio_TINKER, 193
 forcebalance::tinkerio::BindingEnergy_TINKER, 261

forcebalance::tinkerio::Interaction_TINKER, 379
 forcebalance::tinkerio::Liquid_TINKER, 509
 forcebalance::tinkerio::Moments_TINKER, 609
 forcebalance::tinkerio::Vibration_TINKER, 811
 forcebalance::vibration::Vibration, 781
get_H
 forcebalance::abinitio::AbInitio, 84
 forcebalance::abinitio_internal::AbInitio_Internal, 150
 forcebalance::amberio::AbInitio_AMBER, 106
 forcebalance::binding::BindingEnergy, 217
 forcebalance::counterpoise::Counterpoise, 280
 forcebalance::gmxio::AbInitio_GMX, 128
 forcebalance::gmxio::BindingEnergy_GMX, 232
 forcebalance::gmxio::Interaction_GMX, 350
 forcebalance::gmxio::Lipid_GMX, 435
 forcebalance::gmxio::Liquid_GMX, 471
 forcebalance::gmxio::Moments_GMX, 580
 forcebalance::gmxio::Thermo_GMX, 754
 forcebalance::gmxio::Vibration_GMX, 797
 forcebalance::interaction::Interaction, 335
 forcebalance::leastsq::LeastSquares, 399
 forcebalance::lipid::Lipid, 417
 forcebalance::liquid::Liquid, 452
 forcebalance::moments::Moments, 565
 forcebalance::openmmio::AbInitio_OpenMM, 172
 forcebalance::openmmio::BindingEnergy_OpenMM, 247
 forcebalance::openmmio::Interaction_OpenMM, 365
 forcebalance::openmmio::Liquid_OpenMM, 490
 forcebalance::openmmio::Moments_OpenMM, 595
 forcebalance::psi4io::RDVR3_Psi4, 677
 forcebalance::psi4io::THCDF_Psi4, 722
 forcebalance::target::RemoteTarget, 691
 forcebalance::target::Target, 706
 forcebalance::thermo::Thermo, 737
 forcebalance::tinkerio::AbInitio_TINKER, 194
 forcebalance::tinkerio::BindingEnergy_TINKER, 262
 forcebalance::tinkerio::Interaction_TINKER, 380
 forcebalance::tinkerio::Liquid_TINKER, 510
 forcebalance::tinkerio::Moments_TINKER, 610
 forcebalance::tinkerio::Vibration_TINKER, 812
 forcebalance::vibration::Vibration, 782
get_X
 forcebalance::abinitio::AbInitio, 85
 forcebalance::abinitio_internal::AbInitio_Internal, 151
 forcebalance::amberio::AbInitio_AMBER, 107
 forcebalance::binding::BindingEnergy, 218
 forcebalance::counterpoise::Counterpoise, 281
 forcebalance::gmxio::AbInitio_GMX, 129
 forcebalance::gmxio::BindingEnergy_GMX, 233
 forcebalance::gmxio::Interaction_GMX, 351
 forcebalance::gmxio::Lipid_GMX, 436
 forcebalance::gmxio::Liquid_GMX, 472
 forcebalance::gmxio::Moments_GMX, 581

 forcebalance::gmxio::Thermo_GMX, 755
 forcebalance::gmxio::Vibration_GMX, 798
 forcebalance::interaction::Interaction, 336
 forcebalance::leastsq::LeastSquares, 400
 forcebalance::lipid::Lipid, 418
 forcebalance::liquid::Liquid, 453
 forcebalance::moments::Moments, 566
 forcebalance::openmmio::AbInitio_OpenMM, 173
 forcebalance::openmmio::BindingEnergy_OpenMM, 248
 forcebalance::openmmio::Interaction_OpenMM, 366
 forcebalance::openmmio::Liquid_OpenMM, 491
 forcebalance::openmmio::Moments_OpenMM, 596
 forcebalance::psi4io::RDVR3_Psi4, 678
 forcebalance::psi4io::THCDF_Psi4, 723
 forcebalance::target::RemoteTarget, 692
 forcebalance::target::Target, 707
 forcebalance::thermo::Thermo, 738
 forcebalance::tinkerio::AbInitio_TINKER, 195
 forcebalance::tinkerio::BindingEnergy_TINKER, 263
 forcebalance::tinkerio::Interaction_TINKER, 381
 forcebalance::tinkerio::Liquid_TINKER, 511
 forcebalance::tinkerio::Moments_TINKER, 611
 forcebalance::tinkerio::Vibration_TINKER, 813
 forcebalance::vibration::Vibration, 783
get_atom
 forcebalance::Mol2::mol2, 524
get_bonded_atoms
 forcebalance::Mol2::mol2, 525
get_dipole
 forcebalance::openmmio, 60
get_energy_force
 forcebalance::abinitio::AbInitio, 82
 forcebalance::abinitio_internal::AbInitio_Internal, 148
 forcebalance::amberio::AbInitio_AMBER, 104
 forcebalance::gmxio::AbInitio_GMX, 126
 forcebalance::openmmio::AbInitio_OpenMM, 170
 forcebalance::tinkerio::AbInitio_TINKER, 192
get_least_squares
 forcebalance::nifty, 49
get_multipoles
 forcebalance::openmmio, 60
get_resp
 forcebalance::abinitio::AbInitio, 85
 forcebalance::abinitio_internal::AbInitio_Internal, 151
 forcebalance::amberio::AbInitio_AMBER, 107
 forcebalance::gmxio::AbInitio_GMX, 129
 forcebalance::openmmio::AbInitio_OpenMM, 173
 forcebalance::tinkerio::AbInitio_TINKER, 195
get_rotate_translate
 forcebalance::molecule, 40
getElement
 forcebalance::molecule, 40
GetVirtualSiteParameters

```

    forcebalance::openmmio, 60
getWQIds
    forcebalance::nifty, 49
getWorkQueue
    forcebalance::nifty, 49
gmx_defs
    forcebalance::gmlio::GMX, 326
gmlio.py, 827
gmxpath
    forcebalance::gmlio::GMX, 326
gmxsuffix
    forcebalance::gmlio::GMX, 326
GolTo
    forcebalance::nifty, 50
GoodStep
    forcebalance::optimizer, 63
Gp
    forcebalance::gmlio::Lipid_GMX, 444
    forcebalance::gmlio::Liquid_GMX, 481
    forcebalance::gmlio::Thermo_GMX, 763
    forcebalance::lipid::Lipid, 426
    forcebalance::liquid::Liquid, 462
    forcebalance::openmmio::Liquid_OpenMM, 500
    forcebalance::thermo::Thermo, 745
    forcebalance::tinkerio::Liquid_TINKER, 520
Grad
    forcebalance::optimizer::Optimizer, 652
gradd
    forcebalance::psi4io::RDVR3_Psi4, 685
Gradient
    forcebalance::optimizer::Optimizer, 645
group
    forcebalance::molecule, 40
    forcebalance::nifty, 50

H
    forcebalance::optimizer::Optimizer, 652
h
    forcebalance::optimizer::Optimizer, 652
HYP
    forcebalance::objective::Penalty, 655
have_contact
    forcebalance::molecule, 43
hct
    forcebalance::abinitio::AbInitio, 93
    forcebalance::abinitio_internal::AbInitio_Internal, 160
    forcebalance::amber::AbInitio_AMBER, 116
    forcebalance::binding::BindingEnergy, 225
    forcebalance::counterpoise::Counterpoise, 289
    forcebalance::gmlio::AbInitio_GMX, 137
    forcebalance::gmlio::BindingEnergy_GMX, 240
    forcebalance::gmlio::Interaction_GMX, 358
    forcebalance::gmlio::Lipid_GMX, 444
    forcebalance::gmlio::Liquid_GMX, 481
forcebalance::gmlio::Moments_GMX, 588
forcebalance::gmlio::Thermo_GMX, 763
forcebalance::gmlio::Vibration_GMX, 805
forcebalance::interaction::Interaction, 343
forcebalance::leastsq::LeastSquares, 407
forcebalance::lipid::Lipid, 426
forcebalance::liquid::Liquid, 462
forcebalance::moments::Moments, 573
forcebalance::openmmio::AbInitio_OpenMM, 181
forcebalance::openmmio::BindingEnergy_OpenMM,
    255
forcebalance::openmmio::Interaction_OpenMM, 373
forcebalance::openmmio::Liquid_OpenMM, 500
forcebalance::openmmio::Moments_OpenMM, 603
forcebalance::psi4io::RDVR3_Psi4, 685
forcebalance::psi4io::THCDF_Psi4, 730
forcebalance::target::RemoteTarget, 699
forcebalance::target::Target, 714
forcebalance::thermo::Thermo, 746
forcebalance::tinkerio::AbInitio_TINKER, 203
forcebalance::tinkerio::BindingEnergy_TINKER, 270
forcebalance::tinkerio::Interaction_TINKER, 388
forcebalance::tinkerio::Liquid_TINKER, 520
forcebalance::tinkerio::Moments_TINKER, 618
forcebalance::tinkerio::Vibration_TINKER, 820
forcebalance::vibration::Vibration, 790
hdiagd
    forcebalance::psi4io::RDVR3_Psi4, 685
Hess
    forcebalance::optimizer::Optimizer, 652
Hessian
    forcebalance::optimizer::Optimizer, 645

ITERATION
    forcebalance::optimizer, 63
ITERINIT
    forcebalance::optimizer, 63
idnr
    forcebalance::thermo::Point, 659
Implemented.Targets
    forcebalance::objective, 57
in_fd
    forcebalance::finite_difference, 26
in_fd_src
    forcebalance::finite_difference, 27
Indicate
    forcebalance::objective::Objective, 625
indicate
    forcebalance::abinitio::AbInitio, 86
    forcebalance::abinitio_internal::AbInitio_Internal, 152
    forcebalance::amber::AbInitio_AMBER, 108
    forcebalance::binding::BindingEnergy, 219
    forcebalance::gmlio::AbInitio_GMX, 130
    forcebalance::gmlio::BindingEnergy_GMX, 234

```

forcebalance::gmxio::Interaction_GMX, 352
 forcebalance::gmxio::Lipid_GMX, 437
 forcebalance::gmxio::Liquid_GMX, 473
 forcebalance::gmxio::Moments_GMX, 582
 forcebalance::gmxio::Thermo_GMX, 756
 forcebalance::gmxio::Vibration_GMX, 799
 forcebalance::interaction::Interaction, 337
 forcebalance::leastsq::LeastSquares, 401
 forcebalance::lipid::Lipid, 419
 forcebalance::liquid::Liquid, 454
 forcebalance::moments::Moments, 567
 forcebalance::openmmio::AbInitio_OpenMM, 174
 forcebalance::openmmio::BindingEnergy_OpenMM, 249
 forcebalance::openmmio::Interaction_OpenMM, 367
 forcebalance::openmmio::Liquid_OpenMM, 492
 forcebalance::openmmio::Moments_OpenMM, 597
 forcebalance::psi4io::RDVR3_Psi4, 679
 forcebalance::psi4io::THCDF_Psi4, 724
 forcebalance::target::RemoteTarget, 693
 forcebalance::thermo::Thermo, 739
 forcebalance::tinkerio::AbInitio_TINKER, 196
 forcebalance::tinkerio::BindingEnergy_TINKER, 264
 forcebalance::tinkerio::Interaction_TINKER, 382
 forcebalance::tinkerio::Liquid_TINKER, 512
 forcebalance::tinkerio::Moments_TINKER, 612
 forcebalance::tinkerio::Vibration_TINKER, 814
 forcebalance::vibration::Vibration, 784
 inter_opts
 forcebalance::binding::BindingEnergy, 225
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::openmmio::BindingEnergy_OpenMM, 255
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
 interaction.py, 828
 interaction_energy
 forcebalance::gmxio::GMX, 322
 forcebalance::openmmio::OpenMM, 632
 forcebalance::tinkerio::TINKER, 769
 invdists
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
 invert_svd
 forcebalance::nifty, 50
 iocc
 forcebalance::parser, 66
 is_charmm_coord
 forcebalance::molecule, 40
 is_gro_box
 forcebalance::molecule, 41
 is_gro_coord
 forcebalance::molecule, 41
 is_mol2_atom
 forcebalance::amberio, 18
 isdata
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
 isdecimal
 forcebalance::nifty, 50
 isfloat
 forcebalance::molecule, 42
 forcebalance::nifty, 50
 isint
 forcebalance::molecule, 42
 forcebalance::nifty, 50
 itype
 forcebalance::amberio::FrcMod_Reader, 310
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 212
 forcebalance::custom_io::Gen_Reader, 316
 forcebalance::gmxio::ITP_Reader, 393
 forcebalance::mol2io::Mol2_Reader, 535
 forcebalance::openmmio::OpenMM_Reader, 639
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
 forcebalance::qcchemio::QCIn_Reader, 662
 forcebalance::tinkerio::Tinker_Reader, 776
 kb
 forcebalance::nifty, 56
 key
 forcebalance::tinkerio::TINKER, 772
 L
 forcebalance::chemistry, 20
 forcebalance::molecule::MyG, 622
 L2_norm
 forcebalance::objective::Penalty, 655
 LAST_MVALS
 forcebalance::leastsq, 34
 label
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::tinkerio::Interaction_TINKER, 388
 Labels
 forcebalance::gmxio::Lipid_GMX, 444
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::lipid::Lipid, 426
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
 last_amom
 forcebalance::psi4io::GBS_Reader, 313

last_traj
 forcebalance::gmxio::Lipid_GMX, 444
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::lipid::Lipid, 426
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
LastMvals
 forcebalance::leastsq, 34
leastsq.py, 828
Leave
 forcebalance::nifty, 51
Letters
 forcebalance::objective, 58
LfDict
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 481
LfDict_New
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 481
line
 forcebalance::chemistry, 20
linedestroy_save
 forcebalance::forcefield::FF, 304
linedestroy_this
 forcebalance::forcefield::FF, 304
link_dir_contents
 forcebalance::nifty, 51
link_from_tempdir
 forcebalance::abinitio::AbInitio, 86
 forcebalance::abinitio_internal::AbInitio_Internal, 152
 forcebalance::amberio::AbInitio_AMBER, 108
 forcebalance::binding::BindingEnergy, 219
 forcebalance::counterpoise::Counterpoise, 282
 forcebalance::gmxio::AbInitio_GMX, 130
 forcebalance::gmxio::BindingEnergy_GMX, 234
 forcebalance::gmxio::Interaction_GMX, 352
 forcebalance::gmxio::Lipid_GMX, 437
 forcebalance::gmxio::Liquid_GMX, 473
 forcebalance::gmxio::Moments_GMX, 582
 forcebalance::gmxio::Thermo_GMX, 756
 forcebalance::gmxio::Vibration_GMX, 799
 forcebalance::interaction::Interaction, 337
 forcebalance::leastsq::LeastSquares, 401
 forcebalance::lipid::Lipid, 419
 forcebalance::liquid::Liquid, 454
 forcebalance::moments::Moments, 567
 forcebalance::openmmio::AbInitio_OpenMM, 174
 forcebalance::openmmio::BindingEnergy_OpenMM, 249
 forcebalance::openmmio::Interaction_OpenMM, 367
 forcebalance::openmmio::Liquid_OpenMM, 492
 forcebalance::openmmio::Moments_OpenMM, 597
 forcebalance::psi4io::RDVR3_Psi4, 679
 forcebalance::psi4io::THCDF_Psi4, 724
 forcebalance::target::RemoteTarget, 693
 forcebalance::target::Target, 708
 forcebalance::thermo::Thermo, 739
 forcebalance::tinkerio::AbInitio_TINKER, 196
 forcebalance::tinkerio::BindingEnergy_TINKER, 264
 forcebalance::tinkerio::Interaction_TINKER, 382
 forcebalance::tinkerio::Liquid_TINKER, 512
 forcebalance::tinkerio::Moments_TINKER, 612
 forcebalance::tinkerio::Vibration_TINKER, 814
 forcebalance::vibration::Vibration, 784
LinkFile
 forcebalance::nifty, 51
links
 forcebalance::gmxio::GMX, 323
lipid.py, 829
lipid_mol
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::lipid::Lipid, 426
liquid.py, 829
liquid_mol
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
list_map
 forcebalance::forcefield::FF, 301
In
 forcebalance::amberio::FrcMod_Reader, 310
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 212
 forcebalance::custom_io::Gen_Reader, 316
 forcebalance::gmxio::ITP_Reader, 393
 forcebalance::mol2io::Mol2_Reader, 535
 forcebalance::openmmio::OpenMM_Reader, 639
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
 forcebalance::qcchemio::QCIn_Reader, 662
 forcebalance::tinkerio::Tinker_Reader, 776
load_cp
 forcebalance::counterpoise::Counterpoise, 282
load_frames
 forcebalance::molecule::Molecule, 547
loadxyz
 forcebalance::counterpoise::Counterpoise, 282
logger
 forcebalance::abinitio, 16
 forcebalance::amberio, 18
 forcebalance::binding, 19
 forcebalance::counterpoise, 22
 forcebalance::engine, 24
 forcebalance::finite_difference, 27
 forcebalance::forcefield, 29
 forcebalance::gmxio, 33

forcebalance::interaction, 34
 forcebalance::leastsq, 34
 forcebalance::lipid, 35
 forcebalance::liquid, 35
 forcebalance::moments, 44
 forcebalance::nifty, 56
 forcebalance::objective, 58
 forcebalance::openmmio, 61
 forcebalance::optimizer, 63
 forcebalance::parser, 66
 forcebalance::psi4io, 68
 forcebalance::qcchemio, 69
 forcebalance::quantity, 71
 forcebalance::target, 71
 forcebalance::thermo, 71
 forcebalance::tinkerio, 73
 forcebalance::vibration, 74
LookupByMass
 forcebalance::chemistry, 20
lp_dump
 forcebalance::nifty, 51
lp_load
 forcebalance::nifty, 51
MAQ
 forcebalance::leastsq::LeastSquares, 407
 forcebalance::psi4io::THCDF_Psi4, 730
MBarEnergy
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
MP2_Energy
 forcebalance::psi4io::THCDF_Psi4, 730
MTSVVRIntegrator
 forcebalance::openmmio, 60
main
 forcebalance::molecule, 42
MainOptimizer
 forcebalance::optimizer::Optimizer, 645
mainsections
 forcebalance::parser, 67
make
 forcebalance::forcefield::FF, 301
make_redirect
 forcebalance::forcefield::FF, 302
map
 forcebalance::forcefield::FF, 304
mass
 forcebalance::openmmio::OpenMM, 635
maxrd
 forcebalance::abinitio::AbInitio, 87
 forcebalance::abinitio_internal::AbInitio_Internal, 153
 forcebalance::amberio::AbInitio_AMBER, 109
 forcebalance::binding::BindingEnergy, 220
 forcebalance::counterpoise::Counterpoise, 284
 forcebalance::gmxio::AbInitio_GMX, 131
 forcebalance::gmxio::BindingEnergy_GMX, 235
 forcebalance::gmxio::Interaction_GMX, 353
 forcebalance::gmxio::Lipid_GMX, 438
 forcebalance::gmxio::Liquid_GMX, 474
 forcebalance::gmxio::Moments_GMX, 583
 forcebalance::gmxio::Thermo_GMX, 757
 forcebalance::gmxio::Vibration_GMX, 800
 forcebalance::interaction::Interaction, 338
 forcebalance::leastsq::LeastSquares, 401
 forcebalance::lipid::Lipid, 420
 forcebalance::liquid::Liquid, 455
 forcebalance::moments::Moments, 568
 forcebalance::openmmio::AbInitio_OpenMM, 175
 forcebalance::openmmio::BindingEnergy_OpenMM, 250
 forcebalance::openmmio::Interaction_OpenMM, 368
 forcebalance::openmmio::Liquid_OpenMM, 493
 forcebalance::openmmio::Moments_OpenMM, 598
 forcebalance::psi4io::RDVR3_Psi4, 680
 forcebalance::psi4io::THCDF_Psi4, 724
 forcebalance::target::RemoteTarget, 693
 forcebalance::target::Target, 708
 forcebalance::thermo::Thermo, 740
 forcebalance::tinkerio::AbInitio_TINKER, 197
 forcebalance::tinkerio::BindingEnergy_TINKER, 265
 forcebalance::tinkerio::Interaction_TINKER, 383
 forcebalance::tinkerio::Liquid_TINKER, 513
 forcebalance::tinkerio::Moments_TINKER, 613
 forcebalance::tinkerio::Vibration_TINKER, 815
 forcebalance::vibration::Vibration, 785
md
 forcebalance::gmxio::GMX, 323
mdene
 forcebalance::gmxio::GMX, 326
mdp
 forcebalance::gmxio::GMX, 326
mdpx
 forcebalance::gmxio::Thermo_GMX, 763
mdtraj
 forcebalance::gmxio::GMX, 326
 forcebalance::tinkerio::TINKER, 772
mean_stderr
 forcebalance::quantity, 70
measure_dihedrals
 forcebalance::molecule::Molecule, 547
meta_get
 forcebalance::abinitio::AbInitio, 87
 forcebalance::abinitio_internal::AbInitio_Internal, 153
 forcebalance::amberio::AbInitio_AMBER, 109

forcebalance::binding::BindingEnergy, 220
 forcebalance::counterpoise::Counterpoise, 284
 forcebalance::gmxio::AbInitio_GMX, 131
 forcebalance::gmxio::BindingEnergy_GMX, 235
 forcebalance::gmxio::Interaction_GMX, 353
 forcebalance::gmxio::Lipid_GMX, 438
 forcebalance::gmxio::Liquid_GMX, 474
 forcebalance::gmxio::Moments_GMX, 583
 forcebalance::gmxio::Thermo_GMX, 757
 forcebalance::gmxio::Vibration_GMX, 800
 forcebalance::interaction::Interaction, 338
 forcebalance::leastsq::LeastSquares, 402
 forcebalance::lipid::Lipid, 420
 forcebalance::liquid::Liquid, 455
 forcebalance::moments::Moments, 568
 forcebalance::openmmio::AbInitio_OpenMM, 175
 forcebalance::openmmio::BindingEnergy_OpenMM, 250
 forcebalance::openmmio::Interaction_OpenMM, 368
 forcebalance::openmmio::Liquid_OpenMM, 493
 forcebalance::openmmio::Moments_OpenMM, 598
 forcebalance::psi4io::RDVR3_Psi4, 680
 forcebalance::psi4io::THCDF_Psi4, 725
 forcebalance::target::RemoteTarget, 694
 forcebalance::target::Target, 709
 forcebalance::thermo::Thermo, 740
 forcebalance::tinkerio::AbInitio_TINKER, 197
 forcebalance::tinkerio::BindingEnergy_TINKER, 265
 forcebalance::tinkerio::Interaction_TINKER, 383
 forcebalance::tinkerio::Liquid_TINKER, 513
 forcebalance::tinkerio::Moments_TINKER, 613
 forcebalance::tinkerio::Vibration_TINKER, 815
 forcebalance::vibration::Vibration, 785
 meta_indicate
 forcebalance::abinitio::AbInitio, 88
 forcebalance::abinitio_internal::AbInitio_Internal, 154
 forcebalance::amberio::AbInitio_AMBER, 110
 forcebalance::binding::BindingEnergy, 221
 forcebalance::counterpoise::Counterpoise, 285
 forcebalance::gmxio::AbInitio_GMX, 132
 forcebalance::gmxio::BindingEnergy_GMX, 236
 forcebalance::gmxio::Interaction_GMX, 354
 forcebalance::gmxio::Lipid_GMX, 439
 forcebalance::gmxio::Liquid_GMX, 475
 forcebalance::gmxio::Moments_GMX, 584
 forcebalance::gmxio::Thermo_GMX, 758
 forcebalance::gmxio::Vibration_GMX, 801
 forcebalance::interaction::Interaction, 339
 forcebalance::leastsq::LeastSquares, 403
 forcebalance::lipid::Lipid, 421
 forcebalance::liquid::Liquid, 456
 forcebalance::moments::Moments, 569
 forcebalance::openmmio::AbInitio_OpenMM, 176
 forcebalance::openmmio::BindingEnergy_OpenMM, 251
 forcebalance::openmmio::Interaction_OpenMM, 369
 forcebalance::openmmio::Liquid_OpenMM, 494
 forcebalance::openmmio::Moments_OpenMM, 599
 forcebalance::psi4io::RDVR3_Psi4, 681
 forcebalance::psi4io::THCDF_Psi4, 726
 forcebalance::target::RemoteTarget, 695
 forcebalance::target::Target, 710
 forcebalance::thermo::Thermo, 741
 forcebalance::tinkerio::AbInitio_TINKER, 198
 forcebalance::tinkerio::BindingEnergy_TINKER, 266
 forcebalance::tinkerio::Interaction_TINKER, 384
 forcebalance::tinkerio::Liquid_TINKER, 514
 forcebalance::tinkerio::Moments_TINKER, 614
 forcebalance::tinkerio::Vibration_TINKER, 816
 forcebalance::vibration::Vibration, 786
 MetaVariableNames
 forcebalance::molecule, 43
 mfnm
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::moments::Moments, 573
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::tinkerio::Moments_TINKER, 618
 MissingFileInspection
 forcebalance::nifty, 51
 mktransmat
 forcebalance::forcefield::FF, 302
 mmopts
 forcebalance::openmmio::OpenMM, 635
 mod
 forcebalance::openmmio::OpenMM, 635
 mol
 forcebalance::abinitio::AbInitio, 93
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::gmxio::GMX, 326
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::gmxio::ITP_Reader, 393
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::openmmio::OpenMM, 635
 forcebalance::tinkerio::AbInitio_TINKER, 204
 forcebalance::tinkerio::Interaction_TINKER, 388
 forcebalance::tinkerio::TINKER, 772
 Mol2.py, 829
 mol2_pdct
 forcebalance::amberio, 18
 forcebalance::mol2io, 36
 mol2io.py, 830
 mol_name

forcebalance::Mol2::mol2, 527
 mol_type
 forcebalance::Mol2::mol2, 527
 molatom
 forcebalance::amberio::FrcMod_Reader, 310
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 212
 forcebalance::custom_io::Gen_Reader, 316
 forcebalance::gmxio::ITP_Reader, 393
 forcebalance::mol2io::Mol2_Reader, 535
 forcebalance::openmmio::OpenMM_Reader, 639
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
 forcebalance::qchemio::QCIn_Reader, 662
 forcebalance::tinkerio::Tinker_Reader, 776
 molecular_dynamics
 forcebalance::gmxio::GMX, 323
 forcebalance::openmmio::OpenMM, 632
 forcebalance::tinkerio::TINKER, 769
 molecule.py, 830
 Molecules
 forcebalance::amberio::FrcMod_Reader, 310
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 212
 forcebalance::custom_io::Gen_Reader, 316
 forcebalance::gmxio::ITP_Reader, 393
 forcebalance::mol2io::Mol2_Reader, 535
 forcebalance::openmmio::OpenMM_Reader, 639
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
 forcebalance::psi4io::THCDF_Psi4, 730
 forcebalance::qchemio::QCIn_Reader, 662
 forcebalance::tinkerio::Tinker_Reader, 776
 molecules
 forcebalance::molecule::Molecule, 558
 forcebalance::psi4io::RDVR3_Psi4, 685
 moments.py, 832
 monotonic
 forcebalance::nifty, 51
 multiD_statisticalInefficiency
 forcebalance::nifty, 51
 multipole_moments
 forcebalance::gmxio::GMX, 324
 forcebalance::openmmio::OpenMM, 633
 forcebalance::tinkerio::TINKER, 770
 mvals0
 forcebalance::optimizer::Optimizer, 652
 mvals_bak
 forcebalance::optimizer::Optimizer, 652
 n_snaps
 forcebalance::gmxio::GMX, 324
 na
 forcebalance::counterpoise::Counterpoise, 289
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::moments::Moments, 573
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::tinkerio::Moments_TINKER, 618
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
 name
 forcebalance::engine::Engine, 292
 forcebalance::gmxio::GMX, 326
 forcebalance::openmmio::OpenMM, 635
 forcebalance::quantity::Quantity, 664
 forcebalance::quantity::Quantity_Density, 666
 forcebalance::quantity::Quantity_H_vap, 668
 forcebalance::tinkerio::TINKER, 772
 nbcharges
 forcebalance::openmmio::OpenMM, 635
 nbtype
 forcebalance::gmxio::ITP_Reader, 393
 ndof
 forcebalance::openmmio::OpenMM, 635
 ndtypes
 forcebalance::custom_io, 23
 forcebalance::qchemio, 69
 nesp
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
 new_vsites
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
 NewtonCG
 forcebalance::optimizer::Optimizer, 646
 NewtonRaphson
 forcebalance::optimizer::Optimizer, 646
 nf_err
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
 nf_err_pct
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138

forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
nf_ref
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
nftqm
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
nftytes
 forcebalance::gmxio, 33
nifty.py, 832
nnf
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
nodematch
 forcebalance::molecule, 42
nomnom
 forcebalance::nifty::LineChunker, 410
normal_modes
 forcebalance::gmxio::GMX, 324
 forcebalance::openmmio::OpenMM, 633
 forcebalance::tinkerio::TINKER, 770
np
 forcebalance::forcefield::FF, 304
 forcebalance::optimizer::Optimizer, 652
nparticles
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
npt_simulation
 forcebalance::gmxio::Lipid_GMX, 440
 forcebalance::gmxio::Liquid_GMX, 476
 forcebalance::lipid::Lipid, 422
 forcebalance::liquid::Liquid, 457
 forcebalance::openmmio::Liquid_OpenMM, 495
 forcebalance::tinkerio::Liquid_TINKER, 515
nptfiles
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
nptpx
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 520
ns
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::counterpoise::Counterpoise, 289
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::tinkerio::AbInitio_TINKER, 204
 forcebalance::tinkerio::Interaction_TINKER, 388
ntq
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
num_atoms
 forcebalance::Mol2::mol2, 527
num_bonds
 forcebalance::Mol2::mol2, 527
num_compounds
 forcebalance::Mol2::mol2_set, 538
num_feat
 forcebalance::Mol2::mol2, 527
num_sets
 forcebalance::Mol2::mol2, 527
num_subst
 forcebalance::Mol2::mol2, 527
ObjDict
 forcebalance::objective::Objective, 625
ObjDict_Last
 forcebalance::objective::Objective, 625
objd
 forcebalance::psi4io::RDVR3_Psi4, 685
Objective
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 481
 forcebalance::gmxio::Thermo_GMX, 763
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::optimizer::Optimizer, 652
 forcebalance::thermo::Thermo, 746

forcebalance::tinkerio::Liquid_TINKER, 520
objective
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::binding::BindingEnergy, 225
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::interaction::Interaction, 343
 forcebalance::leastsq::LeastSquares, 407
 forcebalance::moments::Moments, 573
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::openmmio::BindingEnergy_OpenMM, 255
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::psi4io::RDVR3_Psi4, 685
 forcebalance::psi4io::THCDF_Psi4, 730
 forcebalance::tinkerio::AbInitio_TINKER, 204
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
 forcebalance::tinkerio::Interaction_TINKER, 388
 forcebalance::tinkerio::Moments_TINKER, 618
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
objective.py, 834
objective_term
 forcebalance::gmxio::Lipid_GMX, 440
 forcebalance::gmxio::Liquid_GMX, 476
 forcebalance::gmxio::Thermo_GMX, 759
 forcebalance::lipid::Lipid, 422
 forcebalance::liquid::Liquid, 457
 forcebalance::openmmio::Liquid_OpenMM, 495
 forcebalance::thermo::Thermo, 742
 forcebalance::tinkerio::Liquid_TINKER, 515
objfiles
 forcebalance::psi4io::RDVR3_Psi4, 685
objvals
 forcebalance::psi4io::RDVR3_Psi4, 685
onefile
 forcebalance::nifty, 52
openmm_boxes
 forcebalance::molecule::Molecule, 547
openmm_positions
 forcebalance::molecule::Molecule, 547
openmmio.py, 835
openmmxml
 forcebalance::forcefield::FF, 304
OptTab
 forcebalance::optimizer::Optimizer, 653
optimize
 forcebalance::gmxio::GMX, 324
 forcebalance::openmmio::OpenMM, 633
 forcebalance::tinkerio::TINKER, 771
optimizer.py, 836
origin_atom_id
 forcebalance::Mol2::mol2_bond, 532
orthogonalize
 forcebalance::nifty, 52
out
 forcebalance::Mol2::mol2, 525
output.py, 837
overlaps
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
PT.py, 838
ParsTab
 forcebalance::parser, 67
parse
 forcebalance::Mol2::mol2, 525
 forcebalance::Mol2::mol2_atom, 528
 forcebalance::Mol2::mol2_bond, 531
 forcebalance::Mol2::mol2_set, 538
parse_atomtype.line
 forcebalance::gmxio, 31
parse_inputs
 forcebalance::parser, 65
parse_interactions
 forcebalance::binding, 19
parser.py, 837
pathwise_rmsd
 forcebalance::molecule::Molecule, 547
patoms
 forcebalance::forcefield::FF, 304
pbc
 forcebalance::gmxio::GMX, 326
 forcebalance::openmmio::OpenMM, 635
 forcebalance::tinkerio::TINKER, 772
pdb
 forcebalance::openmmio::OpenMM, 635
pdict
 forcebalance::amberio::FrcMod_Reader, 310
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 212
 forcebalance::custom_io, 23
 forcebalance::custom_io::Gen_Reader, 316
 forcebalance::gmxio, 33
 forcebalance::gmxio::ITP_Reader, 394
 forcebalance::mol2io::Mol2_Reader, 535
 forcebalance::openmmio, 61
 forcebalance::openmmio::OpenMM_Reader, 639
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
 forcebalance::qchemio, 69

forcebalance::qchemio::QCIn_Reader, 662
 forcebalance::tinkerio, 73
 forcebalance::tinkerio::Tinker_Reader, 776
Pen_Names
 forcebalance::objective::Penalty, 656
Pen_Tab
 forcebalance::objective::Penalty, 656
Penalty
 forcebalance::objective::Objective, 625
 forcebalance::optimizer::Optimizer, 653
PeriodicTable
 forcebalance::chemistry, 20
 forcebalance::molecule, 43
 forcebalance::PT, 68
pfields
 forcebalance::forcefield::FF, 305
ptypes
 forcebalance::gmxio, 33
pgrad
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amber::AbInitio_AMBER, 116
 forcebalance::binding::BindingEnergy, 225
 forcebalance::counterpoise::Counterpoise, 289
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Thermo_GMX, 763
 forcebalance::gmxio::Vibration_GMX, 805
 forcebalance::interaction::Interaction, 343
 forcebalance::leastsq::LeastSquares, 407
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 462
 forcebalance::moments::Moments, 573
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::openmmio::BindingEnergy_OpenMM, 255
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::psi4io::RDVR3_Psi4, 685
 forcebalance::psi4io::THCDF_Psi4, 730
 forcebalance::target::RemoteTarget, 699
 forcebalance::target::Target, 714
 forcebalance::thermo::Thermo, 746
 forcebalance::tinkerio::AbInitio_TINKER, 204
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
 forcebalance::tinkerio::Interaction_TINKER, 388
 forcebalance::tinkerio::Liquid_TINKER, 521
 forcebalance::tinkerio::Moments_TINKER, 618
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
PhasePoints
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 500
 forcebalance::tinkerio::Liquid_TINKER, 521
platform
 forcebalance::openmmio::OpenMM, 635
platname
 forcebalance::openmmio::OpenMM, 635
plist
 forcebalance::forcefield::FF, 305
pmat2d
 forcebalance::nifty, 52
point
 forcebalance::psi4io::Grid_Reader, 329
points
 forcebalance::gmxio::Thermo_GMX, 763
 forcebalance::thermo::Thermo, 746
polarization_correction
 forcebalance::gmxio::Lipid_GMX, 440
 forcebalance::gmxio::Liquid_GMX, 476
 forcebalance::lipid::Lipid, 422
 forcebalance::liquid::Liquid, 457
 forcebalance::openmmio::Liquid_OpenMM, 495
 forcebalance::tinkerio::Liquid_TINKER, 515
positive_resid
 forcebalance::molecule::Molecule, 558
Powell
 forcebalance::optimizer::Optimizer, 647
Pp
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::gmxio::Thermo_GMX, 763
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 462
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::thermo::Thermo, 746
 forcebalance::tinkerio::Liquid_TINKER, 521
precision
 forcebalance::openmmio::OpenMM, 635
prefactor
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::tinkerio::Interaction_TINKER, 388
prepare
 forcebalance::engine::Engine, 292
 forcebalance::gmxio::GMX, 325
 forcebalance::openmmio::OpenMM, 634
 forcebalance::tinkerio::TINKER, 771
prepare_temp_directory

forcebalance::amberio::AbInitio_AMBER, 111
 forcebalance::gmxio::Lipid_GMX, 441
 forcebalance::gmxio::Liquid_GMX, 477
 forcebalance::lipid::Lipid, 423
 forcebalance::liquid::Liquid, 458
 forcebalance::openmmio::Liquid_OpenMM, 496
 forcebalance::psi4io::THCDF_Psi4, 727
 forcebalance::tinkerio::Liquid_TINKER, 516
PrepareVirtualSites
 forcebalance::openmmio, 61
pressure
 forcebalance::quantity::Quantity, 664
 forcebalance::quantity::Quantity_Density, 666
 forcebalance::quantity::Quantity_H_vap, 668
 forcebalance::thermo::Point, 659
prev_bad
 forcebalance::optimizer::Optimizer, 653
print_map
 forcebalance::forcefield::FF, 302
PrintDict
 forcebalance::binding::BindingEnergy, 225
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::openmmio::BindingEnergy_OpenMM,
 255
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
PrintOptionDict
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::BaseClass, 209
 forcebalance::binding::BindingEnergy, 225
 forcebalance::counterpoise::Counterpoise, 289
 forcebalance::engine::Engine, 292
 forcebalance::forcefield::FF, 305
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::gmxio::GMX, 326
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Thermo_GMX, 763
 forcebalance::gmxio::Vibration_GMX, 806
 forcebalance::interaction::Interaction, 343
 forcebalance::leastsq::LeastSquares, 407
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 462
 forcebalance::moments::Moments, 573
 forcebalance::objective::Objective, 626
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::openmmio::BindingEnergy_OpenMM,
 255
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::openmmio::Liquid_OpenMM, 501

forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::openmmio::OpenMM, 636
 forcebalance::optimizer::Optimizer, 653
 forcebalance::psi4io::RDVR3_Psi4, 685
 forcebalance::psi4io::THCDF_Psi4, 731
 forcebalance::target::RemoteTarget, 699
 forcebalance::target::Target, 714
 forcebalance::thermo::Thermo, 746
 forcebalance::tinkerio::AbInitio_TINKER, 204
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
 forcebalance::tinkerio::Interaction_TINKER, 388
 forcebalance::tinkerio::Liquid_TINKER, 521
 forcebalance::tinkerio::Moments_TINKER, 618
 forcebalance::tinkerio::TINKER, 772
 forcebalance::tinkerio::Vibration_TINKER, 821
 forcebalance::vibration::Vibration, 790
printcool
 forcebalance::nifty, 52
printcool_dictionary
 forcebalance::nifty, 53
printcool_table
 forcebalance::abinitio::AbInitio, 89
 forcebalance::abinitio_internal::AbInitio_Internal, 155
 forcebalance::amberio::AbInitio_AMBER, 111
 forcebalance::binding::BindingEnergy, 222
 forcebalance::counterpoise::Counterpoise, 286
 forcebalance::gmxio::AbInitio_GMX, 133
 forcebalance::gmxio::BindingEnergy_GMX, 237
 forcebalance::gmxio::Interaction_GMX, 355
 forcebalance::gmxio::Lipid_GMX, 441
 forcebalance::gmxio::Liquid_GMX, 477
 forcebalance::gmxio::Moments_GMX, 585
 forcebalance::gmxio::Thermo_GMX, 759
 forcebalance::gmxio::Vibration_GMX, 802
 forcebalance::interaction::Interaction, 340
 forcebalance::leastsq::LeastSquares, 404
 forcebalance::lipid::Lipid, 423
 forcebalance::liquid::Liquid, 458
 forcebalance::moments::Moments, 570
 forcebalance::openmmio::AbInitio_OpenMM, 177
 forcebalance::openmmio::BindingEnergy_OpenMM,
 252
 forcebalance::openmmio::Interaction_OpenMM, 370
 forcebalance::openmmio::Liquid_OpenMM, 496
 forcebalance::openmmio::Moments_OpenMM, 600
 forcebalance::psi4io::RDVR3_Psi4, 682
 forcebalance::psi4io::THCDF_Psi4, 727
 forcebalance::target::RemoteTarget, 696
 forcebalance::target::Target, 711
 forcebalance::thermo::Thermo, 742
 forcebalance::tinkerio::AbInitio_TINKER, 199
 forcebalance::tinkerio::BindingEnergy_TINKER, 267
 forcebalance::tinkerio::Interaction_TINKER, 385
 forcebalance::tinkerio::Liquid_TINKER, 516

forcebalance::tinkerio::Moments_TINKER, 615
 forcebalance::tinkerio::Vibration_TINKER, 817
 forcebalance::vibration::Vibration, 787
 printsection
 forcebalance::parser, 65
 prm
 forcebalance::tinkerio::TINKER, 772
 prmdestroy_save
 forcebalance::forcefield::FF, 305
 prmdestroy_this
 forcebalance::forcefield::FF, 305
 process_vectors
 forcebalance::gmxio::Vibration_GMX, 802
 forcebalance::tinkerio::Vibration_TINKER, 817
 forcebalance::vibration::Vibration, 787
 psi4io.py, 838
 ptyp
 forcebalance::objective::Penalty, 656
 push
 forcebalance::nifty::LineChunker, 410
 pvals0
 forcebalance::forcefield::FF, 305
 pvec
 forcebalance::molecule, 42
 pvec1d
 forcebalance::nifty, 54

 QChem_Dielectric_Energy
 forcebalance::qchemio, 69
 qchemio.py, 838
 qfnm
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::gmxio::Interaction_GMX, 358
 forcebalance::interaction::Interaction, 343
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::openmmio::Interaction_OpenMM, 373
 forcebalance::tinkerio::AbInitio_TINKER, 204
 forcebalance::tinkerio::Interaction_TINKER, 388
 qid
 forcebalance::forcefield::FF, 305
 qid2
 forcebalance::forcefield::FF, 305
 qmap
 forcebalance::forcefield::FF, 305
 qmatoms
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 116
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204

 qmboltz_wts
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 160
 forcebalance::amberio::AbInitio_AMBER, 117
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::openmmio::AbInitio_OpenMM, 182
 forcebalance::tinkerio::AbInitio_TINKER, 204
 quantity.py, 839
 QuantumVariableNames
 forcebalance::molecule, 43
 queue_up
 forcebalance::nifty, 54
 queue_up_src_dest
 forcebalance::nifty, 54

 r_options
 forcebalance::target::RemoteTarget, 699
 r_tgt_opts
 forcebalance::target::RemoteTarget, 699
 RMSDDict
 forcebalance::binding::BindingEnergy, 225
 forcebalance::gmxio::BindingEnergy_GMX, 241
 forcebalance::openmmio::BindingEnergy_OpenMM,
 256
 forcebalance::tinkerio::BindingEnergy_TINKER, 271
 radian
 forcebalance::molecule, 43
 Radii
 forcebalance::chemistry, 21
 forcebalance::molecule, 43
 radii
 forcebalance::psi4io::Grid_Reader, 329
 radius_of_gyration
 forcebalance::molecule::Molecule, 548
 rd
 forcebalance::abinitio::AbInitio, 94
 forcebalance::abinitio_internal::AbInitio_Internal, 161
 forcebalance::amberio::AbInitio_AMBER, 117
 forcebalance::binding::BindingEnergy, 225
 forcebalance::counterpoise::Counterpoise, 289
 forcebalance::gmxio::AbInitio_GMX, 138
 forcebalance::gmxio::BindingEnergy_GMX, 240
 forcebalance::gmxio::Interaction_GMX, 359
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::gmxio::Moments_GMX, 588
 forcebalance::gmxio::Thermo_GMX, 763
 forcebalance::gmxio::Vibration_GMX, 806
 forcebalance::interaction::Interaction, 343
 forcebalance::leastsq::LeastSquares, 407
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 462
 forcebalance::moments::Moments, 573
 forcebalance::openmmio::AbInitio_OpenMM, 182

forcebalance::openmmio::BindingEnergy_OpenMM,
 255
 forcebalance::openmmio::Interaction_OpenMM, 374
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::openmmio::Moments_OpenMM, 603
 forcebalance::psi4io::RDVR3_Psi4, 685
 forcebalance::psi4io::THCDF_Psi4, 731
 forcebalance::target::RemoteTarget, 699
 forcebalance::target::Target, 714
 forcebalance::thermo::Thermo, 746
 forcebalance::tinkerio::AbInitio_TINKER, 204
 forcebalance::tinkerio::BindingEnergy_TINKER, 270
 forcebalance::tinkerio::Interaction_TINKER, 389
 forcebalance::tinkerio::Liquid_TINKER, 521
 forcebalance::tinkerio::Moments_TINKER, 618
 forcebalance::tinkerio::Vibration_TINKER, 821
 forcebalance::vibration::Vibration, 791
read
 forcebalance::abinitio::AbInitio, 89
 forcebalance::abinitio_internal::AbInitio_Internal, 155
 forcebalance::amberio::AbInitio_AMBER, 111
 forcebalance::binding::BindingEnergy, 222
 forcebalance::counterpoise::Counterpoise, 286
 forcebalance::gmxio::AbInitio_GMX, 133
 forcebalance::gmxio::BindingEnergy_GMX, 237
 forcebalance::gmxio::Interaction_GMX, 355
 forcebalance::gmxio::Lipid_GMX, 441
 forcebalance::gmxio::Liquid_GMX, 477
 forcebalance::gmxio::Moments_GMX, 585
 forcebalance::gmxio::Thermo_GMX, 760
 forcebalance::gmxio::Vibration_GMX, 803
 forcebalance::interaction::Interaction, 340
 forcebalance::leastsq::LeastSquares, 404
 forcebalance::lipid::Lipid, 423
 forcebalance::liquid::Liquid, 458
 forcebalance::moments::Moments, 570
 forcebalance::openmmio::AbInitio_OpenMM, 177
 forcebalance::openmmio::BindingEnergy_OpenMM,
 252
 forcebalance::openmmio::Interaction_OpenMM, 370
 forcebalance::openmmio::Liquid_OpenMM, 496
 forcebalance::openmmio::Moments_OpenMM, 600
 forcebalance::psi4io::RDVR3_Psi4, 682
 forcebalance::psi4io::THCDF_Psi4, 728
 forcebalance::target::RemoteTarget, 699
 forcebalance::target::Target, 711
 forcebalance::thermo::Thermo, 743
 forcebalance::tinkerio::AbInitio_TINKER, 199
 forcebalance::tinkerio::BindingEnergy_TINKER, 267
 forcebalance::tinkerio::Interaction_TINKER, 385
 forcebalance::tinkerio::Liquid_TINKER, 516
 forcebalance::tinkerio::Moments_TINKER, 615
 forcebalance::tinkerio::Vibration_TINKER, 818
 forcebalance::vibration::Vibration, 788
read_Ograds
 forcebalance::abinitio::AbInitio, 90
 forcebalance::abinitio_internal::AbInitio_Internal, 156
 forcebalance::amberio::AbInitio_AMBER, 112
 forcebalance::binding::BindingEnergy, 223
 forcebalance::counterpoise::Counterpoise, 287
 forcebalance::gmxio::AbInitio_GMX, 134
 forcebalance::gmxio::BindingEnergy_GMX, 238
 forcebalance::gmxio::Interaction_GMX, 356
 forcebalance::gmxio::Lipid_GMX, 442
 forcebalance::gmxio::Liquid_GMX, 478
 forcebalance::gmxio::Moments_GMX, 586
 forcebalance::gmxio::Thermo_GMX, 760
 forcebalance::gmxio::Vibration_GMX, 803
 forcebalance::interaction::Interaction, 341
 forcebalance::leastsq::LeastSquares, 405
 forcebalance::lipid::Lipid, 424
 forcebalance::liquid::Liquid, 459
 forcebalance::moments::Moments, 571
 forcebalance::openmmio::AbInitio_OpenMM, 178
 forcebalance::openmmio::BindingEnergy_OpenMM,
 253
 forcebalance::openmmio::Interaction_OpenMM, 371
 forcebalance::openmmio::Liquid_OpenMM, 497
 forcebalance::openmmio::Moments_OpenMM, 601
 forcebalance::psi4io::RDVR3_Psi4, 683
 forcebalance::psi4io::THCDF_Psi4, 728
 forcebalance::target::RemoteTarget, 697
 forcebalance::target::Target, 712
 forcebalance::thermo::Thermo, 743
 forcebalance::tinkerio::AbInitio_TINKER, 200
 forcebalance::tinkerio::BindingEnergy_TINKER, 268
 forcebalance::tinkerio::Interaction_TINKER, 386
 forcebalance::tinkerio::Liquid_TINKER, 517
 forcebalance::tinkerio::Moments_TINKER, 616
 forcebalance::tinkerio::Vibration_TINKER, 818
 forcebalance::vibration::Vibration, 788
Read_Tab
 forcebalance::molecule::Molecule, 559
read_arc
 forcebalance::molecule::Molecule, 548
read_charmm
 forcebalance::molecule::Molecule, 549
read_com
 forcebalance::molecule::Molecule, 549
read_data
 forcebalance::gmxio::Lipid_GMX, 442
 forcebalance::gmxio::Liquid_GMX, 478
 forcebalance::lipid::Lipid, 424
 forcebalance::liquid::Liquid, 459
 forcebalance::openmmio::Liquid_OpenMM, 497
 forcebalance::tinkerio::Liquid_TINKER, 517
read_dcd
 forcebalance::molecule::Molecule, 550

```

read_gro
    forcebalance::molecule::Molecule, 550
read_indicate
    forcebalance::abinitio::AbInitio, 95
    forcebalance::abinitio_internal::AbInitio_Internal, 161
    forcebalance::amberio::AbInitio_AMBER, 117
    forcebalance::binding::BindingEnergy, 225
    forcebalance::counterpoise::Counterpoise, 289
    forcebalance::gmxio::AbInitio_GMX, 139
    forcebalance::gmxio::BindingEnergy_GMX, 240
    forcebalance::gmxio::Interaction_GMX, 359
    forcebalance::gmxio::Lipid_GMX, 445
    forcebalance::gmxio::Liquid_GMX, 482
    forcebalance::gmxio::Moments_GMX, 588
    forcebalance::gmxio::Thermo_GMX, 763
    forcebalance::gmxio::Vibration_GMX, 806
    forcebalance::interaction::Interaction, 344
    forcebalance::leastsq::LeastSquares, 407
    forcebalance::lipid::Lipid, 427
    forcebalance::liquid::Liquid, 463
    forcebalance::moments::Moments, 573
    forcebalance::openmmio::AbInitio_OpenMM, 183
    forcebalance::openmmio::BindingEnergy_OpenMM,
        255
    forcebalance::openmmio::Interaction_OpenMM, 374
    forcebalance::openmmio::Liquid_OpenMM, 501
    forcebalance::openmmio::Moments_OpenMM, 603
    forcebalance::psi4io::RDVR3_Psi4, 685
    forcebalance::psi4io::THCDF_Psi4, 731
    forcebalance::target::RemoteTarget, 699
    forcebalance::target::Target, 714
    forcebalance::thermo::Thermo, 746
    forcebalance::tinkerio::AbInitio_TINKER, 205
    forcebalance::tinkerio::BindingEnergy_TINKER, 270
    forcebalance::tinkerio::Interaction_TINKER, 389
    forcebalance::tinkerio::Liquid_TINKER, 521
    forcebalance::tinkerio::Moments_TINKER, 618
    forcebalance::tinkerio::Vibration_TINKER, 821
    forcebalance::vibration::Vibration, 791
read_internals
    forcebalance::parser, 66
read_mdcrd
    forcebalance::molecule::Molecule, 550
read_mol2
    forcebalance::molecule::Molecule, 551
read_mvals
    forcebalance::parser, 66
read_objective
    forcebalance::abinitio::AbInitio, 95
    forcebalance::abinitio_internal::AbInitio_Internal, 161
    forcebalance::amberio::AbInitio_AMBER, 117
    forcebalance::binding::BindingEnergy, 225
    forcebalance::counterpoise::Counterpoise, 289
    forcebalance::gmxio::AbInitio_GMX, 139
    forcebalance::gmxio::BindingEnergy_GMX, 240
    forcebalance::gmxio::Interaction_GMX, 359
    forcebalance::gmxio::Lipid_GMX, 445
    forcebalance::gmxio::Liquid_GMX, 482
    forcebalance::gmxio::Moments_GMX, 588
    forcebalance::gmxio::Thermo_GMX, 763
    forcebalance::gmxio::Vibration_GMX, 806
    forcebalance::interaction::Interaction, 344
    forcebalance::leastsq::LeastSquares, 407
    forcebalance::lipid::Lipid, 427
    forcebalance::liquid::Liquid, 463
    forcebalance::moments::Moments, 573
    forcebalance::openmmio::AbInitio_OpenMM, 183
    forcebalance::openmmio::BindingEnergy_OpenMM,
        255
    forcebalance::openmmio::Interaction_OpenMM, 374
    forcebalance::openmmio::Liquid_OpenMM, 501
    forcebalance::openmmio::Moments_OpenMM, 603
    forcebalance::psi4io::RDVR3_Psi4, 686
    forcebalance::psi4io::THCDF_Psi4, 731
    forcebalance::target::RemoteTarget, 700
    forcebalance::target::Target, 714
    forcebalance::thermo::Thermo, 746
    forcebalance::tinkerio::AbInitio_TINKER, 205
    forcebalance::tinkerio::BindingEnergy_TINKER, 270
    forcebalance::tinkerio::Interaction_TINKER, 389
    forcebalance::tinkerio::Liquid_TINKER, 521
    forcebalance::tinkerio::Moments_TINKER, 618
    forcebalance::tinkerio::Vibration_TINKER, 821
    forcebalance::vibration::Vibration, 791
read_pdb
    forcebalance::molecule::Molecule, 551
read_priors
    forcebalance::parser, 66
read_pvls
    forcebalance::parser, 66
read_qcesp
    forcebalance::molecule::Molecule, 551
read_qcin
    forcebalance::molecule::Molecule, 551
read_qcout
    forcebalance::molecule::Molecule, 552
read_qdata
    forcebalance::molecule::Molecule, 552
read_reference_data
    forcebalance::abinitio::AbInitio, 90
    forcebalance::abinitio_internal::AbInitio_Internal, 156
    forcebalance::amberio::AbInitio_AMBER, 112
    forcebalance::gmxio::AbInitio_GMX, 134
    forcebalance::gmxio::Interaction_GMX, 356
    forcebalance::gmxio::Moments_GMX, 586
    forcebalance::gmxio::Vibration_GMX, 803
    forcebalance::interaction::Interaction, 341
    forcebalance::moments::Moments, 571

```

```

forcebalance::openmmio::AbInitio_OpenMM, 178
forcebalance::openmmio::Interaction_OpenMM, 371
forcebalance::openmmio::Moments_OpenMM, 601
forcebalance::tinkerio::AbInitio_TINKER, 200
forcebalance::tinkerio::Interaction_TINKER, 386
forcebalance::tinkerio::Moments_TINKER, 616
forcebalance::tinkerio::Vibration_TINKER, 818
forcebalance::vibration::Vibration, 788
read_xyz
    forcebalance::molecule::Molecule, 552
read_xyz0
    forcebalance::molecule::Molecule, 553
readchk
    forcebalance::optimizer::Optimizer, 647
Readers
    forcebalance::forcefield::FF, 305
readsrc
    forcebalance::engine::Engine, 292
    forcebalance::gmxio::GMX, 325
    forcebalance::openmmio::OpenMM, 634
    forcebalance::tinkerio::TINKER, 771
reassign
    forcebalance::gmxio::Vibration_GMX, 806
    forcebalance::tinkerio::Vibration_TINKER, 821
    forcebalance::vibration::Vibration, 791
recover
    forcebalance::optimizer::Optimizer, 647
redirect
    forcebalance::forcefield::FF, 305
ref
    forcebalance::thermo::Point, 659
ref_eigvals
    forcebalance::gmxio::Moments_GMX, 589
    forcebalance::gmxio::Vibration_GMX, 806
    forcebalance::moments::Moments, 574
    forcebalance::openmmio::Moments_OpenMM, 604
    forcebalance::tinkerio::Moments_TINKER, 619
    forcebalance::tinkerio::Vibration_TINKER, 821
    forcebalance::vibration::Vibration, 791
ref_eigvecs
    forcebalance::gmxio::Moments_GMX, 589
    forcebalance::gmxio::Vibration_GMX, 806
    forcebalance::moments::Moments, 574
    forcebalance::openmmio::Moments_OpenMM, 604
    forcebalance::tinkerio::Moments_TINKER, 619
    forcebalance::tinkerio::Vibration_TINKER, 821
    forcebalance::vibration::Vibration, 791
ref_eigvecs_nrm_mw
    forcebalance::gmxio::Vibration_GMX, 806
    forcebalance::tinkerio::Vibration_TINKER, 821
    forcebalance::vibration::Vibration, 791
ref_moments
    forcebalance::gmxio::Moments_GMX, 589
    forcebalance::moments::Moments, 574
forcebalance::openmmio::Moments_OpenMM, 604
forcebalance::tinkerio::Moments_TINKER, 616
forcebalance::tinkerio::Liquid_TINKER, 517
forcebalance::tinkerio::Vibration_TINKER, 818
forcebalance::vibration::Vibration, 788
forcebalance::openmmio::Moments_OpenMM, 604
forcebalance::tinkerio::Moments_TINKER, 619
ref_rmsd
    forcebalance::molecule::Molecule, 553
RefData
    forcebalance::gmxio::Lipid_GMX, 445
    forcebalance::gmxio::Liquid_GMX, 482
    forcebalance::lipid::Lipid, 427
    forcebalance::liquid::Liquid, 463
    forcebalance::openmmio::Liquid_OpenMM, 501
    forcebalance::tinkerio::Liquid_TINKER, 521
refresh_temp_directory
    forcebalance::abinitio::AbInitio, 91
    forcebalance::abinitio.internal::AbInitio_Internal, 157
    forcebalance::amberio::AbInitio_AMBER, 113
    forcebalance::binding::BindingEnergy, 223
    forcebalance::counterpoise::Counterpoise, 287
    forcebalance::gmxio::AbInitio_GMX, 135
    forcebalance::gmxio::BindingEnergy_GMX, 238
    forcebalance::gmxio::Interaction_GMX, 356
    forcebalance::gmxio::Lipid_GMX, 442
    forcebalance::gmxio::Liquid_GMX, 478
    forcebalance::gmxio::Moments_GMX, 586
    forcebalance::gmxio::Thermo_GMX, 760
    forcebalance::gmxio::Vibration_GMX, 803
    forcebalance::interaction::Interaction, 341
    forcebalance::leastsq::LeastSquares, 405
    forcebalance::lipid::Lipid, 424
    forcebalance::liquid::Liquid, 459
    forcebalance::moments::Moments, 571
    forcebalance::openmmio::AbInitio_OpenMM, 179
    forcebalance::openmmio::BindingEnergy_OpenMM,
        253
    forcebalance::openmmio::Interaction_OpenMM, 371
    forcebalance::openmmio::Liquid_OpenMM, 497
    forcebalance::openmmio::Moments_OpenMM, 601
    forcebalance::psi4io::RDVR3_Psi4, 683
    forcebalance::psi4io::THCDF_Psi4, 728
    forcebalance::target::RemoteTarget, 697
    forcebalance::target::Target, 712
    forcebalance::thermo::Thermo, 743
    forcebalance::tinkerio::AbInitio_TINKER, 201
    forcebalance::tinkerio::BindingEnergy_TINKER, 268
    forcebalance::tinkerio::Interaction_TINKER, 386
    forcebalance::tinkerio::Liquid_TINKER, 517
    forcebalance::tinkerio::Moments_TINKER, 616
    forcebalance::tinkerio::Vibration_TINKER, 818
    forcebalance::vibration::Vibration, 788
remote_indicate
    forcebalance::target::RemoteTarget, 700
remove_if_exists
    forcebalance::nifty, 54
removeHandler
    forcebalance::output::ForceBalanceLogger, 307

```

```

repair
    forcebalance::molecule::Molecule, 553
replace_peratom
    forcebalance::molecule::Molecule, 554
replace_peratom_conditional
    forcebalance::molecule::Molecule, 554
require
    forcebalance::molecule::Molecule, 554
require_boxes
    forcebalance::molecule::Molecule, 554
require_resid
    forcebalance::molecule::Molecule, 554
require_resname
    forcebalance::molecule::Molecule, 554
resdir
    forcebalance::optimizer::Optimizer, 653
ResetVirtualSites
    forcebalance::openmmio, 61
ResetVirtualSites_fast
    forcebalance::openmmio, 61
resid
    forcebalance::molecule::Molecule, 559
residue_distances
    forcebalance::contact, 22
resname
    forcebalance::molecule::Molecule, 559
respterm
    forcebalance::abinitio::AbInitio, 95
    forcebalance::abinitio_internal::AbInitio_Internal, 161
    forcebalance::amberio::AbInitio_AMBER, 117
    forcebalance::gmxio::AbInitio_GMX, 139
    forcebalance::openmmio::AbInitio_OpenMM, 183
    forcebalance::tinkerio::AbInitio_TINKER, 205
retrieve
    forcebalance::gmxio::Thermo_GMX, 760
    forcebalance::thermo::Thermo, 743
rigid
    forcebalance::tinkerio::TINKER, 772
rigid_water
    forcebalance::molecule::Molecule, 554
rm_gmx_baks
    forcebalance::gmxio, 31
rmsd_part
    forcebalance::binding::BindingEnergy, 225
    forcebalance::gmxio::BindingEnergy_GMX, 240
    forcebalance::openmmio::BindingEnergy_OpenMM,
        255
    forcebalance::tinkerio::BindingEnergy_TINKER, 270
root
    forcebalance::engine::Engine, 292
    forcebalance::gmxio::GMX, 326
    forcebalance::openmmio::OpenMM, 636
    forcebalance::tinkerio::TINKER, 772
row
    forcebalance::nifty, 54
rs
    forcebalance::forcefield::FF, 305
rs_override
    forcebalance::forcefield, 28
rsmake
    forcebalance::forcefield::FF, 303
Run
    forcebalance::optimizer::Optimizer, 647
rundir
    forcebalance::abinitio::AbInitio, 95
    forcebalance::abinitio_internal::AbInitio_Internal, 161
    forcebalance::amberio::AbInitio_AMBER, 117
    forcebalance::binding::BindingEnergy, 226
    forcebalance::counterpoise::Counterpoise, 289
    forcebalance::gmxio::AbInitio_GMX, 139
    forcebalance::gmxio::BindingEnergy_GMX, 241
    forcebalance::gmxio::Interaction_GMX, 359
    forcebalance::gmxio::Lipid_GMX, 445
    forcebalance::gmxio::Liquid_GMX, 482
    forcebalance::gmxio::Moments_GMX, 589
    forcebalance::gmxio::Thermo_GMX, 763
    forcebalance::gmxio::Vibration_GMX, 806
    forcebalance::interaction::Interaction, 344
    forcebalance::leastsq::LeastSquares, 407
    forcebalance::lipid::Lipid, 427
    forcebalance::liquid::Liquid, 463
    forcebalance::moments::Moments, 574
    forcebalance::openmmio::AbInitio_OpenMM, 183
    forcebalance::openmmio::BindingEnergy_OpenMM,
        256
    forcebalance::openmmio::Interaction_OpenMM, 374
    forcebalance::openmmio::Liquid_OpenMM, 501
    forcebalance::openmmio::Moments_OpenMM, 604
    forcebalance::psi4io::RDVR3_Psi4, 686
    forcebalance::psi4io::THCDF_Psi4, 731
    forcebalance::target::RemoteTarget, 700
    forcebalance::target::Target, 714
    forcebalance::thermo::Thermo, 746
    forcebalance::tinkerio::AbInitio_TINKER, 205
    forcebalance::tinkerio::BindingEnergy_TINKER, 271
    forcebalance::tinkerio::Interaction_TINKER, 389
    forcebalance::tinkerio::Liquid_TINKER, 521
    forcebalance::tinkerio::Moments_TINKER, 619
    forcebalance::tinkerio::Vibration_TINKER, 821
    forcebalance::vibration::Vibration, 791
save_mvals_to_input
    forcebalance::optimizer::Optimizer, 648
save_vmvalls
    forcebalance::abinitio::AbInitio, 95
    forcebalance::abinitio_internal::AbInitio_Internal, 161
    forcebalance::amberio::AbInitio_AMBER, 117
    forcebalance::gmxio::AbInitio_GMX, 139

```

forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::tinkerio::AbInitio_TINKER, 205
SavedMVal
 forcebalance::gmxio::Lipid_GMX, 445
 forcebalance::lipid::Lipid, 427
SavedTraj
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 463
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::tinkerio::Liquid_TINKER, 521
Scan_Values
 forcebalance::optimizer::Optimizer, 648
ScanMVals
 forcebalance::optimizer::Optimizer, 648
ScanPVals
 forcebalance::optimizer::Optimizer, 649
scd_persnap
 forcebalance::gmxio::GMX, 325
Scipy_BFGS
 forcebalance::optimizer::Optimizer, 649
ScipyOptimizer
 forcebalance::optimizer::Optimizer, 649
scripts
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::gmxio::Thermo_GMX, 763
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::tinkerio::Liquid_TINKER, 521
sec
 forcebalance::custom_io::Gen_Reader, 316
 forcebalance::gmxio::ITP_Reader, 394
 forcebalance::qchemio::QCIn_Reader, 662
section
 forcebalance::amberio::Mol2_Reader, 538
segments
 forcebalance::nifty, 54
select1
 forcebalance::gmxio::Interaction_GMX, 359
 forcebalance::interaction::Interaction, 344
 forcebalance::openmmio::Interaction_OpenMM, 374
 forcebalance::tinkerio::Interaction_TINKER, 389
select2
 forcebalance::gmxio::Interaction_GMX, 359
 forcebalance::interaction::Interaction, 344
 forcebalance::openmmio::Interaction_OpenMM, 374
 forcebalance::tinkerio::Interaction_TINKER, 389
set_atom_id
 forcebalance::Mol2::mol2_atom, 529
set_atom_name
 forcebalance::Mol2::mol2_atom, 529
set_atom_type
 forcebalance::Mol2::mol2_atom, 529
set_bond_id
 forcebalance::Mol2::mol2_bond, 532
set_bond_type
 forcebalance::Mol2::mol2_bond, 532
set_charge
 forcebalance::Mol2::mol2_atom, 529
set_charge_type
 forcebalance::Mol2::mol2, 526
set_crds
 forcebalance::Mol2::mol2_atom, 530
set_donor_acceptor_atoms
 forcebalance::Mol2::mol2, 526
set_mol_name
 forcebalance::Mol2::mol2, 526
set_mol_type
 forcebalance::Mol2::mol2, 527
set_num_atoms
 forcebalance::Mol2::mol2, 527
set_num_bonds
 forcebalance::Mol2::mol2, 527
set_num_feat
 forcebalance::Mol2::mol2, 527
set_num_sets
 forcebalance::Mol2::mol2, 527
set_num_subst
 forcebalance::Mol2::mol2, 527
set_option
 forcebalance::abinitio::AbInitio, 91
 forcebalance::abinitio.internal::AbInitio_Internal, 157
 forcebalance::amberio::AbInitio_AMBER, 113
 forcebalance::BaseClass, 209
 forcebalance::binding::BindingEnergy, 223
 forcebalance::counterpoise::Counterpoise, 287
 forcebalance::engine::Engine, 292
 forcebalance::forcefield::FF, 303
 forcebalance::gmxio::AbInitio_GMX, 135
 forcebalance::gmxio::BindingEnergy_GMX, 238
 forcebalance::gmxio::GMX, 325
 forcebalance::gmxio::Interaction_GMX, 356
 forcebalance::gmxio::Lipid_GMX, 442
 forcebalance::gmxio::Liquid_GMX, 478
 forcebalance::gmxio::Moments_GMX, 586
 forcebalance::gmxio::Thermo_GMX, 761
 forcebalance::gmxio::Vibration_GMX, 803
 forcebalance::interaction::Interaction, 341
 forcebalance::leastsq::LeastSquares, 405
 forcebalance::lipid::Lipid, 424
 forcebalance::liquid::Liquid, 459
 forcebalance::moments::Moments, 571
 forcebalance::objective::Objective, 625
 forcebalance::openmmio::AbInitio_OpenMM, 179
 forcebalance::openmmio::BindingEnergy_OpenMM,
 253
 forcebalance::openmmio::Interaction_OpenMM, 371

forcebalance::openmmio::Liquid_OpenMM, 497
 forcebalance::openmmio::Moments_OpenMM, 601
 forcebalance::openmmio::OpenMM, 634
 forcebalance::optimizer::Optimizer, 650
 forcebalance::psi4io::RDVR3_Psi4, 683
 forcebalance::psi4io::THCDF_Psi4, 728
 forcebalance::target::RemoteTarget, 697
 forcebalance::target::Target, 712
 forcebalance::thermo::Thermo, 744
 forcebalance::tinkerio::AbInitio_TINKER, 201
 forcebalance::tinkerio::BindingEnergy_TINKER, 268
 forcebalance::tinkerio::Interaction_TINKER, 386
 forcebalance::tinkerio::Liquid_TINKER, 517
 forcebalance::tinkerio::Moments_TINKER, 616
 forcebalance::tinkerio::TINKER, 771
 forcebalance::tinkerio::Vibration_TINKER, 818
 forcebalance::vibration::Vibration, 788
 set_origin_atom_id
 forcebalance::Mol2::mol2_bond, 532
 set_positions
 forcebalance::openmmio::OpenMM, 634
 set_status_bit
 forcebalance::Mol2::mol2_atom, 530
 forcebalance::Mol2::mol2_bond, 532
 set_subst_id
 forcebalance::Mol2::mol2_atom, 530
 set_subst_name
 forcebalance::Mol2::mol2_atom, 530
 set_target_atom_id
 forcebalance::Mol2::mol2_bond, 532
 SetAmoebaVirtualExclusions
 forcebalance::openmmio, 61
 setopts
 forcebalance::engine::Engine, 292
 forcebalance::gmxio::GMX, 325
 forcebalance::openmmio::OpenMM, 634
 forcebalance::tinkerio::TINKER, 771
 shell
 forcebalance::qchemio::QCIn_Reader, 662
 simkwargs
 forcebalance::openmmio::OpenMM, 636
 simpfx
 forcebalance::gmxio::Thermo_GMX, 764
 forcebalance::thermo::Thermo, 746
 Simplex
 forcebalance::optimizer::Optimizer, 650
 simulation
 forcebalance::openmmio::OpenMM, 636
 SinglePoint
 forcebalance::optimizer::Optimizer, 650
 snum
 forcebalance::qchemio::QCIn_Reader, 662
 spacings
 forcebalance::objective::Penalty, 656
 specific_dct
 forcebalance::nifty, 56
 specific_lst
 forcebalance::nifty, 56
 Split
 forcebalance::amberio::FrcMod_Reader, 309
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 211
 forcebalance::custom_io::Gen_Reader, 316
 forcebalance::gmxio::ITP_Reader, 393
 forcebalance::mol2io::Mol2_Reader, 534
 forcebalance::openmmio::OpenMM_Reader, 638
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
 forcebalance::qchemio::QCIn_Reader, 661
 forcebalance::tinkerio::Tinker_Reader, 775
 split
 forcebalance::molecule::Molecule, 555
 splitter
 forcebalance::molecule, 43
 sprint_map
 forcebalance::forcefield::FF, 303
 srkdir
 forcebalance::engine::Engine, 292
 forcebalance::gmxio::GMX, 326
 forcebalance::openmmio::OpenMM, 636
 forcebalance::tinkerio::TINKER, 772
 stage
 forcebalance::abinitio::AbInitio, 91
 forcebalance::abinitio_internal::AbInitio_Internal, 157
 forcebalance::amberio::AbInitio_AMBER, 113
 forcebalance::binding::BindingEnergy, 223
 forcebalance::counterpoise::Counterpoise, 287
 forcebalance::gmxio::AbInitio_GMX, 135
 forcebalance::gmxio::BindingEnergy_GMX, 238
 forcebalance::gmxio::Interaction_GMX, 356
 forcebalance::gmxio::Lipid_GMX, 442
 forcebalance::gmxio::Liquid_GMX, 478
 forcebalance::gmxio::Moments_GMX, 586
 forcebalance::gmxio::Thermo_GMX, 761
 forcebalance::gmxio::Vibration_GMX, 803
 forcebalance::interaction::Interaction, 341
 forcebalance::leastsq::LeastSquares, 405
 forcebalance::lipid::Lipid, 424
 forcebalance::liquid::Liquid, 459
 forcebalance::moments::Moments, 571
 forcebalance::openmmio::AbInitio_OpenMM, 179
 forcebalance::openmmio::BindingEnergy_OpenMM,
 253
 forcebalance::openmmio::Interaction_OpenMM, 371
 forcebalance::openmmio::Liquid_OpenMM, 497
 forcebalance::openmmio::Moments_OpenMM, 601
 forcebalance::psi4io::RDVR3_Psi4, 683
 forcebalance::psi4io::THCDF_Psi4, 728

forcebalance::target::RemoteTarget, 697
 forcebalance::target::Target, 712
 forcebalance::thermo::Thermo, 744
 forcebalance::tinkerio::AbInitio_TINKER, 201
 forcebalance::tinkerio::BindingEnergy_TINKER, 268
 forcebalance::tinkerio::Interaction_TINKER, 386
 forcebalance::tinkerio::Liquid_TINKER, 517
 forcebalance::tinkerio::Moments_TINKER, 616
 forcebalance::tinkerio::Vibration_TINKER, 818
 forcebalance::vibration::Vibration, 788
 statisticallnefficiency
 forcebalance::nifty, 55
 status_bit
 forcebalance::Mol2::mol2_atom, 530
 forcebalance::Mol2::mol2_bond, 532
 step
 forcebalance::optimizer::Optimizer, 650
 subdict
 forcebalance::parser, 67
 submit_jobs
 forcebalance::abinitio::AbInitio, 91
 forcebalance::abinitio_internal::AbInitio_Internal, 157
 forcebalance::amberio::AbInitio_AMBER, 114
 forcebalance::binding::BindingEnergy, 224
 forcebalance::counterpoise::Counterpoise, 288
 forcebalance::gmxio::AbInitio_GMX, 135
 forcebalance::gmxio::BindingEnergy_GMX, 239
 forcebalance::gmxio::Interaction_GMX, 357
 forcebalance::gmxio::Lipid_GMX, 443
 forcebalance::gmxio::Liquid_GMX, 479
 forcebalance::gmxio::Moments_GMX, 587
 forcebalance::gmxio::Thermo_GMX, 761
 forcebalance::gmxio::Vibration_GMX, 804
 forcebalance::interaction::Interaction, 342
 forcebalance::leastsq::LeastSquares, 406
 forcebalance::lipid::Lipid, 425
 forcebalance::liquid::Liquid, 460
 forcebalance::moments::Moments, 572
 forcebalance::openmmio::AbInitio_OpenMM, 179
 forcebalance::openmmio::BindingEnergy_OpenMM, 254
 forcebalance::openmmio::Interaction_OpenMM, 372
 forcebalance::openmmio::Liquid_OpenMM, 498
 forcebalance::openmmio::Moments_OpenMM, 602
 forcebalance::psi4io::RDVR3_Psi4, 684
 forcebalance::psi4io::THCDF_Psi4, 729
 forcebalance::target::RemoteTarget, 698
 forcebalance::target::Target, 713
 forcebalance::thermo::Thermo, 744
 forcebalance::tinkerio::AbInitio_TINKER, 201
 forcebalance::tinkerio::BindingEnergy_TINKER, 269
 forcebalance::tinkerio::Interaction_TINKER, 387
 forcebalance::tinkerio::Liquid_TINKER, 518
 forcebalance::tinkerio::Moments_TINKER, 617
 forcebalance::tinkerio::Vibration_TINKER, 819
 forcebalance::vibration::Vibration, 789
 subst_id
 forcebalance::Mol2::mol2_atom, 530
 subst_name
 forcebalance::Mol2::mol2_atom, 530
 suffix
 forcebalance::amberio::FrcMod_Reader, 310
 forcebalance::amberio::Mol2_Reader, 538
 forcebalance::BaseReader, 212
 forcebalance::custom_io::Gen_Reader, 316
 forcebalance::gmxio::ITP_Reader, 394
 forcebalance::mol2io::Mol2_Reader, 535
 forcebalance::openmmio::OpenMM_Reader, 639
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 330
 forcebalance::qchemio::QCIn_Reader, 662
 forcebalance::tinkerio::Tinker_Reader, 776
 suffix_dict
 forcebalance::openmmio, 62
 system
 forcebalance::openmmio::OpenMM, 636
 system_driver
 forcebalance::binding::BindingEnergy, 224
 forcebalance::gmxio::BindingEnergy_GMX, 239
 forcebalance::openmmio::BindingEnergy_OpenMM, 254
 forcebalance::tinkerio::BindingEnergy_TINKER, 269
 target
 forcebalance::engine::Engine, 292
 forcebalance::gmxio::GMX, 326
 forcebalance::openmmio::OpenMM, 636
 forcebalance::tinkerio::TINKER, 772
 target.py, 839
 Target.Terms
 forcebalance::objective::Objective, 625
 target_atom_id
 forcebalance::Mol2::mol2_bond, 532
 Targets
 forcebalance::objective::Objective, 626
 tdir
 forcebalance::psi4io::RDVR3_Psi4, 686
 tdiv
 forcebalance::openmmio::OpenMM, 636
 tempbase
 forcebalance::abinitio::AbInitio, 95
 forcebalance::abinitio_internal::AbInitio_Internal, 161
 forcebalance::amberio::AbInitio_AMBER, 117
 forcebalance::binding::BindingEnergy, 226
 forcebalance::counterpoise::Counterpoise, 289
 forcebalance::gmxio::AbInitio_GMX, 139
 forcebalance::gmxio::BindingEnergy_GMX, 241
 forcebalance::gmxio::Interaction_GMX, 359

forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::gmxio::Moments_GMX, 589
 forcebalance::gmxio::Thermo_GMX, 764
 forcebalance::gmxio::Vibration_GMX, 806
 forcebalance::interaction::Interaction, 344
 forcebalance::leastsq::LeastSquares, 407
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 463
 forcebalance::moments::Moments, 574
 forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::openmmio::BindingEnergy_OpenMM, 256
 forcebalance::openmmio::Interaction_OpenMM, 374
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::openmmio::Moments_OpenMM, 604
 forcebalance::psi4io::RDVR3_Psi4, 686
 forcebalance::psi4io::THCDF_Psi4, 731
 forcebalance::target::RemoteTarget, 700
 forcebalance::target::Target, 714
 forcebalance::thermo::Thermo, 746
 forcebalance::tinkerio::AbInitio_TINKER, 205
 forcebalance::tinkerio::BindingEnergy_TINKER, 271
 forcebalance::tinkerio::Interaction_TINKER, 389
 forcebalance::tinkerio::Liquid_TINKER, 521
 forcebalance::tinkerio::Moments_TINKER, 619
 forcebalance::tinkerio::Vibration_TINKER, 821
 forcebalance::vibration::Vibration, 791
tempdir
 forcebalance::abinitio::AbInitio, 95
 forcebalance::abinitio_internal::AbInitio_Internal, 161
 forcebalance::amberio::AbInitio_AMBER, 117
 forcebalance::binding::BindingEnergy, 226
 forcebalance::counterpoise::Counterpoise, 290
 forcebalance::engine::Engine, 292
 forcebalance::gmxio::AbInitio_GMX, 139
 forcebalance::gmxio::BindingEnergy_GMX, 241
 forcebalance::gmxio::GMX, 326
 forcebalance::gmxio::Interaction_GMX, 359
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::gmxio::Moments_GMX, 589
 forcebalance::gmxio::Thermo_GMX, 764
 forcebalance::gmxio::Vibration_GMX, 806
 forcebalance::interaction::Interaction, 344
 forcebalance::leastsq::LeastSquares, 408
 forcebalance::lipid::Lipid, 427
 forcebalance::liquid::Liquid, 463
 forcebalance::moments::Moments, 574
 forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::openmmio::BindingEnergy_OpenMM, 256
 forcebalance::openmmio::Interaction_OpenMM, 374
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::openmmio::Moments_OpenMM, 604
 forcebalance::openmmio::OpenMM, 636
 forcebalance::psi4io::RDVR3_Psi4, 686
 forcebalance::psi4io::THCDF_Psi4, 731
 forcebalance::target::RemoteTarget, 700
 forcebalance::target::Target, 714
 forcebalance::thermo::Thermo, 746
 forcebalance::tinkerio::AbInitio_TINKER, 205
 forcebalance::tinkerio::BindingEnergy_TINKER, 271
 forcebalance::tinkerio::Interaction_TINKER, 389
 forcebalance::tinkerio::Liquid_TINKER, 521
 forcebalance::tinkerio::Moments_TINKER, 619
 forcebalance::tinkerio::TINKER, 772
 forcebalance::tinkerio::Vibration_TINKER, 821
 forcebalance::vibration::Vibration, 791
temperature
 forcebalance::quantity::Quantity, 664
 forcebalance::quantity::Quantity_Density, 666
 forcebalance::quantity::Quantity_H_vap, 668
 forcebalance::thermo::Point, 659
tgt_opts_defaults
 forcebalance::parser, 67
tgt_opts_types
 forcebalance::parser, 67
thermo.py, 840
throw_outs
 forcebalance::psi4io::THCDF_Psi4, 731
tinkerio.py, 840
tinkerpath
 forcebalance::tinkerio::TINKER, 772
tinkerprm
 forcebalance::forcefield::FF, 305
tm
 forcebalance::forcefield::FF, 305
tml
 forcebalance::forcefield::FF, 305
top
 forcebalance::gmxio::GMX, 326
topology
 forcebalance::molecule::Molecule, 559
tq_err
 forcebalance::abinitio::AbInitio, 95
 forcebalance::abinitio_internal::AbInitio_Internal, 161
 forcebalance::amberio::AbInitio_AMBER, 117
 forcebalance::gmxio::AbInitio_GMX, 139
 forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::tinkerio::AbInitio_TINKER, 205
tq_err_pct
 forcebalance::abinitio::AbInitio, 95
 forcebalance::abinitio_internal::AbInitio_Internal, 161
 forcebalance::amberio::AbInitio_AMBER, 117
 forcebalance::gmxio::AbInitio_GMX, 139
 forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::tinkerio::AbInitio_TINKER, 205

tq_ref
 forcebalance::abinitio::AbInitio, 95
 forcebalance::abinitio_internal::AbInitio_Internal, 161
 forcebalance::amberio::AbInitio_AMBER, 117
 forcebalance::gmxio::AbInitio_GMX, 139
 forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::tinkerio::AbInitio_TINKER, 205
 TruncatedNewton
 forcebalance::optimizer::Optimizer, 651

 uncert
 forcebalance::optimizer::Optimizer, 653
 uncommadash
 forcebalance::nifty, 55
 unpack_moments
 forcebalance::gmxio::Moments_GMX, 587
 forcebalance::moments::Moments, 572
 forcebalance::openmmio::Moments_OpenMM, 602
 forcebalance::tinkerio::Moments_TINKER, 617
 update_simulation
 forcebalance::openmmio::OpenMM, 634
 UpdateSimulationParameters
 forcebalance::openmmio, 61
 use_nft
 forcebalance::abinitio::AbInitio, 95
 forcebalance::abinitio_internal::AbInitio_Internal, 161
 forcebalance::amberio::AbInitio_AMBER, 117
 forcebalance::gmxio::AbInitio_GMX, 139
 forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::tinkerio::AbInitio_TINKER, 205

 Val
 forcebalance::optimizer::Optimizer, 653
 valkwrd
 forcebalance::gmxio::GMX, 326
 forcebalance::openmmio::OpenMM, 636
 forcebalance::tinkerio::TINKER, 772
 verbose
 forcebalance::engine::Engine, 292
 forcebalance::gmxio::GMX, 327
 forcebalance::openmmio::OpenMM, 636
 forcebalance::tinkerio::TINKER, 772
 verbose_options
 forcebalance::abinitio::AbInitio, 95
 forcebalance::abinitio_internal::AbInitio_Internal, 161
 forcebalance::amberio::AbInitio_AMBER, 118
 forcebalance::BaseClass, 209
 forcebalance::binding::BindingEnergy, 226
 forcebalance::counterpoise::Counterpoise, 290
 forcebalance::engine::Engine, 292
 forcebalance::forcefield::FF, 305
 forcebalance::gmxio::AbInitio_GMX, 139
 forcebalance::gmxio::BindingEnergy_GMX, 241
 forcebalance::gmxio::GMX, 327

 forcebalance::gmxio::Interaction_GMX, 359
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::gmxio::Moments_GMX, 589
 forcebalance::gmxio::Thermo_GMX, 764
 forcebalance::gmxio::Vibration_GMX, 806
 forcebalance::interaction::Interaction, 344
 forcebalance::leastsq::LeastSquares, 408
 forcebalance::lipid::Lipid, 428
 forcebalance::liquid::Liquid, 463
 forcebalance::moments::Moments, 574
 forcebalance::objective::Objective, 626
 forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::openmmio::BindingEnergy_OpenMM,
 256
 forcebalance::openmmio::Interaction_OpenMM, 374
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::openmmio::Moments_OpenMM, 604
 forcebalance::openmmio::OpenMM, 636
 forcebalance::optimizer::Optimizer, 653
 forcebalance::psi4io::RDVR3_Psi4, 686
 forcebalance::psi4io::THCDF_Psi4, 731
 forcebalance::target::RemoteTarget, 700
 forcebalance::target::Target, 714
 forcebalance::thermo::Thermo, 747
 forcebalance::tinkerio::AbInitio_TINKER, 205
 forcebalance::tinkerio::BindingEnergy_TINKER, 271
 forcebalance::tinkerio::Interaction_TINKER, 389
 forcebalance::tinkerio::Liquid_TINKER, 521
 forcebalance::tinkerio::Moments_TINKER, 619
 forcebalance::tinkerio::TINKER, 773
 forcebalance::tinkerio::Vibration_TINKER, 821
 forcebalance::vibration::Vibration, 791
 vfnm
 forcebalance::gmxio::Vibration_GMX, 806
 forcebalance::tinkerio::Vibration_TINKER, 821
 forcebalance::vibration::Vibration, 791
 vibration.py, 841
 vibration_driver
 forcebalance::gmxio::Vibration_GMX, 804
 forcebalance::tinkerio::Vibration_TINKER, 819
 forcebalance::vibration::Vibration, 789
 vsinfo
 forcebalance::openmmio::OpenMM, 636
 vsprm
 forcebalance::openmmio::OpenMM, 636

 w_al
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::lipid::Lipid, 428
 w_alpha
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 482
 forcebalance::lipid::Lipid, 428

forcebalance::liquid::Liquid, 463
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::tinkerio::Liquid_TINKER, 521
w_cp
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 483
 forcebalance::lipid::Lipid, 428
 forcebalance::liquid::Liquid, 463
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::tinkerio::Liquid_TINKER, 522
w_energy
 forcebalance::abinitio::AbInitio, 95
 forcebalance::abinitio_internal::AbInitio_Internal, 161
 forcebalance::amberio::AbInitio_AMBER, 118
 forcebalance::gmxio::AbInitio_GMX, 139
 forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::tinkerio::AbInitio_TINKER, 205
w_eps0
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 483
 forcebalance::lipid::Lipid, 428
 forcebalance::liquid::Liquid, 463
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::tinkerio::Liquid_TINKER, 522
w_force
 forcebalance::abinitio::AbInitio, 95
 forcebalance::abinitio_internal::AbInitio_Internal, 162
 forcebalance::amberio::AbInitio_AMBER, 118
 forcebalance::gmxio::AbInitio_GMX, 139
 forcebalance::openmmio::AbInitio_OpenMM, 183
 forcebalance::tinkerio::AbInitio_TINKER, 205
w_hvap
 forcebalance::gmxio::Liquid_GMX, 483
 forcebalance::liquid::Liquid, 463
 forcebalance::openmmio::Liquid_OpenMM, 501
 forcebalance::tinkerio::Liquid_TINKER, 522
w_kappa
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 483
 forcebalance::lipid::Lipid, 428
 forcebalance::liquid::Liquid, 463
 forcebalance::openmmio::Liquid_OpenMM, 502
 forcebalance::tinkerio::Liquid_TINKER, 522
w_netforce
 forcebalance::abinitio::AbInitio, 96
 forcebalance::abinitio_internal::AbInitio_Internal, 162
 forcebalance::amberio::AbInitio_AMBER, 118
 forcebalance::gmxio::AbInitio_GMX, 140
 forcebalance::openmmio::AbInitio_OpenMM, 184
 forcebalance::tinkerio::AbInitio_TINKER, 206
w_resp
 forcebalance::abinitio::AbInitio, 96
 forcebalance::abinitio_internal::AbInitio_Internal, 162
 forcebalance::amberio::AbInitio_AMBER, 118
 forcebalance::gmxio::AbInitio_GMX, 140
 forcebalance::openmmio::AbInitio_OpenMM, 184
 forcebalance::tinkerio::AbInitio_TINKER, 206
w_rho
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 483
 forcebalance::lipid::Lipid, 428
 forcebalance::liquid::Liquid, 463
 forcebalance::openmmio::Liquid_OpenMM, 502
 forcebalance::tinkerio::Liquid_TINKER, 522
w_scd
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::lipid::Lipid, 428
w_torque
 forcebalance::abinitio::AbInitio, 96
 forcebalance::abinitio_internal::AbInitio_Internal, 162
 forcebalance::amberio::AbInitio_AMBER, 118
 forcebalance::gmxio::AbInitio_GMX, 140
 forcebalance::openmmio::AbInitio_OpenMM, 184
 forcebalance::tinkerio::AbInitio_TINKER, 206
WORK_QUEUE
 forcebalance::nifty, 56
WQIDS
 forcebalance::nifty, 57
WTot
 forcebalance::objective::Objective, 626
warn_once
 forcebalance::nifty, 55
warn_press_key
 forcebalance::nifty, 55
warn_vn
 forcebalance::tinkerio::TINKER, 773
warnngmx
 forcebalance::gmxio::GMX, 325
weight
 forcebalance::gmxio::Interaction_GMX, 359
 forcebalance::interaction::Interaction, 344
 forcebalance::openmmio::Interaction_OpenMM, 374
 forcebalance::tinkerio::Interaction_TINKER, 389
weight_info
 forcebalance::lipid, 35
 forcebalance::liquid, 35
weighted_variance
 forcebalance::abinitio, 16
weighted_variance2
 forcebalance::abinitio, 16
weights
 forcebalance::gmxio::Thermo_GMX, 764
 forcebalance::thermo::Thermo, 747
whamboltz
 forcebalance::abinitio::AbInitio, 96
 forcebalance::abinitio_internal::AbInitio_Internal, 162
 forcebalance::amberio::AbInitio_AMBER, 118
 forcebalance::gmxio::AbInitio_GMX, 140

forcebalance::openmmio::AbInitio_OpenMM, 184
 forcebalance::tinkerio::AbInitio_TINKER, 206
 which
 forcebalance::nifty, 55
 Whites
 forcebalance::amberio::FrcMod_Reader, 310
 forcebalance::amberio::Mol2_Reader, 537
 forcebalance::BaseReader, 211
 forcebalance::custom_io::Gen_Reader, 316
 forcebalance::gmxio::ITP_Reader, 393
 forcebalance::mol2io::Mol2_Reader, 534
 forcebalance::openmmio::OpenMM_Reader, 638
 forcebalance::psi4io::GBS_Reader, 313
 forcebalance::psi4io::Grid_Reader, 329
 forcebalance::qchemio::QCIn_Reader, 661
 forcebalance::tinkerio::Tinker_Reader, 775
 wopen
 forcebalance::nifty, 55
 Wp
 forcebalance::gmxio::Lipid_GMX, 446
 forcebalance::gmxio::Liquid_GMX, 483
 forcebalance::gmxio::Thermo_GMX, 764
 forcebalance::lipid::Lipid, 428
 forcebalance::liquid::Liquid, 463
 forcebalance::openmmio::Liquid_OpenMM, 502
 forcebalance::thermo::Thermo, 747
 forcebalance::tinkerio::Liquid_TINKER, 522
 wq_complete
 forcebalance::abinitio::AbInitio, 92
 forcebalance::abinitio_internal::AbInitio_Internal, 158
 forcebalance::amberio::AbInitio_AMBER, 114
 forcebalance::binding::BindingEnergy, 224
 forcebalance::counterpoise::Counterpoise, 288
 forcebalance::gmxio::AbInitio_GMX, 136
 forcebalance::gmxio::BindingEnergy_GMX, 239
 forcebalance::gmxio::Interaction_GMX, 357
 forcebalance::gmxio::Lipid_GMX, 443
 forcebalance::gmxio::Liquid_GMX, 480
 forcebalance::gmxio::Moments_GMX, 587
 forcebalance::gmxio::Thermo_GMX, 762
 forcebalance::gmxio::Vibration_GMX, 804
 forcebalance::interaction::Interaction, 342
 forcebalance::leastsq::LeastSquares, 406
 forcebalance::lipid::Lipid, 425
 forcebalance::liquid::Liquid, 461
 forcebalance::moments::Moments, 572
 forcebalance::openmmio::AbInitio_OpenMM, 180
 forcebalance::openmmio::BindingEnergy_OpenMM, 254
 forcebalance::openmmio::Interaction_OpenMM, 372
 forcebalance::openmmio::Liquid_OpenMM, 499
 forcebalance::openmmio::Moments_OpenMM, 602
 forcebalance::psi4io::RDVR3_Psi4, 684
 forcebalance::psi4io::THCDF_Psi4, 729
 forcebalance::target::RemoteTarget, 699
 forcebalance::target::Target, 713
 forcebalance::thermo::Thermo, 745
 forcebalance::tinkerio::AbInitio_TINKER, 202
 forcebalance::tinkerio::BindingEnergy_TINKER, 269
 forcebalance::tinkerio::Interaction_TINKER, 387
 forcebalance::tinkerio::Liquid_TINKER, 519
 forcebalance::tinkerio::Moments_TINKER, 617
 forcebalance::tinkerio::Vibration_TINKER, 820
 forcebalance::vibration::Vibration, 790
 Write_Tab

```

    forcebalance::molecule::Molecule, 559
write_arc
    forcebalance::molecule::Molecule, 555
write_dcd
    forcebalance::molecule::Molecule, 555
write_gro
    forcebalance::molecule::Molecule, 555
write_indicate
    forcebalance::abinitio::AbInitio, 96
    forcebalance::abinitio_internal::AbInitio_Internal, 162
    forcebalance::amberio::AbInitio_AMBER, 118
    forcebalance::binding::BindingEnergy, 226
    forcebalance::counterpoise::Counterpoise, 290
    forcebalance::gmxio::AbInitio_GMX, 140
    forcebalance::gmxio::BindingEnergy_GMX, 241
    forcebalance::gmxio::Interaction_GMX, 359
    forcebalance::gmxio::Lipid_GMX, 446
    forcebalance::gmxio::Liquid_GMX, 483
    forcebalance::gmxio::Moments_GMX, 589
    forcebalance::gmxio::Thermo_GMX, 764
    forcebalance::gmxio::Vibration_GMX, 806
    forcebalance::interaction::Interaction, 344
    forcebalance::leastsq::LeastSquares, 408
    forcebalance::lipid::Lipid, 428
    forcebalance::liquid::Liquid, 464
    forcebalance::moments::Moments, 574
    forcebalance::openmmio::AbInitio_OpenMM, 184
    forcebalance::openmmio::BindingEnergy_OpenMM,
        256
    forcebalance::openmmio::Interaction_OpenMM, 374
    forcebalance::openmmio::Liquid_OpenMM, 502
    forcebalance::openmmio::Moments_OpenMM, 604
    forcebalance::psi4io::RDVR3_Psi4, 686
    forcebalance::psi4io::THCDF_Psi4, 731
    forcebalance::target::RemoteTarget, 700
    forcebalance::target::Target, 714
    forcebalance::thermo::Thermo, 747
    forcebalance::tinkerio::AbInitio_TINKER, 206
    forcebalance::tinkerio::BindingEnergy_TINKER, 271
    forcebalance::tinkerio::Interaction_TINKER, 389
    forcebalance::tinkerio::Liquid_TINKER, 522
    forcebalance::tinkerio::Moments_TINKER, 619
    forcebalance::tinkerio::Vibration_TINKER, 821
    forcebalance::vibration::Vibration, 791
write_key
    forcebalance::tinkerio, 72
write_mdcrd
    forcebalance::molecule::Molecule, 556
write_mdp
    forcebalance::gmxio, 31
write_molproq
    forcebalance::molecule::Molecule, 556
write_ndx
    forcebalance::gmxio, 32
write_nested_destroy
    forcebalance::psi4io::THCDF_Psi4, 730
write_objective
    forcebalance::abinitio::AbInitio, 96
    forcebalance::abinitio_internal::AbInitio_Internal, 162
    forcebalance::amberio::AbInitio_AMBER, 118
    forcebalance::binding::BindingEnergy, 226
    forcebalance::counterpoise::Counterpoise, 290
    forcebalance::gmxio::AbInitio_GMX, 140
    forcebalance::gmxio::BindingEnergy_GMX, 241
    forcebalance::gmxio::Interaction_GMX, 359
    forcebalance::gmxio::Lipid_GMX, 446
    forcebalance::gmxio::Liquid_GMX, 483
    forcebalance::gmxio::Moments_GMX, 589
    forcebalance::gmxio::Thermo_GMX, 764
    forcebalance::gmxio::Vibration_GMX, 807
    forcebalance::interaction::Interaction, 344
    forcebalance::leastsq::LeastSquares, 408
    forcebalance::lipid::Lipid, 428
    forcebalance::liquid::Liquid, 464
    forcebalance::moments::Moments, 574
    forcebalance::openmmio::AbInitio_OpenMM, 184
    forcebalance::openmmio::BindingEnergy_OpenMM,
        256
    forcebalance::openmmio::Interaction_OpenMM, 374
    forcebalance::openmmio::Liquid_OpenMM, 502
    forcebalance::openmmio::Moments_OpenMM, 604
    forcebalance::psi4io::RDVR3_Psi4, 686
    forcebalance::psi4io::THCDF_Psi4, 731
    forcebalance::target::RemoteTarget, 700
    forcebalance::target::Target, 715
    forcebalance::thermo::Thermo, 747
    forcebalance::tinkerio::AbInitio_TINKER, 206
    forcebalance::tinkerio::BindingEnergy_TINKER, 271
    forcebalance::tinkerio::Interaction_TINKER, 389
    forcebalance::tinkerio::Liquid_TINKER, 522
    forcebalance::tinkerio::Moments_TINKER, 619
    forcebalance::tinkerio::Vibration_TINKER, 822
    forcebalance::vibration::Vibration, 791
write_pdb
    forcebalance::molecule::Molecule, 556
write_qcin
    forcebalance::molecule::Molecule, 557
write_qdata
    forcebalance::molecule::Molecule, 557
write_xyz
    forcebalance::molecule::Molecule, 558
write_techk
    forcebalance::optimizer::Optimizer, 651
x
    forcebalance::Mol2::mol2_atom, 530
    forcebalance::molecule::MyG, 622
x.best

```

forcebalance::optimizer::Optimizer, 653
 x_prev
 forcebalance::optimizer::Optimizer, 653
 XMLFILE
 forcebalance::nifty, 57
 xct
 forcebalance::abinitio::AbInitio, 96
 forcebalance::abinitio_internal::AbInitio_Internal, 162
 forcebalance::amberio::AbInitio_AMBER, 118
 forcebalance::binding::BindingEnergy, 226
 forcebalance::counterpoise::Counterpoise, 290
 forcebalance::gmxi::AbInitio_GMX, 140
 forcebalance::gmxi::BindingEnergy_GMX, 241
 forcebalance::gmxi::Interaction_GMX, 360
 forcebalance::gmxi::Lipid_GMX, 446
 forcebalance::gmxi::Liquid_GMX, 483
 forcebalance::gmxi::Moments_GMX, 589
 forcebalance::gmxi::Thermo_GMX, 764
 forcebalance::gmxi::Vibration_GMX, 807
 forcebalance::interaction::Interaction, 344
 forcebalance::leastsq::LeastSquares, 408
 forcebalance::lipid::Lipid, 428
 forcebalance::liquid::Liquid, 464
 forcebalance::moments::Moments, 574
 forcebalance::openmmio::AbInitio_OpenMM, 184
 forcebalance::openmmio::BindingEnergy_OpenMM,
 256
 forcebalance::openmmio::Interaction_OpenMM, 375
 forcebalance::openmmio::Liquid_OpenMM, 502
 forcebalance::openmmio::Moments_OpenMM, 604
 forcebalance::psi4io::RDVR3_Psi4, 686
 forcebalance::psi4io::THCDF_Psi4, 731
 forcebalance::target::RemoteTarget, 700
 forcebalance::target::Target, 715
 forcebalance::thermo::Thermo, 747
 forcebalance::tinkerio::AbInitio_TINKER, 206
 forcebalance::tinkerio::BindingEnergy_TINKER, 271
 forcebalance::tinkerio::Interaction_TINKER, 390
 forcebalance::tinkerio::Liquid_TINKER, 522
 forcebalance::tinkerio::Moments_TINKER, 619
 forcebalance::tinkerio::Vibration_TINKER, 822
 forcebalance::vibration::Vibration, 792
 xk_prev
 forcebalance::optimizer::Optimizer, 653
 Xp
 forcebalance::gmxi::Lipid_GMX, 446
 forcebalance::gmxi::Liquid_GMX, 483
 forcebalance::gmxi::Thermo_GMX, 764
 forcebalance::lipid::Lipid, 428
 forcebalance::liquid::Liquid, 464
 forcebalance::openmmio::Liquid_OpenMM, 502
 forcebalance::thermo::Thermo, 747
 forcebalance::tinkerio::Liquid_TINKER, 522
 xyz_omms