

ForceBalance Developer API Guide version 1.1

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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.

1.1 Short Term (summer 2013)

- Create and expand project unit testing framework to encourage a test driven development approach
- Improve/consolidate existing documentation

1.2 Long Term

- Development of a ForceBalance GUI interface to complement the current command line interface
- More comprehensive tutorial to walk users through the initial process of setting up targets and preparing for a successful ForceBalance run

2 Todo List

Member `forcebalance.abinitio.AbInitio.__init__`

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

Member `forcebalance.abinitio.AbInitio.get_energy_force__`

Parallelization over snapshots is not implemented yet

Member `forcebalance.abinitio.AbInitio.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.

Member `forcebalance.abinitio_gmxx2.AbInitio_GMXX2.get_energy_force__`

Some of these files don't need to be printed, they can be passed to GROMACS as arguments. Let's think about this some more.

Currently I have no way to pass out the qualitative indicators.

Member `forcebalance.abinitio_gmxx2.AbInitio_GMXX2.prepare_temp_directory`

Someday I'd like to use WHAM to put AIMD simulations in. :)

The fitatoms shouldn't be the first however many atoms, it should be a list.

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.

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

Class [forcebalance.gmxio.OTP_Reader](#)

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

Member [forcebalance.liquid.Liquid.__init__](#)

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

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.

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):

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[forcebalance](#)

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[forcebalance.abinitio](#)

Ab-initio fitting module (energies, forces, resp) 14

[forcebalance.abinitio_gmxx2](#)

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[forcebalance.abinitio_internal](#)

Internal implementation of energy matching (for TIP3P water only) 15

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| forcebalance.amberio | |
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| forcebalance.basereader | |
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| forcebalance.binding | |
| Binding energy fitting module | 18 |
| forcebalance.chemistry | 18 |
| 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 | 22 |
| forcebalance.finite_difference | 24 |
| forcebalance.fitsim | 26 |
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| Contains the dictionary of usable Target classes | 33 |
| forcebalance.interaction | |
| Interaction energy fitting module | 34 |
| forcebalance.interactions | 34 |
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| Matching of liquid bulk properties | 36 |
| forcebalance.Mol2 | 36 |
| forcebalance.mol2io | |
| Mol2 I/O | 37 |
| forcebalance.molecule | 37 |
| forcebalance.moments | |
| Multipole moment fitting module | 45 |

| | |
|--|----|
| forcebalance.nifty | |
| Nifty functions, intended to be imported by any module within ForceBalance | 45 |
| forcebalance.objective | |
| ForceBalance objective function | 57 |
| forcebalance.openmmio | |
| OpenMM input/output | 58 |
| forcebalance.optimizer | |
| Optimization algorithms | 61 |
| forcebalance.output | |
| | 62 |
| forcebalance.parser | |
| Input file parser for ForceBalance jobs | 63 |
| forcebalance.psi4io | |
| PSI4 force field input/output | 67 |
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| | 67 |
| forcebalance.qchemio | |
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| | 69 |
| forcebalance.target | |
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| forcebalance.tinkerio | |
| TINKER input/output | 70 |
| forcebalance.vibration | |
| Vibrational mode fitting module | 72 |
| interaction | |
| Interaction energy fitting module | 73 |
| simtab | |
| Contains the dictionary of fitting simulation classes | 73 |

4 Hierarchical Index

4.1 Class Hierarchy

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

dict

| | |
|--|-----|
| forcebalance.forcefield.BackedUpDict | 94 |
| FileHandler | |
| forcebalance.output.CleanFileHandler | 100 |
| forcebalance.output.RawFileHandler | 195 |

| | |
|---|------------|
| forcebalance.Mol2.mol2 | 146 |
| forcebalance.Mol2.mol2_atom | 150 |
| forcebalance.Mol2.mol2_bond | 153 |
| forcebalance.Mol2.mol2_set | 158 |
| object | |
| forcebalance.baseclass.ForceBalanceBaseClass | 116 |
| forcebalance.forcefield.FF | 103 |
| forcebalance.objective.Objective | 178 |
| forcebalance.target.Target | 198 |
| forcebalance.abinitio.AbInitio | 73 |
| forcebalance.abinitio_internal.AbInitio_Internal | 89 |
| forcebalance.amberio.AbInitio_AMBER | 82 |
| forcebalance.gmxio.AbInitio_GMX | 84 |
| forcebalance.openmmio.AbInitio_OpenMM | 90 |
| forcebalance.tinkerio.AbInitio_TINKER | 92 |
| forcebalance.binding.BindingEnergy | 97 |
| forcebalance.tinkerio.BindingEnergy_TINKER | 98 |
| forcebalance.counterpoise.Counterpoise | 100 |
| forcebalance.gmxqpio.Monomer_QTPIE | 176 |
| forcebalance.interaction.Interaction | 124 |
| forcebalance.gmxio.Interaction_GMX | 127 |
| forcebalance.openmmio.Interaction_OpenMM | 129 |
| forcebalance.tinkerio.Interaction_TINKER | 130 |
| forcebalance.leastsq.LeastSquares | 136 |
| forcebalance.psi4io.THCDF_Psi4 | 203 |
| forcebalance.liquid.Liquid | 137 |
| forcebalance.gmxio.Liquid_GMX | 141 |
| forcebalance.openmmio.Liquid_OpenMM | 143 |
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| forcebalance.moments.Moments | 173 |

| | |
|---|------------|
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| forcebalance.psi4io.RDVR3_Psi4 | 196 |
| forcebalance.vibration.Vibration | 208 |
| forcebalance.basereader.BaseReader | 95 |
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| forcebalance.amberio.Mol2_Reader | 155 |
| forcebalance.custom_io.Gen_Reader | 121 |
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| forcebalance.openmmio.OpenMM_Reader | 180 |
| forcebalance.psi4io.GBS_Reader | 119 |
| forcebalance.psi4io.Grid_Reader | 122 |
| forcebalance.qchemio.QCIn_Reader | 193 |
| forcebalance.tinkerio.Tinker_Reader | 205 |
| forcebalance.molecule.Molecule | 160 |
| forcebalance.objective.Penalty | 189 |
| Pickler | |
| forcebalance.nifty.Pickler_LP | 192 |
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| forcebalance.output.RawStreamHandler | 195 |
| Structure | |
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| Unpickler | |
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| AbInitio | |
| forcebalance.abinitio_gmxx2.AbInitio_GMXX2 | 86 |
| BaseReader | |
| forcebalance.mol2io.Mol2_Reader | 157 |
| ForceBalanceBaseClass | |
| forcebalance.fitsim.FittingSimulation | 112 |
| forcebalance.optimizer.Optimizer | 181 |
| Target | |
| forcebalance.interactions.Interactions | 131 |
| Vibration | |
| forcebalance.tinkerio.Vibration_TINKER | 210 |

5 Class Index

5.1 Class List

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

| | |
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| <code>forcebalance.abinitio.AbInitio</code> | |
| Subclass of Target for fitting force fields to ab initio data | 73 |
| <code>forcebalance.amberio.AbInitio_AMBER</code> | |
| Subclass of Target for force and energy matching using AMBER | 82 |
| <code>forcebalance.gmxio.AbInitio_GMX</code> | |
| Subclass of AbInitio for force and energy matching using normal GROMACS | 84 |
| <code>forcebalance.abinitio_gmxx2.AbInitio_GMXX2</code> | |
| ForceBalance class for force and energy matching with the modified GROMACS | 86 |
| <code>forcebalance.abinitio_internal.AbInitio_Internal</code> | |
| Subclass of Target for force and energy matching using an internal implementation | 89 |
| <code>forcebalance.openmmio.AbInitio_OpenMM</code> | |
| Subclass of AbInitio for force and energy matching using OpenMM | 90 |
| <code>forcebalance.tinkerio.AbInitio_TINKER</code> | |
| Subclass of Target for force and energy matching using TINKER | 92 |
| <code>forcebalance.forcefield.BackedUpDict</code> | 94 |
| <code>forcebalance.basereader.BaseReader</code> | |
| The 'reader' class | 95 |
| <code>forcebalance.binding.BindingEnergy</code> | |
| Improved subclass of Target for fitting force fields to binding energies | 97 |
| <code>forcebalance.tinkerio.BindingEnergy_TINKER</code> | |
| Subclass of BindingEnergy for binding energy matching using TINKER | 98 |
| <code>forcebalance.output.CleanFileHandler</code> | |
| File handler that does not write terminal escape codes to files | 100 |
| <code>forcebalance.counterpoise.Counterpoise</code> | |
| Target subclass for matching the counterpoise correction | 100 |
| <code>forcebalance.forcefield.FF</code> | |
| Force field class | 103 |
| <code>forcebalance.fitsim.FittingSimulation</code> | |
| Base class for all fitting simulations | 112 |
| <code>forcebalance.baseclass.ForceBalanceBaseClass</code> | |
| Provides some nifty functions that are common to all ForceBalance classes | 116 |
| <code>forcebalance.amberio.FrcMod_Reader</code> | |
| Finite state machine for parsing FrcMod force field file | 117 |

| | |
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| forcebalance.psi4io.GBS_Reader | |
| Interaction type -> Parameter Dictionary | 119 |
| forcebalance.custom_io.Gen_Reader | |
| Finite state machine for parsing custom GROMACS force field files | 121 |
| forcebalance.psi4io.Grid_Reader | |
| Finite state machine for parsing DVR grid files | 122 |
| forcebalance.interaction.Interaction | |
| Subclass of Target for fitting force fields to interaction energies | 124 |
| forcebalance.gmxio.Interaction_GMX | |
| Subclass of Interaction for interaction energy matching using GROMACS | 127 |
| forcebalance.openmmio.Interaction_OpenMM | |
| Subclass of Target for interaction matching using OpenMM | 129 |
| forcebalance.tinkerio.Interaction_TINKER | |
| Subclass of Target for interaction matching using TINKER | 130 |
| forcebalance.interactions.Interactions | |
| Improved subclass of Target for fitting force fields to interaction energies | 131 |
| forcebalance.gmxio.OTP_Reader | |
| Finite state machine for parsing GROMACS force field files | 133 |
| forcebalance.leastsq.LeastSquares | |
| Subclass of Target for general least squares fitting | 136 |
| forcebalance.liquid.Liquid | |
| Subclass of Target for liquid property matching | 137 |
| forcebalance.gmxio.Liquid_GMX | 141 |
| forcebalance.openmmio.Liquid_OpenMM | 143 |
| forcebalance.tinkerio.Liquid_TINKER | 145 |
| forcebalance.Mol2.mol2 | |
| This is to manage one mol2 series of lines on the form: | 146 |
| 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 | 150 |
| forcebalance.Mol2.mol2_bond | |
| This is to manage mol2 bond lines on the form: 1 1 2 ar | 153 |
| forcebalance.amberio.Mol2_Reader | |
| Finite state machine for parsing Mol2 force field file | 155 |
| forcebalance.mol2io.Mol2_Reader | |
| Finite state machine for parsing Mol2 force field file | 157 |
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| forcebalance.molecule.Molecule | |
| Lee-Ping's general file format conversion class | 160 |
| forcebalance.molecule.MolfileTimestep | |
| Wrapper for the timestep C structure used in molfile plugins | 172 |
| forcebalance.moments.Moments | |
| Subclass of Target for fitting force fields to multipole moments (from experiment or theory) | 173 |
| forcebalance.tinkerio.Moments_TINKER | |
| Subclass of Target for multipole moment matching using TINKER | 175 |
| forcebalance.gmxqpio.Monomer_QTPIE | |
| Subclass of Target for monomer properties of QTPIE (implemented within gromacs WCV branch) | 176 |
| forcebalance.objective.Objective | |
| Objective function | 178 |
| forcebalance.openmmio.OpenMM_Reader | |
| Class for parsing OpenMM force field files | 180 |
| forcebalance.optimizer.Optimizer | |
| Optimizer class | 181 |
| forcebalance.objective.Penalty | |
| Penalty functions for regularizing the force field optimizer | 189 |
| forcebalance.nifty.Pickler_LP | |
| A subclass of the python Pickler that implements pickling of _ElementTree types | 192 |
| forcebalance.qchemio.QCIn_Reader | |
| Finite state machine for parsing Q-Chem input files | 193 |
| forcebalance.output.RawFileHandler | |
| Exactly like output.FileHandler except it does no extra formatting before sending logging messages to the file | 195 |
| forcebalance.output.RawStreamHandler | |
| Exactly like output.StreamHandler except it does no extra formatting before sending logging messages to the stream | 195 |
| forcebalance.psi4io.RDVR3_Psi4 | |
| Subclass of Target for R-DVR3 grid fitting | 196 |
| forcebalance.target.Target | |
| Base class for all fitting targets | 198 |
| forcebalance.psi4io.THCDF_Psi4 | |
| | 203 |
| forcebalance.tinkerio.Tinker_Reader | |
| Finite state machine for parsing TINKER force field files | 205 |
| forcebalance.nifty.Unpickler_LP | |
| A subclass of the python Unpickler that implements unpickling of _ElementTree types | 207 |
| forcebalance.vibration.Vibration | |
| Subclass of Target for fitting force fields to vibrational spectra (from experiment or theory) | 208 |

| | |
|--|-----|
| forcebalance.tinkerio.Vibration_TINKER | |
| Subclass of Target for vibrational frequency matching using TINKER | 210 |

6 File Index

6.1 File List

Here is a list of all files with brief descriptions:

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7 Namespace Documentation

7.1 abinitio_gmxx2 Namespace Reference

Force and energy matching with interface to modified GROMACS.

7.1.1 Detailed Description

Force and energy matching with interface to modified GROMACS. In order for us to obtain the objective function in force and energy matching, we loop through the snapshots, compute the energy and force (as well as its derivatives), and sum them up. The details of the process are complicated and I won't document them here. The contents of this package (mainly the `AbInitio_GMXX2` class) allows us to call the modified GROMACS to compute the objective function for us.

Author

Lee-Ping Wang

Date

12/2011

7.2 forcebalance Namespace Reference

Namespaces

- namespace [abinitio](#)
Ab-initio fitting module (energies, forces, resp).
- namespace [abinitio_gmxx2](#)
- namespace [abinitio_internal](#)
Internal implementation of energy matching (for TIP3P water only)
- namespace [amberio](#)
AMBER force field input/output.
- namespace [baseclass](#)
- namespace [basereader](#)
Base class for force field line reader.
- namespace [binding](#)
Binding energy fitting module.
- namespace [chemistry](#)
- namespace [contact](#)
- namespace [counterpoise](#)
Match an empirical potential to the counterpoise correction for basis set superposition error (BSSE).
- namespace [custom_io](#)
Custom force field parser.
- namespace [finite_difference](#)
- namespace [fitsim](#)
- namespace [forcefield](#)
Force field module.
- namespace [gmxxio](#)
GROMACS input/output.
- namespace [gmxxpio](#)
- namespace [implemented](#)
Contains the dictionary of usable Target classes.
- namespace [interaction](#)
Interaction energy fitting module.
- namespace [interactions](#)
- namespace [leastsq](#)
- namespace [liquid](#)
Matching of liquid bulk properties.
- namespace [Mol2](#)
- namespace [mol2io](#)
Mol2 I/O.
- namespace [molecule](#)
- namespace [moments](#)
Multipole moment fitting module.
- namespace [nifty](#)
Nifty functions, intended to be imported by any module within ForceBalance.
- namespace [objective](#)
ForceBalance objective function.
- namespace [openmmio](#)

OpenMM input/output.

- namespace [optimizer](#)

Optimization algorithms.

- namespace [output](#)
- namespace [parser](#)

Input file parser for ForceBalance jobs.

- namespace [psi4io](#)

PSI4 force field input/output.

- namespace [PT](#)
- namespace [qchemio](#)

Q-Chem input file parser.

- namespace [simtab](#)
- namespace [target](#)
- namespace [tinkerio](#)

TINKER input/output.

- namespace [vibration](#)

Vibrational mode fitting module.

Variables

- [WORK_QUEUE](#) None
- tuple [WQIDS](#) defaultdict(list)

7.2.1 Variable Documentation

7.2.1.1 forcebalance.WORK_QUEUE None

Definition at line 17 of file `__init__.py`.

7.2.1.2 tuple forcebalance.WQIDS defaultdict(list)

Definition at line 20 of file `__init__.py`.

7.3 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.

7.3.1 Detailed Description

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

Author

Lee-Ping Wang

Date

05/2012

7.3.2 Function Documentation

7.3.2.1 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 1151 of file abinitio.py.

7.3.2.2 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 1121 of file abinitio.py.

Here is the call graph for this function:

7.3.2.3 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 1135 of file abinitio.py.

Here is the call graph for this function:

7.4 forcebalance.abinitio_gmxx2 Namespace Reference

Classes

- class [AbInitio_GMXX2](#)

ForceBalance class for force and energy matching with the modified GROMACS.

7.5 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.

7.5.1 Detailed Description

Internal implementation of energy matching (for TIP3P water only)

Author

Lee-Ping Wang

Date

04/2012

7.6 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

- dictionary [mol2_pdict](#) {'COUL':{'Atom':[1], 8:""}}
- dictionary [frcmod_pdict](#)

7.6.1 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

7.6.2 Function Documentation

7.6.2.1 def forcebalance.amberio.is_mol2_atom (line)

Definition at line 32 of file amberio.py.

Here is the call graph for this function:

7.6.3 Variable Documentation

7.6.3.1 dictionary forcebalance.amberio.frcmod_pdict

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 20 of file amberio.py.

7.6.3.2 dictionary forcebalance.amberio.mol2_pdict {'COUL': {'Atom': [1], 8: ''}}

Definition at line 18 of file amberio.py.

7.7 forcebalance.baseclass Namespace Reference

Classes

- class [ForceBalanceBaseClass](#)

Provides some nifty functions that are common to all ForceBalance classes.

7.8 forcebalance.basereader Namespace Reference

Base class for force field line reader.

Classes

- class [BaseReader](#)

The 'reader' class.

7.8.1 Detailed Description

Base class for force field line reader.

Author

Lee-Ping Wang

Date

12/2011

7.9 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.

7.9.1 Detailed Description

Binding energy fitting module.

Author

Lee-Ping Wang

Date

05/2012

7.9.2 Function Documentation

7.9.2.1 def forcebalance.binding.parse_interactions (*input_file*)

Parse through the interactions input file.

Parameters

| | | |
|-----------|-------------------|-----------------------------|
| <i>in</i> | <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:

7.10 forcebalance.chemistry Namespace Reference

Functions

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

Variables

- tuple [BondEnergies](#) defaultdict(lambda:defaultdict(dict))
- list [Radii](#)
Covalent radii from Cordero et al.
- dictionary [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])

7.10.1 Function Documentation

7.10.1.1 `def forcebalance.chemistry.BondStrengthByLength (A, B, length, atol = 0.33, bias = 0.0)`

Definition at line 164 of file chemistry.py.

7.10.1.2 `def forcebalance.chemistry.LookupByMass (mass)`

Definition at line 155 of file chemistry.py.

7.10.2 Variable Documentation

7.10.2.1 `list forcebalance.chemistry.A atoms[0]`

Definition at line 149 of file chemistry.py.

7.10.2.2 `tuple forcebalance.chemistry.atoms re.split('[=3]', line.split()[0])`

Definition at line 148 of file chemistry.py.

7.10.2.3 `list forcebalance.chemistry.B atoms[1]`

Definition at line 150 of file chemistry.py.

7.10.2.4 `tuple forcebalance.chemistry.BE float(line.split()[1])`

Definition at line 146 of file chemistry.py.

7.10.2.5 `tuple forcebalance.chemistry.bo BondChars.index(re.findall('[=3]', line.split()[0])[0])`

Definition at line 151 of file chemistry.py.

7.10.2.6 list forcebalance.chemistry.BondChars ['-', '=', ':', '3']

Definition at line 49 of file chemistry.py.

7.10.2.7 tuple forcebalance.chemistry.BondEnergies defaultdict(lambda:defaultdict(dict))

Definition at line 7 of file chemistry.py.

7.10.2.8 string forcebalance.chemistry.data_from_web

Definition at line 51 of file chemistry.py.

7.10.2.9 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.

7.10.2.10 tuple forcebalance.chemistry.L float(line.split()[2])

Definition at line 147 of file chemistry.py.

7.10.2.11 tuple forcebalance.chemistry.line line.expandtabs()

Definition at line 145 of file chemistry.py.

7.10.2.12 dictionary forcebalance.chemistry.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' : 140.12,
   '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' : 190.23, '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,
14         'Lr' : 262, 'Rf' : 261, 'Db' : 262, 'Sg' : 266, 'Bh' : 264, '
    Hs' : 277, 'Mt' : 268}

```

Definition at line 25 of file chemistry.py.

7.10.2.13 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, 1.22, 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.

7.11 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.

7.11.1 Function Documentation

7.11.1.1 def forcebalance.contact.atom_distances (xyzlist, atom_contacts)

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.

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 26 of file contact.py.

Here is the call graph for this function:

7.11.1.2 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_lenth 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 85 of file contact.py.

7.12 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.

7.12.1 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

7.13 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.

7.13.1 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

7.13.2 Variable Documentation

7.13.2.1 list forcebalance.custom_io.cptypes [None, 'CPGAUSS', 'CPEXPG', 'CPGEXP']

Types of counterpoise correction.

Definition at line 16 of file custom_io.py.

7.13.2.2 dictionary forcebalance.custom_io.fdict

Initial value:

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

Section -> Interaction type dictionary.

Definition at line 21 of file custom_io.py.

7.13.2.3 list forcebalance.custom_io.ndtypes [None]

Types of NDDO correction.

Definition at line 18 of file custom_io.py.

7.13.2.4 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.

7.14 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 [in_fd](#)
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.

7.14.1 Function Documentation

7.14.1.1 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 107 of file finite_difference.py.

Here is the call graph for this function:

7.14.1.2 `def forcebalance.finite_difference.f12d7p (f, h)`

Definition at line 73 of file finite_difference.py.

Here is the call graph for this function:

7.14.1.3 `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 27 of file finite_difference.py.

Here is the call graph for this function:

7.14.1.4 `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-differences/>

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 58 of file finite_difference.py.

Here is the call graph for this function:

7.14.1.5 `def forcebalance.finite_difference.f1d7p (f, h)`

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

Definition at line 68 of file finite_difference.py.

Here is the call graph for this function:

7.14.1.6 `def forcebalance.finite_difference.fwrap (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 145 of file finite_difference.py.

Here is the call graph for this function:

7.14.1.7 `def forcebalance.finite_difference.fwrap_G (tgt, mvals0, pidx)`

A driver to fwrap for gradients (see documentation for fwrap) 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 164 of file finite_difference.py.

Here is the call graph for this function:

7.14.1.8 `def forcebalance.finite_difference.fwrap_H (tgt, mvals0, pidx)`

A driver to fwrap for Hessians (see documentation for fwrap) 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 175 of file finite_difference.py.

7.14.1.9 `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 119 of file finite_difference.py.

7.15 forcebalance.fitsim Namespace Reference

Classes

- class [FittingSimulation](#)
Base class for all fitting simulations.

7.16 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

- dictionary [FF_Extensions](#)
- dictionary [FF_IOModules](#)

7.16.1 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

7.16.2 Function Documentation

7.16.2.1 `def forcebalance.forcefield.determine_fftype (fname, 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 143 of file forcefield.py.

7.16.2.2 `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

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

Definition at line 1171 of file forcefield.py.

7.16.3 Variable Documentation

7.16.3.1 dictionary forcebalance.forcefield.FF_Extensions

Initial value:

```

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

Definition at line 115 of file forcefield.py.

7.16.3.2 dictionary forcebalance.forcefield.FF_IOModules

Initial value:

```

1 {"gmx": gmxiio. ITP_Reader ,
2   "qchem": qchemio.QCIn_Reader ,
3   "tinker": tinkerio.Tinker_Reader ,
4   "custom": custom_io.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 127 of file forcefield.py.

7.17 forcebalance.gmxio Namespace Reference

GROMACS input/output.

Classes

- class [ITP_Reader](#)
Finite state machine for parsing GROMACS force field files.
- class [AbInitio_GMX](#)
Subclass of AbInitio for force and energy matching using normal GROMACS.
- class [Liquid_GMX](#)
- class [Interaction_GMX](#)
Subclass of Interaction for interaction energy matching using GROMACS.

Functions

- def [edit_mdp](#)
Create or edit a Gromacs MDP file.
- def [parse_atomtype_line](#)
Parses the 'atomtype' line.
- def [rm_gmx_baks](#)

Variables

- 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', 'PDIHMULS']
Dihedral interaction function types.
- dictionary [fdict](#)
Section -> Interaction type dictionary.
- dictionary [pdict](#)
Interaction type -> Parameter Dictionary.

7.17.1 Detailed Description

GROMACS input/output.

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

Author

Lee-Ping Wang

Date

12/2011

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

Author

Lee-Ping Wang

Date

12/2011

7.17.2 Function Documentation

7.17.2.1 `def forcebalance.gmxio.edit_mdp(fin, fout, options, verbose=False)`

Create or edit a Gromacs MDP file.

Parameters

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

Definition at line 32 of file gmxio.py.

Here is the call graph for this function:

7.17.2.2 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 ; PARM
5 6
```

Look at all the variety!

Parameters

| | | |
|-----------|-------------|-------------|
| <i>in</i> | <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 178 of file gmxio.py.

Here is the call graph for this function:

7.17.2.3 def forcebalance.gmxio.rm_gmx_baks (*dir*)

Definition at line 425 of file gmxio.py.

7.17.3 Variable Documentation

7.17.3.1 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 88 of file gmxio.py.

7.17.3.2 list forcebalance.gmxio.bftypes [None, 'BONDS', 'G96BONDS', 'MORSE']

Bonded interaction function types.

Definition at line 86 of file gmxio.py.

7.17.3.3 list forcebalance.gmxio.dftypes [None, 'PDIHS', 'IDIHS', 'RBDIHS', 'PIMPDHS', 'FOURDIHS', None, None, 'TABDIHS', 'PDIHMULS']

Dihedral interaction function types.

Definition at line 91 of file gmxio.py.

7.17.3.4 dictionary forcebalance.gmxio.fdict

Initial value:

```

1 {
2   'atomtypes'      : nftypes,
3   'nonbond_params' : pftypes,
4   'bonds'          : bftypes,
5   'bondtypes'      : bftypes,
6   'angles'         : aftypes,
7   'angletypes'     : aftypes,
8   'dihedrals'      : dftypes,
9   'dihedraltypes'  : dftypes,
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 99 of file gmxio.py.

7.17.3.5 list forcebalance.gmxio.nftypes [None, 'VDW', 'VDW_BHAM']

VdW interaction function types.

Definition at line 82 of file gmxio.py.

7.17.3.6 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 122 of file gmxio.py.

7.17.3.7 list forcebalance.gmxio.pftypes [None, 'VPAIR', 'VPAIR_BHAM']

Pairwise interaction function types.

Definition at line 84 of file gmxio.py.

7.18 forcebalance.gmxqpio Namespace Reference

Classes

- class [Monomer_QTPIE](#)
Subclass of Target for monomer properties of QTPIE (implemented within gromacs WCV branch).

Functions

- def [get_monomer_properties](#)

7.18.1 Function Documentation

7.18.1.1 def forcebalance.gmxqpio.get_monomer_properties (print_stuff = 0)

Definition at line 25 of file gmxqpio.py.

Here is the call graph for this function:

7.19 forcebalance.implemented Namespace Reference

Contains the dictionary of usable Target classes.

Variables

- dictionary [Implemented_Targets](#)
The table of implemented Targets.

7.19.1 Detailed Description

Contains the dictionary of usable Target classes.

7.19.2 Variable Documentation

7.19.2.1 dictionary forcebalance.implemented.Implemented_Targets

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   'LIQUID_OPENMM':Liquid_OpenMM,

```

```
9     'LIQUID_TINKER':Liquid_TINKER,  
10     'COUNTERPOISE':Counterpoise,  
11     'THCDF_PSI4':THCDF_Psi4,  
12     'RDVR3_PSI4':RDVR3_Psi4,  
13     'INTERACTION_TINKER':Interaction_TINKER,  
14     'INTERACTION_OPENMM':Interaction_OpenMM,  
15     'BINDINGENERGY_TINKER':BindingEnergy_TINKER,  
16     'MOMENTS_TINKER':Moments_TINKER,  
17     'MONOMER_QTPIE':Monomer_QTPIE,  
18     }
```

The table of implemented Targets.

Definition at line 55 of file implemented.py.

7.20 forcebalance.interaction Namespace Reference

[Interaction](#) energy fitting module.

Classes

- class [Interaction](#)
Subclass of Target for fitting force fields to interaction energies.

7.20.1 Detailed Description

[Interaction](#) energy fitting module.

Author

Lee-Ping Wang

Date

05/2012

7.21 forcebalance.interactions Namespace Reference

Classes

- class [Interactions](#)
Improved subclass of Target for fitting force fields to interaction energies.

Functions

- def [parse_interactions](#)
Parse through the interactions input file.

7.21.1 Function Documentation

7.21.1.1 def forcebalance.interactions.parse_interactions (*input_file*)

Parse through the interactions input file.

Parameters

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

Definition at line 30 of file interactions.py.

Here is the call graph for this function:

7.22 forcebalance.leastsq Namespace Reference

Classes

- class [LeastSquares](#)
Subclass of Target for general least squares fitting.

Functions

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

Variables

- [CHECK_BASIS](#) False
- [LAST_MVALS](#) None

7.22.1 Function Documentation

7.22.1.1 def forcebalance.leastsq.CheckBasis ()

Definition at line 21 of file leastsq.py.

7.22.1.2 def forcebalance.leastsq.LastMvals ()

Definition at line 26 of file leastsq.py.

7.22.2 Variable Documentation

7.22.2.1 forcebalance.leastsq.CHECK_BASIS False

Definition at line 20 of file leastsq.py.

7.22.2.2 forcebalance.leastsq.LAST_MVALS None

Definition at line 25 of file leastsq.py.

7.23 forcebalance.liquid Namespace Reference

Matching of liquid bulk properties.

Classes

- class [Liquid](#)
Subclass of Target for liquid property matching.

Functions

- def [weight_info](#)

7.23.1 Detailed Description

Matching of liquid bulk properties. Under development.

Author

Lee-Ping Wang

Date

04/2012

7.23.2 Function Documentation

7.23.2.1 `def forcebalance.liquid.weight_info (W, PT, N.k, verbose = True)`

Definition at line 29 of file liquid.py.

7.24 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"])`

7.24.1 Variable Documentation

7.24.1.1 tuple forcebalance.Mol2.data mol2_set(sys.argv[1], subset=["RNase.xray.inh8.1QHC"])

Definition at line 651 of file Mol2.py.

7.25 forcebalance.mol2io Namespace Reference

Mol2 I/O.

Classes

- class [Mol2_Reader](#)
Finite state machine for parsing [Mol2](#) force field file.

Variables

- dictionary [mol2_pdict](#) {'COUL':{'Atom':[1], 6:"}}

7.25.1 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

7.25.2 Variable Documentation

7.25.2.1 dictionary forcebalance.mol2io.mol2_pdict {'COUL':{'Atom':[1], 6:"}}

Definition at line 18 of file mol2io.py.

7.26 forcebalance.molecule Namespace Reference

Classes

- 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 [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 [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 [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', '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
- [Alive](#)

7.26.1 Function Documentation

7.26.1.1 `def forcebalance.molecule.add_strip_to_mat (mat, strip)`

Definition at line 438 of file molecule.py.

Here is the call graph for this function:

7.26.1.2 `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 541 of file molecule.py.

Here is the call graph for this function:

7.26.1.3 `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 553 of file molecule.py.

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

Definition at line 476 of file molecule.py.

7.26.1.5 `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 258 of file molecule.py.

Here is the call graph for this function:

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

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

The hash function is something we can use to discard two things that are obviously not equal. Here we neglect the hash. Return a list of the sorted atom numbers in this graph. Return a string of atoms, which serves as a rudimentary 'fingerprint' : '99,100,103,151' . Return an array of the elements. For instance ['H' 'C' 'C' 'H']. Create an Empirical Formula Get a list of the coordinates.

Definition at line 273 of file molecule.py.

7.26.1.7 `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 524 of file molecule.py.

Here is the call graph for this function:

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

Definition at line 479 of file molecule.py.

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

Definition at line 487 of file molecule.py.

7.26.1.10 `def forcebalance.molecule.EulerMatrix (T1, T2, T3)`

Constructs an Euler matrix from three Euler angles.

Definition at line 496 of file molecule.py.

Here is the call graph for this function:

7.26.1.11 `def forcebalance.molecule.even_list (totlen, splitsize)`

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

Definition at line 458 of file molecule.py.

Here is the call graph for this function:

7.26.1.12 `def forcebalance.molecule.format_gro_box (box)`

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

Parameters

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

Definition at line 389 of file molecule.py.

Here is the call graph for this function:

7.26.1.13 `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.

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 368 of file molecule.py.

Here is the call graph for this function:

7.26.1.14 `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 352 of file molecule.py.

Here is the call graph for this function:

7.26.1.15 `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 380 of file molecule.py.

Here is the call graph for this function:

7.26.1.16 `def forcebalance.molecule.get_rotate_translate (matrix1, matrix2)`

Definition at line 576 of file molecule.py.

7.26.1.17 `def forcebalance.molecule.getElement (mass)`

Definition at line 191 of file molecule.py.

7.26.1.18 `def forcebalance.molecule.grouper (n, iterable)`

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

Definition at line 452 of file molecule.py.

Here is the call graph for this function:

7.26.1.19 `def forcebalance.molecule.is_charmm_coord (line)`

Determines whether a line contains CHARMM data or not.

Parameters

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

Definition at line 416 of file molecule.py.

Here is the call graph for this function:

7.26.1.20 `def forcebalance.molecule.is_gro_box (line)`

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

Parameters

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

Definition at line 429 of file molecule.py.

Here is the call graph for this function:

7.26.1.21 `def forcebalance.molecule.is_gro_coord (line)`

Determines whether a line contains GROMACS data or not.

Parameters

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

Definition at line 401 of file molecule.py.

Here is the call graph for this function:

7.26.1.22 `def forcebalance.molecule.isfloat (word)`

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

Definition at line 247 of file molecule.py.

7.26.1.23 `def forcebalance.molecule.isint (word)`

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

Definition at line 242 of file molecule.py.

Here is the call graph for this function:

7.26.1.24 `def forcebalance.molecule.main ()`

Definition at line 2489 of file molecule.py.

7.26.1.25 `def forcebalance.molecule.nodematch (node1, node2)`

Definition at line 236 of file molecule.py.

Here is the call graph for this function:

7.26.1.26 `def forcebalance.molecule.pvec (vec)`

Definition at line 447 of file molecule.py.

7.26.2 Variable Documentation

7.26.2.1 forcebalance.molecule.Alive

Definition at line 302 of file molecule.py.

7.26.2.2 forcebalance.molecule.AllVariableNames QuantumVariableNames|AtomVariableNames|MetaVariableNames|FrameVariableNames

Definition at line 139 of file molecule.py.

7.26.2.3 tuple forcebalance.molecule.AtomVariableNames set(['elem', 'partial_charge', 'atomname', 'atomtype', 'tinkersuf', 'resid', 'resname', 'qcsuf', 'qm_ghost', 'chain', 'altloc', 'icode'])

Definition at line 122 of file molecule.py.

7.26.2.4 float forcebalance.molecule.bohrang 0.529177249

One bohr equals this many angstroms.

Definition at line 234 of file molecule.py.

7.26.2.5 tuple forcebalance.molecule.Box namedtuple('Box', ['a', 'b', 'c', 'alpha', 'beta', 'gamma', 'A', 'B', 'C', 'V'])

Definition at line 254 of file molecule.py.

7.26.2.6 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 166 of file molecule.py.

7.26.2.7 tuple forcebalance.molecule.FrameVariableNames

Initial value:

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

Definition at line 108 of file molecule.py.

7.26.2.8 tuple forcebalance.molecule.MetaVariableNames set(['fnm', 'ftype', 'qcrems', 'qctemplate', 'charge', 'mult', 'bonds'])

Definition at line 135 of file molecule.py.

7.26.2.9 tuple forcebalance.molecule.PeriodicTable

Initial value:

```

1 OrderedDict([('H' , 1.0079), ('He' , 4.0026),
2              ('Li' , 6.941), ('Be' , 9.0122), ('B' , 10.811), (
3              'C' , 12.0107), ('N' , 14.0067), ('O' , 15.9994), ('F' , 18.9984), ('Ne' , 20.17
4              97),
5              ('Na' , 22.9897), ('Mg' , 24.305), ('Al' , 26.9815
6              ), ('Si' , 28.0855), ('P' , 30.9738), ('S' , 32.065), ('Cl' , 35.453), ('Ar' , 3
7              9.948),
8              ('K' , 39.0983), ('Ca' , 40.078), ('Sc' , 44.9559)
9              , ('Ti' , 47.867), ('V' , 50.9415), ('Cr' , 51.9961), ('Mn' , 54.938), ('Fe' , 5
10             5.845), ('Co' , 58.9332),
11             ('Ni' , 58.6934), ('Cu' , 63.546), ('Zn' , 65.39),
12             ('Ga' , 69.723), ('Ge' , 72.64), ('As' , 74.9216), ('Se' , 78.96), ('Br' , 79.9
13             04), ('Kr' , 83.8),
14             ('Rb' , 85.4678), ('Sr' , 87.62), ('Y' , 88.9059),
15             ('Zr' , 91.224), ('Nb' , 92.9064), ('Mo' , 95.94), ('Tc' , 98), ('Ru' , 101.07)
16             , ('Rh' , 102.9055),
17             ('Pd' , 106.42), ('Ag' , 107.8682), ('Cd' , 112.41
18             1), ('In' , 114.818), ('Sn' , 118.71), ('Sb' , 121.76), ('Te' , 127.6), ('I' , 1
19             26.9045), ('Xe' , 131.293),
20             ('Cs' , 132.9055), ('Ba' , 137.327), ('La' , 138.9
21             055), ('Ce' , 140.116), ('Pr' , 140.9077), ('Nd' , 144.24), ('Pm' , 145), ('Sm'
22             , 150.36),
23             ('Eu' , 151.964), ('Gd' , 157.25), ('Tb' , 158.925
24             3), ('Dy' , 162.5), ('Ho' , 164.9303), ('Er' , 167.259), ('Tm' , 168.9342), ('Yb
25             ' , 173.04),
26             ('Lu' , 174.967), ('Hf' , 178.49), ('Ta' , 180.947
27             9), ('W' , 183.84), ('Re' , 186.207), ('Os' , 190.23), ('Ir' , 192.217), ('Pt' ,
28             195.078),
29             ('Au' , 196.9665), ('Hg' , 200.59), ('Tl' , 204.38
30             33), ('Pb' , 207.2), ('Bi' , 208.9804), ('Po' , 209), ('At' , 210), ('Rn' , 222)
31             ,
32             ('Fr' , 223), ('Ra' , 226), ('Ac' , 227), ('Th' ,
33             232.0381), ('Pa' , 231.0359), ('U' , 238.0289), ('Np' , 237), ('Pu' , 244),
34             ('Am' , 243), ('Cm' , 247), ('Bk' , 247), ('Cf' ,
35             251), ('Es' , 252), ('Fm' , 257), ('Md' , 258), ('No' , 259),
36             ('Lr' , 262), ('Rf' , 261), ('Db' , 262), ('Sg' ,
37             266), ('Bh' , 264), ('Hs' , 277), ('Mt' , 268)])

```

Definition at line 176 of file molecule.py.

7.26.2.10 tuple forcebalance.molecule.QuantumVariableNames set(['qcrems', 'qctemplate', 'charge', 'mult', 'qcsuf', 'qm_ghost'])

Definition at line 137 of file molecule.py.

7.26.2.11 int forcebalance.molecule.radian 180

Definition at line 255 of file molecule.py.

7.26.2.12 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, 1.22, 1.20, 1.19, 1.20, 1.20, 1.16, # Third row
6     elements, K through Kr
7     2.20, 1.95, 1.90, 1.75, 1.64, 1.54, 1.47, 1.46, 1.42,
8     1.39, 1.45, 1.44, 1.42, 1.39, 1.39, 1.38, 1.39, 1.40, # Fourth row
9     elements, Rb through Xe
10    2.44, 2.15, 2.07, 2.04, 2.03, 2.01, 1.99, 1.98,
11    1.98, 1.96, 1.94, 1.92, 1.92, 1.89, 1.90, 1.87, # Fifth row elements,
12    s and f blocks
13    1.87, 1.75, 1.70, 1.62, 1.51, 1.44, 1.41, 1.36,
14    1.36, 1.32, 1.45, 1.46, 1.48, 1.40, 1.50, 1.50, # Fifth row elements,
15    d and p blocks
16    2.60, 2.21, 2.15, 2.06, 2.00, 1.96, 1.90, 1.87, 1.80, 1.69]

```


Definition at line 152 of file molecule.py.

7.26.2.13 tuple forcebalance.molecule.splitter re.compile(r'(\s+|\S+)')

Definition at line 251 of file molecule.py.

7.27 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).

7.27.1 Detailed Description

Multipole moment fitting module.

Author

Lee-Ping Wang

Date

09/2012

7.28 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.

Functions

- def [pvec1d](#)
Printout of a 1-D vector.
- def [pmat2d](#)
Printout of a 2-D matrix.
- def [encode](#)
- def [segments](#)
- def [commadash](#)
- def [uncommadash](#)

- 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 [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 [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 [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 [GoInto](#)
- def [allsplit](#)
- def [Leave](#)
- def [MissingFileInspection](#)
- 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()`.

- def `multiopen`

This function be given any of several variable types (single file name, file object, or list of lines, or a list of the above) and give a list of files:

Variables

- 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.

- list `specific_lst`
- tuple `specific_dct` dict(list(itertools.chain(*[[j,i[1]] for j in i[0]] for i in `specific_lst`))))

7.28.1 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

7.28.2 Function Documentation

7.28.2.1 `def forcebalance.nifty.allsplit (Dir)`

Definition at line 701 of file nifty.py.

Here is the call graph for this function:

7.28.2.2 `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 267 of file nifty.py.

Here is the call graph for this function:

7.28.2.3 `def forcebalance.nifty.commadash (l)`

Definition at line 78 of file nifty.py.

Here is the call graph for this function:

7.28.2.4 `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 904 of file nifty.py.

7.28.2.5 `def forcebalance.nifty.CopyFile (src, dest)`

Definition at line 749 of file nifty.py.

Here is the call graph for this function:

7.28.2.6 `def forcebalance.nifty.createWorkQueue (wq_port)`

Definition at line 569 of file nifty.py.

Here is the call graph for this function:

7.28.2.7 `def forcebalance.nifty.encode (l)`

Definition at line 69 of file nifty.py.

Here is the call graph for this function:

7.28.2.8 `def forcebalance.nifty.flat (vec)`

Given any list, array, or matrix, return a single-index array.

Parameters

| | | |
|-----------------|------------------|--------------------------|
| <code>in</code> | <code>vec</code> | The data to be flattened |
|-----------------|------------------|--------------------------|

Returns

answer The flattened data

Definition at line 286 of file nifty.py.

Here is the call graph for this function:

7.28.2.9 `def forcebalance.nifty.floatornan (word)`

Returns a big number if we encounter NaN.

Parameters

| | | |
|----|-------------|----------------------------|
| in | <i>word</i> | 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 249 of file nifty.py.

Here is the call graph for this function:

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

```

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

```

Parameters

| | | |
|-----|-------------|---|
| in | <i>X</i> | (2-D array) An array of X-values (see above) |
| in | <i>Y</i> | (array) An array of Y-values (only used in getting the least squares coefficients) |
| in | <i>w</i> | (array) An array of weights, hopefully normalized to one. |
| out | <i>Beta</i> | The least-squares coefficients |
| out | <i>Hat</i> | The hat matrix that takes linear combinations of data y-values to give fitted y-values (weights) |
| out | <i>yfit</i> | The fitted y-values |
| out | <i>MPPI</i> | 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 354 of file nifty.py.

Here is the call graph for this function:

7.28.2.11 `def forcebalance.nifty.getWorkQueue ()`

Definition at line 563 of file nifty.py.

7.28.2.12 `def forcebalance.nifty.getWQlds ()`

Definition at line 566 of file nifty.py.

7.28.2.13 `def forcebalance.nifty.GoInto (Dir)`

Definition at line 693 of file nifty.py.

7.28.2.14 `def forcebalance.nifty.invert_svd (X, thresh = 1e-12)`

Invert a matrix using singular value decomposition.

Parameters

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

Returns

Xt The inverted matrix

Definition at line 313 of file nifty.py.

Here is the call graph for this function:

7.28.2.15 `def forcebalance.nifty.isdecimal (word)`

Matches things with a decimal only; see isint and isfloat.

Parameters

| | | |
|-----------|-------------|---|
| <i>in</i> | <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 239 of file nifty.py.

Here is the call graph for this function:

7.28.2.16 `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

| | | |
|-----------|-------------|---|
| <i>in</i> | <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 229 of file nifty.py.

Here is the call graph for this function:

7.28.2.17 `def forcebalance.nifty.isint (word)`

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

Parameters

| | | |
|-----------|-------------|---|
| <i>in</i> | <i>word</i> | 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 218 of file nifty.py.

Here is the call graph for this function:

7.28.2.18 `def forcebalance.nifty.Leave (Dir)`

Definition at line 707 of file nifty.py.

7.28.2.19 `def forcebalance.nifty.link_dir_contents (absrsrcdir, absdestdir)`

Definition at line 759 of file nifty.py.

7.28.2.20 `def forcebalance.nifty.LinkFile (src, dest)`

Definition at line 738 of file nifty.py.

Here is the call graph for this function:

7.28.2.21 `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 546 of file nifty.py.

Here is the call graph for this function:

7.28.2.22 `def forcebalance.nifty.lp.load (file)`

Use this instead of pickle.load for unpickling anything that contains `_ElementTree` types.

Definition at line 551 of file nifty.py.

Here is the call graph for this function:

7.28.2.23 `def forcebalance.nifty.MissingFileInspection (fnm)`

Definition at line 728 of file nifty.py.

Here is the call graph for this function:

7.28.2.24 `def forcebalance.nifty.multiopen (arg)`

This function be given any of several variable types (single file name, file object, or list of lines, or a list of the above) and give a list of files:

```
[file1, file2, file3 ... ]
```

each of which can then be iterated over:

```
[[file1_line1, file1_line2 ... ], [file2_line1, file2_line2 ... ]]
```

Definition at line 934 of file nifty.py.

7.28.2.25 `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

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

Returns

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

Definition at line 300 of file nifty.py.

7.28.2.26 `def forcebalance.nifty.pmat2d (mat2d, precision = 1)`

Printout of a 2-D matrix.

Parameters

| | | |
|-----------------|--------------------|--------------|
| <code>in</code> | <code>mat2d</code> | a 2-D matrix |
|-----------------|--------------------|--------------|

Definition at line 62 of file nifty.py.

Here is the call graph for this function:

7.28.2.27 `def forcebalance.nifty.printcool (text, sym = "#", bold = False, color = 2, ansi = None, bottom = '-', minwidth = 50, center = True)`

Cool-looking printout for slick formatting of output.

Parameters

| | | |
|-----------------|-----------------------|--|
| <code>in</code> | <code>text</code> | 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 ### ##### |
| <code>in</code> | <code>sym</code> | The surrounding symbol |
| <code>in</code> | <code>bold</code> | Whether to use bold print |
| <code>in</code> | <code>color</code> | The ANSI color: 1 red 2 green 3 yellow 4 blue 5 magenta 6 cyan 7 white |
| <code>in</code> | <code>bottom</code> | The symbol for the bottom bar |
| <code>in</code> | <code>minwidth</code> | 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 151 of file nifty.py.

Here is the call graph for this function:

```
7.28.2.28 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 194 of file nifty.py.

Here is the call graph for this function:

```
7.28.2.29 def forcebalance.nifty.pvec1d ( vec1d, precision = 1 )
```

Printout of a 1-D vector.

Parameters

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

Definition at line 51 of file nifty.py.

Here is the call graph for this function:

```
7.28.2.30 def forcebalance.nifty.queue_up ( wq, command, input_files, output_files, 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 585 of file nifty.py.

Here is the call graph for this function:

```
7.28.2.31 def forcebalance.nifty.queue_up_src_dest ( wq, command, input_files, output_files, 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 616 of file nifty.py.

7.28.2.32 `def forcebalance.nifty.remove_if_exists (fnm)`

Remove the file if it exists (doesn't return an error).

Definition at line 770 of file nifty.py.

7.28.2.33 `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 277 of file nifty.py.

Here is the call graph for this function:

7.28.2.34 `def forcebalance.nifty.segments (e)`

Definition at line 72 of file nifty.py.

Here is the call graph for this function:

7.28.2.35 `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 τ is the correlation time). We enforce $g \geq 1.0$.

Definition at line 430 of file nifty.py.

7.28.2.36 `def forcebalance.nifty.uncommadash (s)`

Definition at line 88 of file nifty.py.

Here is the call graph for this function:

7.28.2.37 `def forcebalance.nifty.warn_once (warning, warnhash = None)`

Prints a warning but will only do so once in a given run.

Definition at line 880 of file nifty.py.

Here is the call graph for this function:

7.28.2.38 `def forcebalance.nifty.warn_press_key (warning, timeout = 10)`

Definition at line 865 of file nifty.py.

Here is the call graph for this function:

7.28.2.39 `def forcebalance.nifty.which (fnm)`

Definition at line 774 of file nifty.py.

Here is the call graph for this function:

7.28.2.40 `def forcebalance.nifty.wq_wait (wq, verbose = False)`

This function waits until the work queue is completely empty.

Definition at line 686 of file nifty.py.

Here is the call graph for this function:

7.28.2.41 `def forcebalance.nifty.wq_wait1 (wq, wait_time = 10, verbose = False)`

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

Definition at line 636 of file nifty.py.

Here is the call graph for this function:

7.28.3 Variable Documentation

7.28.3.1 float forcebalance.nifty.bohrang 0.529177249

One bohr equals this many angstroms.

Definition at line 41 of file nifty.py.

7.28.3.2 float forcebalance.nifty.eqcgmx 2625.5002

Q-Chem to GMX unit conversion for energy.

Definition at line 37 of file nifty.py.

7.28.3.3 float forcebalance.nifty.fqcgmx 49621.9

Q-Chem to GMX unit conversion for force.

Definition at line 39 of file nifty.py.

7.28.3.4 float forcebalance.nifty.kb 0.0083144100163

Boltzmann constant.

Definition at line 35 of file nifty.py.

7.28.3.5 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 726 of file nifty.py.

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

```

Definition at line 714 of file nifty.py.

7.28.3.7 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 492 of file nifty.py.

7.29 forcebalance.objective Namespace Reference

ForceBalance objective function.

Classes

- class [Objective](#)
Objective function.
- class [Penalty](#)
Penalty functions for regularizing the force field optimizer.

Variables

- dictionary [Implemented_Targets](#)
The table of implemented Targets.
- list [Letters](#) ['X','G','H']
This is the canonical lettering that corresponds to : objective function, gradient, Hessian.

7.29.1 Detailed Description

ForceBalance objective function.

7.29.2 Variable Documentation

7.29.2.1 dictionary forcebalance.objective.Implemented_Targets

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     'LIQUID_OPENMM':Liquid_OpenMM,
9     'LIQUID_TINKER':Liquid_TINKER,
10    'LIQUID_GMX':Liquid_GMX,
11    'COUNTERPOISE':Counterpoise,
12    'THCDF_PSI4':THCDF_Psi4,
13    'RDVR3_PSI4':RDVR3_Psi4,
14    'INTERACTION_TINKER':Interaction_TINKER,
15    'INTERACTION_OPENMM':Interaction_OpenMM,
16    'BINDINGENERGY_TINKER':BindingEnergy_TINKER,
17    'MOMENTS_TINKER':Moments_TINKER,
18    'MONOMER_QTPIE':Monomer_QTPIE,
19 }
```

The table of implemented Targets.

Definition at line 67 of file objective.py.

7.29.2.2 list forcebalance.objective.Letters ['X','G','H']

This is the canonical lettering that corresponds to : objective function, gradient, Hessian.

Definition at line 88 of file objective.py.

7.30 forcebalance.openmmio Namespace Reference

OpenMM input/output.

Classes

- class [OpenMM_Reader](#)
Class for parsing OpenMM force field files.
- class [Liquid_OpenMM](#)
- class [AbInitio_OpenMM](#)
Subclass of AbInitio for force and energy matching using OpenMM.
- class [Interaction_OpenMM](#)
Subclass of Target for interaction matching using OpenMM.

Functions

- def [get_dipole](#)
Return the current dipole moment in Debye.
- def [ResetVirtualSites](#)
Given a set of OpenMM-compatible positions and a System object, compute the correct virtual site positions according to 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 [MTSVVVRIntegrator](#)
Create a multiple timestep velocity verlet with velocity randomization (VVVR) integrator.

Variables

- dictionary [suffix_dict](#)
- string [pdict](#) "XML_Override"
pdict is a useless variable if the force field is XML.

7.30.1 Detailed Description

OpenMM input/output.

Author

Lee-Ping Wang

Date

04/2012

7.30.2 Function Documentation

7.30.2.1 `def forcebalance.openmmio.CopyAmoebaAngleParameters (src, dest)`

Definition at line 109 of file openmmio.py.

Here is the call graph for this function:

7.30.2.2 `def forcebalance.openmmio.CopyAmoebaBondParameters (src, dest)`

Definition at line 95 of file openmmio.py.

Here is the call graph for this function:

7.30.2.3 `def forcebalance.openmmio.CopyAmoebaInPlaneAngleParameters (src, dest)`

Definition at line 118 of file openmmio.py.

Here is the call graph for this function:

7.30.2.4 `def forcebalance.openmmio.CopyAmoebaMultipoleParameters (src, dest)`

Definition at line 131 of file openmmio.py.

Here is the call graph for this function:

7.30.2.5 `def forcebalance.openmmio.CopyAmoebaOutOfPlaneBendParameters (src, dest)`

Definition at line 101 of file openmmio.py.

Here is the call graph for this function:

7.30.2.6 `def forcebalance.openmmio.CopyAmoebaVdwParameters (src, dest)`

Definition at line 127 of file openmmio.py.

Here is the call graph for this function:

7.30.2.7 `def forcebalance.openmmio.CopyHarmonicAngleParameters (src, dest)`

Definition at line 139 of file openmmio.py.

Here is the call graph for this function:

7.30.2.8 `def forcebalance.openmmio.CopyHarmonicBondParameters (src, dest)`

Definition at line 135 of file openmmio.py.

Here is the call graph for this function:

7.30.2.9 `def forcebalance.openmmio.CopyNonbondedParameters (src, dest)`

Definition at line 147 of file openmmio.py.

Here is the call graph for this function:

7.30.2.10 `def forcebalance.openmmio.CopyPeriodicTorsionParameters (src, dest)`

Definition at line 143 of file openmmio.py.

Here is the call graph for this function:

7.30.2.11 `def forcebalance.openmmio.CopySystemParameters (src, dest)`

Copy parameters from one system (i.e.

that which is created by a new force field) to another system (i.e. the one stored inside the Target object). DANGER: These need to be implemented manually!!!

Definition at line 161 of file openmmio.py.

Here is the call graph for this function:

7.30.2.12 `def forcebalance.openmmio.do_nothing (src, dest)`

Definition at line 154 of file openmmio.py.

7.30.2.13 `def forcebalance.openmmio.get_dipole (simulation, q=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 34 of file openmmio.py.

Here is the call graph for this function:

7.30.2.14 `def forcebalance.openmmio.MTSVVVRIntegrator (temperature, collision_rate, timestep, system, ninnersteps=4)`

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

ARGUMENTS

temperature (numpy.unit.Quantity compatible with kelvin) - the temperature collision_rate (numpy.unit.Quantity compatible with 1/picoseconds) - the collision rate timestep (numpy.unit.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 219 of file openmmio.py.

7.30.2.15 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 64 of file openmmio.py.

Here is the call graph for this function:

7.30.2.16 def forcebalance.openmmio.UpdateSimulationParameters (*src_system*, *dest_simulation*)

Definition at line 180 of file openmmio.py.

Here is the call graph for this function:

7.30.3 Variable Documentation

7.30.3.1 string forcebalance.openmmio.pdict "XML_Override"

pdict is a useless variable if the force field is XML.

Definition at line 298 of file openmmio.py.

7.30.3.2 dictionary forcebalance.openmmio.suffix_dict

Initial value:

```

1 { "HarmonicBondForce" : {"Bond" : ["class1","class2"]},
2   "HarmonicAngleForce" : {"Angle" : ["class1","class2","class3"],
3     },
4   "PeriodicTorsionForce" : {"Proper" : ["class1","class2","class3",
5     "","class4"],},
6   "NonbondedForce" : {"Atom": ["type"]},
7   "AmoebaBondForce" : {"Bond" : ["class1","class2"]},
8   "AmoebaAngleForce" : {"Angle" : ["class1","class2","class3"]},
9   "AmoebaStretchBendForce" : {"StretchBend" : ["class1","class2",
10     "class3"]},
11   "AmoebaVdwForce" : {"Vdw" : ["class"]},
12   "AmoebaMultipoleForce" : {"Multipole" : ["type","kz","kx"], "
    Polarize" : ["type"]},
13   "AmoebaUreyBradleyForce" : {"UreyBradley" : ["class1","class2",
14     "class3"]},
15   "Residues.Residue" : {"VirtualSite" : ["index"]}
16 }
```

Definition at line 284 of file openmmio.py.

7.31 forcebalance.optimizer Namespace Reference

Optimization algorithms.

Classes

- class [Optimizer](#)

Optimizer class.

Functions

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

Variables

- int [ITERATION_NUMBER](#) 0
- int [GOODSTEP](#) 0

7.31.1 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

7.31.2 Function Documentation

7.31.2.1 `def forcebalance.optimizer.Counter ()`

Definition at line 27 of file optimizer.py.

Here is the call graph for this function:

7.31.2.2 `def forcebalance.optimizer.GoodStep ()`

Definition at line 31 of file optimizer.py.

7.31.3 Variable Documentation

7.31.3.1 `int forcebalance.optimizer.GOODSTEP 0`

Definition at line 25 of file optimizer.py.

7.31.3.2 `int forcebalance.optimizer.ITERATION_NUMBER 0`

Definition at line 23 of file optimizer.py.

7.32 forcebalance.output Namespace Reference

Classes

- 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 [CleanFileHandler](#)

File handler that does not write terminal escape codes to files.

Variables

- tuple [logger](#) getLogger('forcebalance')

7.32.1 Variable Documentation

7.32.1.1 tuple forcebalance.output.logger getLogger('forcebalance')

Definition at line 5 of file output.py.

7.33 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

- dictionary [gen_opts_types](#)
Default general options.
- dictionary [tgt_opts_types](#)
Default fitting target options.
- dictionary [gen_opts_defaults](#) {}
Default general options - basically a collapsed veresion of gen_opts_types.
- dictionary [subdict](#) {}
- dictionary [tgt_opts_defaults](#) {}
Default target options - basically a collapsed version of tgt_opts_types.
- dictionary [bkwd](#) {"simtype" : "type"}
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.

7.33.1 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

7.33.2 Function Documentation

7.33.2.1 `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

| | | |
|-----------|-------------------|-----------------------------|
| <i>in</i> | <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 372 of file parser.py.

Here is the call graph for this function:

7.33.2.2 `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

| | | |
|-----------|-----------------|---|
| <i>in</i> | <i>heading</i> | Heading, either \$options or \$target |
| <i>in</i> | <i>optdict</i> | Options dictionary or None. |
| <i>in</i> | <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 275 of file parser.py.

Here is the call graph for this function:

7.33.2.3 `def forcebalance.parser.read_internals (fobj)`

Definition at line 249 of file parser.py.

7.33.2.4 `def forcebalance.parser.read_mvals (fobj)`

Definition at line 224 of file parser.py.

Here is the call graph for this function:

7.33.2.5 `def forcebalance.parser.read_priors (fobj)`

Definition at line 240 of file parser.py.

Here is the call graph for this function:

7.33.2.6 `def forcebalance.parser.read_pvals (fobj)`

Definition at line 232 of file parser.py.

Here is the call graph for this function:

7.33.3 Variable Documentation**7.33.3.1** dictionary `forcebalance.parser.bkwd` `{"simtype" : "type"}`

Option maps for maintaining backward compatibility.

Definition at line 219 of file parser.py.

7.33.3.2 dictionary `forcebalance.parser.gen_opts_defaults` `{}`

Default general options - basically a collapsed veresion of `gen_opts_types`.

Definition at line 203 of file parser.py.

7.33.3.3 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 62 of file parser.py.

7.33.3.4 list `forcebalance.parser.mainsections` `["SIMULATION","TARGET","OPTIONS","END","NONE"]`

Listing of sections in the input file.

Definition at line 222 of file parser.py.

7.33.3.5 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 253 of file parser.py.

7.33.3.6 dictionary forcebalance.parser.subdict {}

Definition at line 205 of file parser.py.

7.33.3.7 dictionary forcebalance.parser.tgt_opts_defaults {}

Default target options - basically a collapsed version of tgt_opts_types.

Definition at line 211 of file parser.py.

7.33.3.8 dictionary forcebalance.parser.tgt_opts_types

Default fitting target options.

Definition at line 123 of file parser.py.

7.34 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.

7.34.1 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

7.35 forcebalance.PT Namespace Reference

Variables

- dictionary [PeriodicTable](#)
- list [Elements](#)

7.35.1 Variable Documentation

7.35.1.1 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',
5   'As', 'Se', 'Br', 'Kr',
6   'Rb', 'Sr', 'Y', 'Zr', 'Nb', 'Mo', 'Tc', 'Ru', 'Rh', 'Pd', 'Ag', 'Cd', 'In', 'Sn',
7   'Sb', 'Te', 'I', 'Xe',
8   'Cs', 'Ba', 'La', 'Ce', 'Pr', 'Nd', 'Pm', 'Sm', 'Eu', 'Gd', 'Tb', 'Dy', 'Ho', 'Er', 'Tm', 'Yb',
9   'Lu', 'Hf', 'Ta', 'W', 'Re', 'Os', 'Ir', 'Pt', 'Au', 'Hg', 'Tl', 'Pb', 'Bi', 'Po',
10  'At', 'Rn',
11  'Fr', 'Ra', 'Ac', 'Th', 'Pa', 'U', 'Np', 'Pu', 'Am', 'Cm', 'Bk', 'Cf', 'Es', 'Fm',
12  'Md', 'No', 'Lr', 'Rf', 'Db', 'Sg', 'Bh', 'Hs', 'Mt']

```

Definition at line 18 of file PT.py.

7.35.1.2 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'
3   : 14.0067, 'O' : 15.9994, 'F' : 18.9984, 'Ne' : 20.1797,
4   'Na' : 22.9897, 'Mg' : 24.305, 'Al' : 26.9815, 'Si' : 28.0855,
5   'P' : 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' : 50.9415,
7   'Cr' : 51.9961, 'Mn' : 54.938, 'Fe' : 55.845, 'Co' : 58.9332, 'Ni' : 58.6934,
8   'Cu' : 63.546, 'Zn' : 65.39, 'Ga' : 69.723, 'Ge' : 72.64, 'As' : 74.9216,
9   'Se' : 78.96, 'Br' : 79.904, 'Kr' : 83.8, 'Rb' : 85.4678, 'Sr' : 87.62,
10  'Y' : 88.9059, 'Zr' : 91.224, 'Nb' : 92.9064, 'Mo' : 95.94, 'Tc' : 98, 'Ru' : 101.07,
11  'Rh' : 102.9055, 'Pd' : 106.42, 'Ag' : 107.8682, 'Cd' : 112.411, 'In' : 114.818,
12  'Sn' : 118.71, 'Sb' : 121.76, 'Te' : 127.6, 'I' : 126.9045, 'Xe' : 131.293,
13  'Cs' : 132.9055, 'Ba' : 137.327, 'La' : 138.9055, 'Ce' : 140.116, 'Pr' : 140.9077,
14  'Nd' : 144.24, 'Pm' : 145, 'Sm' : 150.36, 'Eu' : 151.964, 'Gd' : 157.25,
15  'Tb' : 158.9253, 'Dy' : 162.5, 'Ho' : 164.9303, 'Er' : 167.259, 'Tm' : 168.9342,
16  'Yb' : 173.04, 'Lu' : 174.967, 'Hf' : 178.49, 'Ta' : 180.9479, 'W' : 183.84,
17  'Re' : 186.207, 'Os' : 190.23, 'Ir' : 192.217, 'Pt' : 195.078, 'Au' : 196.9665,
18  'Hg' : 200.59, 'Tl' : 204.3833, 'Pb' : 207.2, 'Bi' : 208.9804, 'Po' : 209,
19  'At' : 210, 'Rn' : 222, 'Fr' : 223, 'Ra' : 226, 'Ac' : 227, 'Th' : 232.0381,
20  'Pa' : 231.0359, 'U' : 238.0289, 'Np' : 237, 'Pu' : 244, 'Am' : 243, 'Cm' : 247,
21  'Bk' : 247, 'Cf' : 251, 'Es' : 252, 'Fm' : 257, 'Md' : 258, 'No' : 259, 'Lr' : 262,
22  'Rf' : 261, 'Db' : 262, 'Sg' : 266, 'Bh' : 264, 'Hs' : 277, 'Mt' : 268}

```

Definition at line 3 of file PT.py.

7.36 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

- list [ndtypes](#) [None]
Types of counterpoise correction cotypes = [None, 'BASS', 'BASSP'] Types of NDDO correction.
- dictionary [pdict](#)
Section -> Interaction type dictionary.

7.36.1 Detailed Description

Q-Chem input file parser.

7.36.2 Function Documentation

7.36.2.1 def forcebalance.qchemio.QChem_Dielectric_Energy (*fnm*, *wq*)

Definition at line 71 of file qchemio.py.

Here is the call graph for this function:

7.36.3 Variable Documentation

7.36.3.1 list forcebalance.qchemio.ndtypes [None]

Types of counterpoise correction cotypes = [None, 'BASS', 'BASSP'] Types of NDDO correction.

Definition at line 13 of file qchemio.py.

7.36.3.2 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 20 of file qchemio.py.

7.37 forcebalance.simtab Namespace Reference

Variables

- dictionary [SimTab](#)
The table of fitting simulations.

7.37.1 Variable Documentation

7.37.1.1 dictionary forcebalance.simtab.SimTab

Initial value:

```

1 {
2     'ABINITIO_GMX':AbInitio_GMX,
3     'INTERACTION_GMX':Interaction_GMX,
4     'ABINITIO_TINKER':AbInitio_TINKER,
5     'ABINITIO_OPENMM':AbInitio_OpenMM,
6     'ABINITIO_AMBER':AbInitio_AMBER,
7     'ABINITIO_GMXX2':AbInitio_GMXX2,
8     'ABINITIO_INTERNAL':AbInitio_Internal,
9     'VIBRATION_TINKER':Vibration_TINKER,
10    'LIQUID_OPENMM':Liquid_OpenMM,
11    'COUNTERPOISE':Counterpoise,
12    'THCDF_PSI4':THCDF_Psi4,
13    'INTERACTIONS_TINKER':Interactions_TINKER,
14    'MOMENTS_TINKER':Moments_TINKER,
15    'MONOMER_QTPIE':Monomer_QTPIE,
16 }
```

The table of fitting simulations.

Definition at line 54 of file simtab.py.

7.38 forcebalance.target Namespace Reference

Classes

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

7.39 forcebalance.tinkerio Namespace Reference

TINKER input/output.

Classes

- class [Tinker_Reader](#)
Finite state machine for parsing TINKER force field files.
- class [Liquid_TINKER](#)
- class [AbInitio_TINKER](#)
Subclass of Target for force and energy matching using TINKER.
- class [Vibration_TINKER](#)
Subclass of Target for vibrational frequency matching using TINKER.
- class [Moments_TINKER](#)
Subclass of Target for multipole moment matching using TINKER.
- class [BindingEnergy_TINKER](#)
Subclass of BindingEnergy for binding energy matching using TINKER.
- class [Interaction_TINKER](#)
Subclass of Target for interaction matching using TINKER.

Functions

- def [write_key_with_prm](#)
Copies a TINKER .key file but changes the parameter keyword as necessary to reflect the ForceBalance settings.
- def [modify_key](#)
Performs in-place modification of a TINKER .key file.

Variables

- dictionary [pdict](#)

7.39.1 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

7.39.2 Function Documentation

7.39.2.1 `def forcebalance.tinkerio.modify_key (src, in_dict)`

Performs in-place modification of a TINKER .key file.

The input dictionary contains key:value pairs such as "polarization direct". If the key exists in the TINKER file, then that line is modified such that it contains the value in the dictionary. Note that this "key" is not to be confused with the .key extension in the TINKER file that we're modifying.

Sometimes keys like 'archive' do not have a value, in which case the dictionary should contain a None value or a blank space.

If the key doesn't exist in the TINKER file, then the key:value pair will be printed at the end.

Parameters

| | | |
|-----------------|----------------------|---|
| <code>in</code> | <code>src</code> | Name of the TINKER file to be modified. |
| <code>in</code> | <code>in_dict</code> | Dictionary containing key-value pairs used to modify the TINKER file. |

Definition at line 199 of file `tinkerio.py`.

7.39.2.2 `def forcebalance.tinkerio.write_key_with_prm (src, dest, prmfnm=None, fobj=None)`

Copies a TINKER .key file but changes the parameter keyword as necessary to reflect the ForceBalance settings.

Definition at line 143 of file `tinkerio.py`.

Here is the call graph for this function:

7.39.3 Variable Documentation

7.39.3.1 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   'UREYBRAD'     : {'Atom':[1,2,3], 4:'K',5:'B'},    # Urey-Bradley force
   constant and equilibrium distance (Angstrom)
5   'MCHARGE'      : {'Atom':[1,2,3], 4:''},          # Atomic charge
6   'DIPOLE'       : {0:'X',1:'Y',2:'Z'},             # Dipole moment in
   local frame
7   'QUADX'        : {0:'X'},                          # Quadrupole moment,
   X component
8   'QUADY'        : {0:'X',1:'Y'},                   # Quadrupole moment,
   Y component
9   'QUADZ'        : {0:'X',1:'Y',2:'Z'},             # Quadrupole moment,
   Y component
10  'POLARIZE'      : {'Atom':[1], 2:'A',3:'T'},      # Atomic dipole
   polarizability
11  'BOND-CUBIC'    : {'Atom':[], 0:''},              # Below are global parameters.
12  'BOND-QUARTIC'  : {'Atom':[], 0:''},
13  'ANGLE-CUBIC'   : {'Atom':[], 0:''},
14  'ANGLE-QUARTIC' : {'Atom':[], 0:''},
15  'ANGLE-PENTIC'  : {'Atom':[], 0:''},
16  'ANGLE-SEXTIC'  : {'Atom':[], 0:''},
17  'DIELECTRIC'    : {'Atom':[], 0:''},
18  'POLAR-SOR'     : {'Atom':[], 0:''}
19
   coupling, out-of-plane bending,
20
   pi-torsion, torsion-torsion
21 }

```

Definition at line 31 of file tinkerio.py.

7.40 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).

7.40.1 Detailed Description

Vibrational mode fitting module.

Author

Lee-Ping Wang

Date

08/2012

7.41 interaction Namespace Reference

Interaction energy fitting module.

7.41.1 Detailed Description

Interaction energy fitting module.

Author

Lee-Ping Wang

Date

05/2012

7.42 simtab Namespace Reference

Contains the dictionary of fitting simulation classes.

7.42.1 Detailed Description

Contains the dictionary of fitting simulation classes. This is in a separate file to facilitate importing. I would happily put it somewhere else.

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 [read_topology](#)
- 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 [prepare_temp_directory](#)
Prepare the temporary directory, by default does nothing.
- def [indicate](#)
- def [energy_force_transformer_all](#)
- def [energy_force_transformer](#)

- def [get_energy_force_](#)
LPW 06-30-2013.
- def [get_resp_](#)
Electrostatic potential fitting.
- def [get](#)

Public Attributes

- [whamboltz_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.
- [traj](#)
- [nparticles](#)
The number of (atoms + drude particles + virtual sites)
- [AtomLists](#)
This is a default-dict containing a number of atom-wise lists, such as the residue number of each atom, the mass of each atom, and so on.

- [new_vsites](#)
Read in the topology.
- [save_vmvals](#)
Save the mvals from the last time we updated the vsites.
- [topology_flag](#)
- [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](#)

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 44 of file abinitio.py.

8.1.2 Constructor & Destructor Documentation

8.1.2.1 `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 54 of file abinitio.py.

Here is the call graph for this function:

8.1.3 Member Function Documentation

8.1.3.1 `def forcebalance.abinitio.AbInitio.build_invdist (self, mvals)`

Definition at line 165 of file abinitio.py.

Here is the call graph for this function:

8.1.3.2 `def forcebalance.abinitio.AbInitio.compute_netforce_torque (self, xyz, force, QM=False)`

Definition at line 201 of file abinitio.py.

8.1.3.3 `def forcebalance.abinitio.AbInitio.energy_force_transformer (self, i)`

Definition at line 455 of file abinitio.py.

Here is the call graph for this function:

8.1.3.4 `def forcebalance.abinitio.AbInitio.energy_force_transformer_all (self)`

Definition at line 439 of file abinitio.py.

Here is the call graph for this function:

8.1.3.5 `def forcebalance.abinitio.AbInitio.get (self, mvals, AGrad=False, AHess=False)`

Definition at line 1095 of file abinitio.py.

Here is the call graph for this function:

8.1.3.6 `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 $[E \ F_{1x} \ F_{1y} \ F_{1z} \ F_{2x} \ F_{2y} \ \dots]$, 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

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 529 of file abinitio.py.

8.1.3.7 `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 996 of file abinitio.py.

8.1.3.8 `def forcebalance.abinitio.AbInitio.indicate (self)`

Definition at line 419 of file abinitio.py.

Here is the call graph for this function:

8.1.3.9 `def forcebalance.abinitio.AbInitio.prepare_temp_directory (self, options, tgt_opts)`

Prepare the temporary directory, by default does nothing.

Definition at line 416 of file abinitio.py.

8.1.3.10 `def forcebalance.abinitio.AbInitio.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:

$$S = -1 * \sum_i (P_i * \log(P_i)) \quad \text{InfoContent} = \exp(-S)$$

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

Definition at line 314 of file abinitio.py.

8.1.3.11 `def forcebalance.abinitio.AbInitio.read_topology (self)`

Definition at line 161 of file abinitio.py.

Here is the call graph for this function:

8.1.4 Member Data Documentation

8.1.4.1 forcebalance.abinitio.AbInitio.AtomLists

This is a default-dict containing a number of atom-wise lists, such as the residue number of each atom, the mass of each atom, and so on.

Definition at line 147 of file abinitio.py.

8.1.4.2 forcebalance.abinitio.AbInitio.e_err

Qualitative Indicator: average energy error (in kJ/mol)

Definition at line 125 of file abinitio.py.

8.1.4.3 forcebalance.abinitio.AbInitio.e_err_pct

Definition at line 126 of file abinitio.py.

8.1.4.4 forcebalance.abinitio.AbInitio.e_ref

Definition at line 973 of file abinitio.py.

8.1.4.5 forcebalance.abinitio.AbInitio.emd0

Energies of the sampling simulation.

Definition at line 113 of file abinitio.py.

8.1.4.6 forcebalance.abinitio.AbInitio.eqm

Reference (QM) energies.

Definition at line 111 of file abinitio.py.

8.1.4.7 forcebalance.abinitio.AbInitio.esp_err

Qualitative Indicator: "relative RMS" for electrostatic potential.

Definition at line 131 of file abinitio.py.

8.1.4.8 forcebalance.abinitio.AbInitio.espval

ESP values.

Definition at line 119 of file abinitio.py.

8.1.4.9 forcebalance.abinitio.AbInitio.espxyz

ESP grid points.

Definition at line 117 of file abinitio.py.

8.1.4.10 forcebalance.abinitio.AbInitio.f_err

Qualitative Indicator: average force error (fractional)

Definition at line 128 of file abinitio.py.

8.1.4.11 forcebalance.abinitio.AbInitio.f_err_pct

Definition at line 129 of file abinitio.py.

8.1.4.12 forcebalance.abinitio.AbInitio.f_ref

Definition at line 977 of file abinitio.py.

8.1.4.13 forcebalance.abinitio.AbInitio.fitatoms

Definition at line 351 of file abinitio.py.

8.1.4.14 forcebalance.abinitio.AbInitio.force

Definition at line 346 of file abinitio.py.

8.1.4.15 forcebalance.abinitio.AbInitio.force_map

Definition at line 209 of file abinitio.py.

8.1.4.16 forcebalance.abinitio.AbInitio.fqm

Reference (QM) forces.

Definition at line 115 of file abinitio.py.

8.1.4.17 forcebalance.abinitio.AbInitio.fref

Definition at line 410 of file abinitio.py.

8.1.4.18 forcebalance.abinitio.AbInitio.invdists

Definition at line 1004 of file abinitio.py.

8.1.4.19 forcebalance.abinitio.AbInitio.nesp

Definition at line 348 of file abinitio.py.

8.1.4.20 forcebalance.abinitio.AbInitio.new_vsites

Read in the topology.

Read in the reference data Prepare the temporary directory 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 156 of file abinitio.py.

8.1.4.21 forcebalance.abinitio.AbInitio.nf_err

Definition at line 132 of file abinitio.py.

8.1.4.22 forcebalance.abinitio.AbInitio.nf_err_pct

Definition at line 133 of file abinitio.py.

8.1.4.23 forcebalance.abinitio.AbInitio.nf_ref

Definition at line 981 of file abinitio.py.

8.1.4.24 forcebalance.abinitio.AbInitio.nftqm

Definition at line 406 of file abinitio.py.

8.1.4.25 forcebalance.abinitio.AbInitio.nnf

Definition at line 252 of file abinitio.py.

8.1.4.26 forcebalance.abinitio.AbInitio.nparticles

The number of (atoms + drude particles + virtual sites)

Definition at line 144 of file abinitio.py.

8.1.4.27 forcebalance.abinitio.AbInitio.ns

Read in the trajectory file.

Definition at line 138 of file abinitio.py.

8.1.4.28 forcebalance.abinitio.AbInitio.ntq

Definition at line 253 of file abinitio.py.

8.1.4.29 forcebalance.abinitio.AbInitio.objective

Definition at line 1115 of file abinitio.py.

8.1.4.30 forcebalance.abinitio.AbInitio.qfnm

The qdata.txt file that contains the QM energies and forces.

Definition at line 121 of file abinitio.py.

8.1.4.31 forcebalance.abinitio.AbInitio.qmatoms

The number of atoms in the QM calculation (Irrelevant if not fitting forces)

Definition at line 123 of file abinitio.py.

8.1.4.32 forcebalance.abinitio.AbInitio.qmboltz_wts

QM Boltzmann weights.

Definition at line 109 of file abinitio.py.

8.1.4.33 forcebalance.abinitio.AbInitio.respterm

Definition at line 1083 of file abinitio.py.

8.1.4.34 forcebalance.abinitio.AbInitio.save_vmvals

Save the mvals from the last time we updated the vsites.

Definition at line 158 of file abinitio.py.

8.1.4.35 forcebalance.abinitio.AbInitio.topology_flag

Definition at line 163 of file abinitio.py.

8.1.4.36 forcebalance.abinitio.AbInitio.tq_err

Definition at line 985 of file abinitio.py.

8.1.4.37 forcebalance.abinitio.AbInitio.tq_err_pct

Definition at line 134 of file abinitio.py.

8.1.4.38 forcebalance.abinitio.AbInitio.tq_ref

Definition at line 984 of file abinitio.py.

8.1.4.39 forcebalance.abinitio.AbInitio.traj

Definition at line 139 of file abinitio.py.

8.1.4.40 forcebalance.abinitio.AbInitio.use_nft

Whether to compute net forces and torques, or not.

Definition at line 136 of file abinitio.py.

8.1.4.41 forcebalance.abinitio.AbInitio.w_energy

Definition at line 568 of file abinitio.py.

8.1.4.42 forcebalance.abinitio.AbInitio.w_force

Definition at line 347 of file abinitio.py.

8.1.4.43 forcebalance.abinitio.AbInitio.w_netforce

Definition at line 568 of file abinitio.py.

8.1.4.44 forcebalance.abinitio.AbInitio.w_resp

Definition at line 997 of file abinitio.py.

8.1.4.45 forcebalance.abinitio.AbInitio.w_torque

Definition at line 568 of file abinitio.py.

8.1.4.46 forcebalance.abinitio.AbInitio.whamboltz

Definition at line 367 of file abinitio.py.

8.1.4.47 forcebalance.abinitio.AbInitio.whamboltz_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) WHAM Boltzmann weights

Definition at line 107 of file abinitio.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`

Public Attributes

- `trajnm`
Name of the trajectory, we need this BEFORE initializing the SuperClass.
- `all_at_once`
all_at_once is not implemented.

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 168 of file amberio.py.

8.2.2 Constructor & Destructor Documentation

8.2.2.1 `def forcebalance.amberio.AbInitio_AMBER.__init__(self, options, tgt_opts, forcefield)`

Definition at line 171 of file amberio.py.

8.2.3 Member Function Documentation

8.2.3.1 `def forcebalance.amberio.AbInitio_AMBER.energy_force_driver_all(self)`

Definition at line 225 of file amberio.py.

8.2.3.2 `def forcebalance.amberio.AbInitio_AMBER.energy_force_driver_all_external_(self)`

Definition at line 187 of file amberio.py.

Here is the call graph for this function:

8.2.3.3 `def forcebalance.amberio.AbInitio_AMBER.prepare_temp_directory(self, options, tgt_opts)`

Definition at line 178 of file amberio.py.

Here is the call graph for this function:

8.2.4 Member Data Documentation

8.2.4.1 `forcebalance.amberio.AbInitio_AMBER.all_at_once`

`all_at_once` is not implemented.

Definition at line 176 of file amberio.py.

8.2.4.2 forcebalance.amberio.AbInitio_AMBER.trajfnm

Name of the trajectory, we need this BEFORE initializing the SuperClass.

Definition at line 173 of file amberio.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 normal GROMACS.

Inheritance diagram for forcebalance.gmxio.AbInitio_GMX:

Collaboration diagram for forcebalance.gmxio.AbInitio_GMX:

Public Member Functions

- [def __init__](#)
- [def read_topology](#)
This function parses the GROMACS topology file (.top) which contains a listing of the molecules in the simulation.
- [def prepare_temp_directory](#)
- [def energy_force_driver](#)
Computes the energy and force using GROMACS for a single snapshot.
- [def energy_force_driver_all](#)
Computes the energy and force using GROMACS for a trajectory.
- [def generate_vsite_positions](#)
Call mdrun in order to update the virtual site positions.

Public Attributes

- [trajfnm](#)
Name of the trajectory.
- [topfnm](#)
- [AtomMask](#)
- [topology_flag](#)

8.3.1 Detailed Description

Subclass of AbInitio for force and energy matching using normal GROMACS.

Implements the prepare_temp_directory and energy_force_driver methods.

Definition at line 435 of file gmxio.py.

8.3.2 Constructor & Destructor Documentation

8.3.2.1 `def forcebalance.gmxio.AbInitio_GMX.__init__(self, options, tgt_opts, forcefield)`

Definition at line 437 of file gmxio.py.

Here is the call graph for this function:

8.3.3 Member Function Documentation

8.3.3.1 `def forcebalance.gmxio.AbInitio_GMX.energy_force_driver (self, shot)`

Computes the energy and force using GROMACS for a single snapshot.

This does not require GROMACS-X2.

Definition at line 515 of file gmxio.py.

Here is the call graph for this function:

8.3.3.2 `def forcebalance.gmxio.AbInitio_GMX.energy_force_driver_all (self)`

Computes the energy and force using GROMACS for a trajectory.

This does not require GROMACS-X2.

Definition at line 536 of file gmxio.py.

Here is the call graph for this function:

8.3.3.3 `def forcebalance.gmxio.AbInitio_GMX.generate_vsite_positions (self)`

Call mdrun in order to update the virtual site positions.

Definition at line 559 of file gmxio.py.

Here is the call graph for this function:

8.3.3.4 `def forcebalance.gmxio.AbInitio_GMX.prepare_temp_directory (self, options, tgt_opts)`

Definition at line 490 of file gmxio.py.

Here is the call graph for this function:

8.3.3.5 `def forcebalance.gmxio.AbInitio_GMX.read_topology (self)`

This function parses the GROMACS topology file (.top) which contains a listing of the molecules in the simulation.

For each molecule, it loads up a "FFMolecule" dictionary which contains information about each atom in the molecule - which residue (i.e. molecular fragment) the atom belongs in, the charge group, the particle type etc.

This allows us to do things like condense the gradients into net forces and torques, determine which particles are real atoms and which are virtual sites, and so on.

Definition at line 452 of file gmxio.py.

Here is the call graph for this function:

8.3.4 Member Data Documentation

8.3.4.1 `forcebalance.gmxio.AbInitio_GMX.AtomMask`

Definition at line 486 of file gmxio.py.

8.3.4.2 `forcebalance.gmxio.AbInitio_GMX.topfnm`

Definition at line 440 of file gmxio.py.

8.3.4.3 forcebalance.gmxio.AbInitio_GMX.topology_flag

Definition at line 487 of file gmxio.py.

8.3.4.4 forcebalance.gmxio.AbInitio_GMX.trajfnm

Name of the trajectory.

Definition at line 439 of file gmxio.py.

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

- [gmxio.py](#)

8.4 forcebalance.abinitio_gmxx2.AbInitio_GMXX2 Class Reference

ForceBalance class for force and energy matching with the modified GROMACS.

Inheritance diagram for forcebalance.abinitio_gmxx2.AbInitio_GMXX2:

Collaboration diagram for forcebalance.abinitio_gmxx2.AbInitio_GMXX2:

Public Member Functions

- `def __init__`
Instantiation of [AbInitio_GMXX2](#).
- `def prepare_temp_directory`
Prepare the temporary directory for running the modified GROMACS.
- `def get_energy_force_`
Calls the modified GROMACS and collects the objective function contribution.
- `def callgmxx2`
Call the modified GROMACS!

Public Attributes

- `trajfnm`
Set the software to GROMACS no matter what.
- `whamboltz`
- `sampcorr`
- `covariance`
- `e_err`
- `f_err`

8.4.1 Detailed Description

ForceBalance class for force and energy matching with the modified GROMACS.

This class allows us to use a heavily modified version of GROMACS (a major component of this program) to compute the objective function contribution. The modified GROMACS does the looping through snapshots, computes the interactions as well as the derivatives, and sums them up to build the objective function. I will write that documentation elsewhere, perhaps when I port GROMACS over to version 4.5.4.

This class implements the 'get_energy_force_' method. When it is called, the force field is printed to the temporary directory along with several files containing the information needed by the modified GROMACS (the Boltzmann weights, the parameters that need derivatives and their values, the QM energies and forces, and the energy / force weighting.)

The modified GROMACS is called with the arguments '-rerun all.gro -fortune -rerunvsite' to loop over the snapshots, turn on force matching functionality and reconstruct virtual site positions (an important consideration if we're changing the virtual site positions in the optimization). Its outputs are 'e2f2bc' which means 'energy squared, force squared, boltzmann corrected' and contains the objective function, 'a1dbc' and 'a2dbc' containing analytic first and second derivatives, 'gmxboltz' containing the Boltzmann weights used, and possibly some other stuff.

Most importantly, 'e2f2bc', 'a1dbc' and 'a2dbc' are read by 'get' after GROMACS is called and returned directly as the objective function contributions.

Other methods implemented in this class are related to the preparation of the temp directory.

Definition at line 62 of file abinitio_gmxx2.py.

8.4.2 Constructor & Destructor Documentation

8.4.2.1 `def forcebalance.abinitio_gmxx2.Ablnitio_GMXX2.__init__(self, options, sim_opts, forcefield)`

Instantiation of [Ablnitio_GMXX2](#).

Several important things happen here:

- We load in the coordinates from 'all.gro'.
- We prepare the temporary directory.

Definition at line 73 of file abinitio_gmxx2.py.

8.4.3 Member Function Documentation

8.4.3.1 `def forcebalance.abinitio_gmxx2.Ablnitio_GMXX2.callgmxx2(self)`

Call the modified GROMACS!

Definition at line 258 of file abinitio_gmxx2.py.

8.4.3.2 `def forcebalance.abinitio_gmxx2.Ablnitio_GMXX2.get_energy_force_(self, mvals, AGrad=False, AHess=False)`

Calls the modified GROMACS and collects the objective function contribution.

First we create the force field using the parameter values that were passed in. Note that we may pass in physical parameters directly and bypass the coordinate transformation by setting self.usepvals to True.

The physical parameters are printed to 'pvals' for GROMACS to read - of course GROMACS knows the parameters already, but this facilitates retrieval from the low level subroutines.

Several switches are printed to files, such as:

- 'FirstDerivativesOnly' to prevent computation of the Hessian
- 'NoDerivatives' to prevent computation of the Hessian AND the gradient

GROMACS is called in the [callgmxx2\(\)](#) method.

The output files are then parsed for the objective function and its derivatives are read in. The answer is passed out as a dictionary: {'X': Objective Function, 'G': Gradient, 'H': Hessian}

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

Todo Some of these files don't need to be printed, they can be passed to GROMACS as arguments. Let's think about this some more.

Currently I have no way to pass out the qualitative indicators.

Definition at line 203 of file abinitio_gmxx2.py.

Here is the call graph for this function:

8.4.3.3 `def forcebalance.abinitio_gmxx2.AbInitio_GMXX2.prepare_temp_directory (self, options, sim_opts)`

Prepare the temporary directory for running the modified GROMACS.

This method creates the temporary directory, links in the necessary files for running (except for the force field), and writes the coordinate file for the snapshots we've chosen.

There are also files that specific to our *modified* GROMACS, including:

- qmboltz : The QM Boltzmann weights
- bp : The QM vs. MM Boltzmann weight proportionality factor
- whamboltz : The WHAM Boltzmann weights (i.e. MM Boltzmann weights passed from outside)
- sampcorr : Boolean for the 'sampling correction', i.e. updating the Boltzmann factors when the force field is updated. This required a TON of implementation into the modified Gromacs, but in the end we didn't find it to be very useful. It basically emphasizes energy minima and gets barrier heights wrong. Blah! :)
- fitatoms : The number of atoms that we're fitting, which may be less than the total number in the QM calculation (i.e. if we are fitting something to be compatible with a water model ...)
- energyqm : QM reference energies
- forcesqm : QM reference forces
- ztemp : Template for Z-matrix coordinates (for internal coordinate forces)
- pids : Information for building interaction name -> parameter number hashtable

Todo Someday I'd like to use WHAM to put AIMD simulations in. :)

The fitatoms shouldn't be the first however many atoms, it should be a list.

Definition at line 111 of file abinitio_gmxx2.py.

Here is the call graph for this function:

8.4.4 Member Data Documentation

8.4.4.1 forcebalance.abinitio_gmxx2.AbInitio_GMXX2.covariance

Definition at line 141 of file abinitio_gmxx2.py.

8.4.4.2 forcebalance.abinitio_gmxx2.AbInitio_GMXX2.e_err

Definition at line 229 of file abinitio_gmxx2.py.

8.4.4.3 forcebalance.abinitio_gmxx2.AbInitio_GMXX2.f_err

Definition at line 232 of file abinitio_gmxx2.py.

8.4.4.4 forcebalance.abinitio_gmxx2.AbInitio_GMXX2.sampcorr

Definition at line 137 of file abinitio_gmxx2.py.

8.4.4.5 forcebalance.abinitio_gmxx2.AbInitio_GMXX2.traifnm

Set the software to GROMACS no matter what.

Definition at line 78 of file abinitio_gmxx2.py.

8.4.4.6 forcebalance.abinitio_gmxx2.AbInitio_GMXX2.whamboltz

Definition at line 133 of file abinitio_gmxx2.py.

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

- [abinitio_gmxx2.py](#)

8.5 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.

Public Attributes

- [traifnm](#)

Name of the trajectory, we need this BEFORE initializing the SuperClass.

8.5.1 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.

8.5.2 Constructor & Destructor Documentation

8.5.2.1 def forcebalance.abinitio_internal.AbInitio_Internal.__init__(self, options, tgt_opts, forcefield)

Definition at line 40 of file abinitio_internal.py.

8.5.3 Member Function Documentation

8.5.3.1 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.

8.5.4 Member Data Documentation

8.5.4.1 forcebalance.abinitio_internal.AbInitio_Internal.trafnm

Name of the trajectory, we need this BEFORE initializing the SuperClass.

Definition at line 42 of file abinitio_internal.py.

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

- [abinitio_internal.py](#)

8.6 forcebalance.openmmio.AbInitio_OpenMM Class Reference

Subclass of AbInitio for 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 [read_topology](#)
- def [prepare_temp_directory](#)
- def [energy_force_driver_all_external_](#)
- def [energy_force_driver_all_internal_](#)
- *Loop through the snapshots and compute the energies and forces using OpenMM.*
- def [energy_force_driver_all](#)

Public Attributes

- [trajfnm](#)
Name of the trajectory, we need this BEFORE initializing the SuperClass.
- [platform](#)
Initialize the SuperClass!
- [simulation](#)
Create the simulation object within this class itself.
- [xyz_omms](#)
- [topology_flag](#)

8.6.1 Detailed Description

Subclass of AbInitio for force and energy matching using OpenMM.

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

Definition at line 398 of file openmmio.py.

8.6.2 Constructor & Destructor Documentation

8.6.2.1 `def forcebalance.openmmio.AbInitio_OpenMM.__init__(self, options, tgt_opts, forcefield)`

Definition at line 401 of file openmmio.py.

8.6.3 Member Function Documentation

8.6.3.1 `def forcebalance.openmmio.AbInitio_OpenMM.energy_force_driver_all(self)`

Definition at line 525 of file openmmio.py.

Here is the call graph for this function:

8.6.3.2 `def forcebalance.openmmio.AbInitio_OpenMM.energy_force_driver_all_external_(self)`

Definition at line 469 of file openmmio.py.

8.6.3.3 `def forcebalance.openmmio.AbInitio_OpenMM.energy_force_driver_all_internal_(self)`

Loop through the snapshots and compute the energies and forces using OpenMM.

Definition at line 478 of file openmmio.py.

Here is the call graph for this function:

8.6.3.4 `def forcebalance.openmmio.AbInitio_OpenMM.prepare_temp_directory(self, options, tgt_opts)`

Definition at line 464 of file openmmio.py.

Here is the call graph for this function:

8.6.3.5 `def forcebalance.openmmio.AbInitio_OpenMM.read_topology(self)`

Definition at line 454 of file openmmio.py.

Here is the call graph for this function:

8.6.4 Member Data Documentation

8.6.4.1 forcebalance.openmmio.AbInitio_OpenMM.platform

Initialize the SuperClass!

Set the device to the environment variable or zero otherwise.

Set the simulation platform

Definition at line 410 of file openmmio.py.

8.6.4.2 forcebalance.openmmio.AbInitio_OpenMM.simulation

Create the simulation object within this class itself.

Definition at line 442 of file openmmio.py.

8.6.4.3 forcebalance.openmmio.AbInitio_OpenMM.topology_flag

Definition at line 461 of file openmmio.py.

8.6.4.4 forcebalance.openmmio.AbInitio_OpenMM.trajfnm

Name of the trajectory, we need this BEFORE initializing the SuperClass.

Definition at line 403 of file openmmio.py.

8.6.4.5 forcebalance.openmmio.AbInitio_OpenMM.xyz_omms

Definition at line 444 of file openmmio.py.

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

- [openmmio.py](#)

8.7 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 prepare_temp_directory](#)
- [def energy_force_driver](#)
- [def energy_driver_all](#)
- [def energy_force_driver_all](#)

Public Attributes

- [trajfnm](#)

Name of the trajectory.

- [all_at_once](#)

all_at_once is not implemented.

8.7.1 Detailed Description

Subclass of Target for force and energy matching using TINKER.

Implements the prepare and energy_force_driver methods.

Definition at line 294 of file tinkerio.py.

8.7.2 Constructor & Destructor Documentation

8.7.2.1 def forcebalance.tinkerio.AbInitio_TINKER.__init__(self, options, tgt_opts, forcefield)

Definition at line 297 of file tinkerio.py.

Here is the call graph for this function:

8.7.3 Member Function Documentation

8.7.3.1 def forcebalance.tinkerio.AbInitio_TINKER.energy_driver_all (self)

Definition at line 330 of file tinkerio.py.

Here is the call graph for this function:

8.7.3.2 def forcebalance.tinkerio.AbInitio_TINKER.energy_force_driver (self, shot)

Definition at line 314 of file tinkerio.py.

Here is the call graph for this function:

8.7.3.3 def forcebalance.tinkerio.AbInitio_TINKER.energy_force_driver_all (self)

Definition at line 343 of file tinkerio.py.

Here is the call graph for this function:

8.7.3.4 def forcebalance.tinkerio.AbInitio_TINKER.prepare_temp_directory (self, options, tgt_opts)

Definition at line 306 of file tinkerio.py.

Here is the call graph for this function:

8.7.4 Member Data Documentation

8.7.4.1 forcebalance.tinkerio.AbInitio_TINKER.all_at_once

all_at_once is not implemented.

Definition at line 304 of file tinkerio.py.

8.7.4.2 forcebalance.tinkerio.AbInitio_TINKER.trafnm

Name of the trajectory.

Definition at line 299 of file tinkerio.py.

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

- [tinkerio.py](#)

8.8 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](#)

8.8.1 Detailed Description

Definition at line 173 of file forcefield.py.

8.8.2 Constructor & Destructor Documentation

8.8.2.1 `def forcebalance.forcefield.BackedUpDict.__init__(self, backup_dict)`

Definition at line 174 of file forcefield.py.

Here is the call graph for this function:

8.8.3 Member Function Documentation

8.8.3.1 `def forcebalance.forcefield.BackedUpDict.__missing__(self, key)`

Definition at line 177 of file forcefield.py.

Here is the call graph for this function:

8.8.4 Member Data Documentation

8.8.4.1 `forcebalance.forcefield.BackedUpDict.backup_dict`

Definition at line 176 of file forcefield.py.

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

- [forcefield.py](#)

8.9 forcebalance.basereader.BaseReader Class Reference

The 'reader' class.

Inheritance diagram for forcebalance.basereader.BaseReader:

Collaboration diagram for forcebalance.basereader.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 25 of file basereader.py.

8.9.2 Constructor & Destructor Documentation

8.9.2.1 def forcebalance.basereader.BaseReader.__init__(self, fnm)

Definition at line 27 of file basereader.py.

8.9.3 Member Function Documentation

8.9.3.1 def forcebalance.basereader.BaseReader.build_pid (self, pfld)

Returns the parameter type (e.g.

K in BONDSK) based on the current interaction type.

Both the 'pdict' dictionary (see [gmio.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 68 of file basereader.py.

8.9.3.2 def forcebalance.basereader.BaseReader.feed (self, line)

Definition at line 49 of file basereader.py.

Here is the call graph for this function:

8.9.3.3 def forcebalance.basereader.BaseReader.Split (self, line)

Definition at line 43 of file basereader.py.

Here is the call graph for this function:

8.9.3.4 def forcebalance.basereader.BaseReader.Whites (self, line)

Definition at line 46 of file basereader.py.

Here is the call graph for this function:

8.9.4 Member Data Documentation

8.9.4.1 forcebalance.basereader.BaseReader.adict

The mapping of (this residue, atom number) to (atom name) for building atom-specific interactions in [bonds], [angles] etc.

Definition at line 33 of file basereader.py.

8.9.4.2 forcebalance.basereader.BaseReader.AtomTypes

Definition at line 41 of file basereader.py.

8.9.4.3 forcebalance.basereader.BaseReader.itype

Definition at line 29 of file basereader.py.

8.9.4.4 forcebalance.basereader.BaseReader.In

Definition at line 28 of file basereader.py.

8.9.4.5 forcebalance.basereader.BaseReader.molatom

The mapping of (molecule name) to a dictionary of of atom types for the atoms in that residue.

self.moleculdict = OrderedDict() The listing of 'RES:ATOMNAMES' for atom names in the line This is obviously a placeholder.

Definition at line 38 of file basereader.py.

8.9.4.6 forcebalance.basereader.BaseReader.Molecules

Definition at line 40 of file basereader.py.

8.9.4.7 forcebalance.basereader.BaseReader.pdict

Definition at line 31 of file basereader.py.

8.9.4.8 forcebalance.basereader.BaseReader.suffix

Definition at line 30 of file basereader.py.

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

- [basereader.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 [indicate](#)
- def [get](#)

Public Attributes

- [inter_opts](#)
- [PrintDict](#)
- [RMSDDict](#)
- [rmsd_part](#)
- [energy_part](#)
- [objective](#)

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

8.10.2.1 `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

8.10.3.1 `def forcebalance.binding.BindingEnergy.get (self, mvals, AGrad=False, AHess=False)`

Definition at line 161 of file binding.py.

8.10.3.2 `def forcebalance.binding.BindingEnergy.indicate (self)`

Definition at line 155 of file binding.py.

Here is the call graph for this function:

8.10.4 Member Data Documentation

8.10.4.1 `forcebalance.binding.BindingEnergy.energy_part`

Definition at line 201 of file binding.py.

8.10.4.2 `forcebalance.binding.BindingEnergy.inter_opts`

Definition at line 128 of file binding.py.

8.10.4.3 `forcebalance.binding.BindingEnergy.objective`

Definition at line 225 of file binding.py.

8.10.4.4 `forcebalance.binding.BindingEnergy.PrintDict`

Definition at line 163 of file binding.py.

8.10.4.5 `forcebalance.binding.BindingEnergy.rmsd_part`

Definition at line 199 of file binding.py.

8.10.4.6 `forcebalance.binding.BindingEnergy.RMSDDict`

Definition at line 164 of file binding.py.

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

- [binding.py](#)

8.11 forcebalance.tinkerio.BindingEnergy_TINKER Class Reference

Subclass of BindingEnergy for 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 prepare_temp_directory](#)
- [def system_driver](#)

Public Attributes

- [optprog](#)

8.11.1 Detailed Description

Subclass of BindingEnergy for binding energy matching using TINKER.

Definition at line 483 of file tinkerio.py.

8.11.2 Constructor & Destructor Documentation

8.11.2.1 `def forcebalance.tinkerio.BindingEnergy_TINKER.__init__(self, options, tgt_opts, forcefield)`

Definition at line 486 of file tinkerio.py.

Here is the call graph for this function:

8.11.3 Member Function Documentation

8.11.3.1 `def forcebalance.tinkerio.BindingEnergy_TINKER.prepare_temp_directory(self, options, tgt_opts)`

Definition at line 490 of file tinkerio.py.

8.11.3.2 `def forcebalance.tinkerio.BindingEnergy_TINKER.system_driver(self, sysname)`

Definition at line 544 of file tinkerio.py.

Here is the call graph for this function:

8.11.4 Member Data Documentation

8.11.4.1 `forcebalance.tinkerio.BindingEnergy_TINKER.optprog`

Definition at line 493 of file tinkerio.py.

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

- [tinkerio.py](#)

8.12 forcebalance.output.CleanFileHandler Class Reference

File handler that does not write terminal escape codes to files.

Inheritance diagram for forcebalance.output.CleanFileHandler:

Collaboration diagram for forcebalance.output.CleanFileHandler:

Public Member Functions

- def [emit](#)

8.12.1 Detailed Description

File handler that does not write terminal escape codes to files.

Use this when writing to a file that will probably not be viewed in a terminal

Definition at line 36 of file output.py.

8.12.2 Member Function Documentation

8.12.2.1 def forcebalance.output.CleanFileHandler.emit (self, record)

Definition at line 37 of file output.py.

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

- [output.py](#)

8.13 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.

Public Attributes

- [xyzs](#)
Number of snapshots.
- [cpqm](#)
Counterpoise correction data.
- [na](#)
Number of atoms.
- [ns](#)

8.13.1 Detailed Description

Target subclass for matching the counterpoise correction.

Definition at line 31 of file counterpoise.py.

8.13.2 Constructor & Destructor Documentation

8.13.2.1 `def forcebalance.counterpoise.Counterpoise.__init__(self, options, tgt_opts, forcefield)`

To instantiate [Counterpoise](#), we read the coordinates and counterpoise data.

Definition at line 35 of file counterpoise.py.

Here is the call graph for this function:

8.13.3 Member Function Documentation

8.13.3.1 `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

| | | |
|-----------------|--------------------|---|
| <code>in</code> | <code>mvals</code> | Mathematical parameter values |
| <code>in</code> | <code>AGrad</code> | Switch to turn on analytic gradient (not implemented) |
| <code>in</code> | <code>AHess</code> | Switch to turn on analytic Hessian (not implemented) |

Returns

Answer Contribution to the objective function

Definition at line 122 of file counterpoise.py.

8.13.3.2 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 93 of file counterpoise.py.

8.13.3.3 def forcebalance.counterpoise.Counterpoise.loadxyz (self, fnm)

Parse an XYZ file which contains several xyz coordinates, and return their elements.

Parameters

| | | |
|-----------|------------|-------------------------|
| <i>in</i> | <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 61 of file counterpoise.py.

8.13.4 Member Data Documentation

8.13.4.1 forcebalance.counterpoise.Counterpoise.cpqm

[Counterpoise](#) correction data.

Definition at line 51 of file counterpoise.py.

8.13.4.2 forcebalance.counterpoise.Counterpoise.na

Number of atoms.

Definition at line 74 of file counterpoise.py.

8.13.4.3 forcebalance.counterpoise.Counterpoise.ns

Definition at line 87 of file counterpoise.py.

8.13.4.4 forcebalance.counterpoise.Counterpoise.xyzs

Number of snapshots.

XYZ elements and coordinates

Definition at line 49 of file counterpoise.py.

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

- [counterpoise.py](#)

8.14 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](#)
Parse a text force field and create several important instance variables.
- def [addff_xml](#)
Parse an XML force field file and create 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 [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__](#)

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).

- [parmdestroy_save](#)

- [linedestroy_this](#)

- [parmdestroy_this](#)

- [tinkerprm](#)

- [openmmxml](#)

- [qmap](#)

- [qid](#)

- [qid2](#)

8.14.1 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 194 of file forcefield.py.

8.14.2 Constructor & Destructor Documentation

8.14.2.1 `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 202 of file `forcefield.py`.

Here is the call graph for this function:

8.14.3 Member Function Documentation

8.14.3.1 `def forcebalance.forcefield.FF.__eq__(self, other)`

Definition at line 1144 of file `forcefield.py`.

8.14.3.2 `def forcebalance.forcefield.FF.addff(self, ffname)`

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` -> `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 `# PARM 3` (where `#` denotes a comment, the word `PARM` 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 | <i>ffname</i> | Name of the force field file |
|----|---------------|------------------------------|

Definition at line 393 of file forcefield.py.

Here is the call graph for this function:

8.14.3.3 def forcebalance.forcefield.FF.addff_txt (self, ffname, fftype)

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 'PARM' 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 'PARM' 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 463 of file forcefield.py.

Here is the call graph for this function:

8.14.3.4 def forcebalance.forcefield.FF.addff_xml (self, ffname)

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 571 of file forcefield.py.

Here is the call graph for this function:

8.14.3.5 `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 | <i>idx</i> | The index of the parameter. |
| in | <i>fnm</i> | The file name of the parameter field. |
| in | <i>ln</i> | The line number within the file (or the node index in the flattened xml) |
| in | <i>pfld</i> | The field within the line (or the name of the attribute in the xml) |
| in | <i>mult</i> | The multiplier (this is usually 1.0) |

Definition at line 1138 of file forcefield.py.

Here is the call graph for this function:

8.14.3.6 `def forcebalance.forcefield.FF.assign_p0(self, idx, val)`

Assign physical parameter values to the 'pvals0' array.

Parameters

| | | |
|----|------------|---|
| in | <i>idx</i> | The index to which we assign the parameter value. |
| in | <i>val</i> | The parameter value to be inserted. |

Definition at line 1120 of file forcefield.py.

Here is the call graph for this function:

8.14.3.7 `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 854 of file forcefield.py.

Here is the call graph for this function:

8.14.3.8 `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

| | | |
|-----------|--------------|-----------------------------|
| <i>in</i> | <i>mvals</i> | The mathematical parameters |
|-----------|--------------|-----------------------------|

Returns

pvals The physical parameters

Definition at line 817 of file forcefield.py.

Here is the call graph for this function:

8.14.3.9 `def forcebalance.forcefield.FF.find_spacings (self)`

Definition at line 772 of file forcefield.py.

Here is the call graph for this function:

8.14.3.10 `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 1097 of file forcefield.py.

Here is the call graph for this function:

8.14.3.11 `def forcebalance.forcefield.FF.make (self, vals, 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

| | | |
|-----------|------------------|--|
| <i>in</i> | <i>printdir</i> | The directory that the force fields are printed to; as usual this is relative to the project root directory. |
| <i>in</i> | <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. |
| <i>in</i> | <i>use_pvals</i> | Switch for whether to bypass the coordinate transformation and use physical parameters directly. |

Definition at line 619 of file forcefield.py.

Here is the call graph for this function:

8.14.3.12 `def forcebalance.forcefield.FF.make_redirect (self, mvals)`

Definition at line 731 of file forcefield.py.

Here is the call graph for this function:

8.14.3.13 `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 947 of file forcefield.py.

8.14.3.14 `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 1109 of file forcefield.py.

Here is the call graph for this function:

8.14.3.15 `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

Parameters

| | | |
|-----------------|------------------------|---|
| <code>in</code> | <code>printfacs</code> | List for printing out the resealing factors |
|-----------------|------------------------|---|

Definition at line 871 of file forcefield.py.

Here is the call graph for this function:

8.14.4 Member Data Documentation

8.14.4.1 forcebalance.forcefield.FF.atomnames

A list of atom names (this is new, for ESP fitting)

Definition at line 263 of file forcefield.py.

8.14.4.2 forcebalance.forcefield.FF.excision

Indices to exclude from optimization / Hessian inversion.

Some customized constraints here.

Quadrupoles must be traceless

Definition at line 255 of file forcefield.py.

8.14.4.3 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 273 of file forcefield.py.

8.14.4.4 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. 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 235 of file forcefield.py.

8.14.4.5 forcebalance.forcefield.FF.ffdata.isxml

Definition at line 236 of file forcefield.py.

8.14.4.6 forcebalance.forcefield.FF.FFMolecules

Definition at line 286 of file forcefield.py.

8.14.4.7 forcebalance.forcefield.FF.linedestroy_save

Destruction dictionary (experimental).

Definition at line 314 of file forcefield.py.

8.14.4.8 forcebalance.forcefield.FF.linedestroy_this

Definition at line 316 of file forcefield.py.

8.14.4.9 forcebalance.forcefield.FF.map

The mapping of interaction type -> parameter number.

Definition at line 238 of file forcefield.py.

8.14.4.10 forcebalance.forcefield.FF.np

The total number of parameters.

Definition at line 257 of file forcefield.py.

8.14.4.11 forcebalance.forcefield.FF.openmmxml

Definition at line 409 of file forcefield.py.

8.14.4.12 forcebalance.forcefield.FF.parmdestroy_save

Definition at line 315 of file forcefield.py.

8.14.4.13 forcebalance.forcefield.FF.parmdestroy_this

Definition at line 317 of file forcefield.py.

8.14.4.14 forcebalance.forcefield.FF.patoms

A listing of parameter number -> atoms involved.

Definition at line 242 of file forcefield.py.

8.14.4.15 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 247 of file forcefield.py.

8.14.4.16 forcebalance.forcefield.FF.plist

The listing of parameter number -> interaction types.

Definition at line 240 of file forcefield.py.

8.14.4.17 forcebalance.forcefield.FF.pvals0

Initial value of physical parameters.

Definition at line 259 of file forcefield.py.

8.14.4.18 forcebalance.forcefield.FF.qid

Definition at line 949 of file forcefield.py.

8.14.4.19 forcebalance.forcefield.FF.qid2

Definition at line 950 of file forcefield.py.

8.14.4.20 forcebalance.forcefield.FF.qmap

Definition at line 948 of file forcefield.py.

8.14.4.21 forcebalance.forcefield.FF.Readers

A dictionary of force field reader classes.

Definition at line 261 of file forcefield.py.

8.14.4.22 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 312 of file forcefield.py.

8.14.4.23 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','BOND-SK','VDWS','VDWT'].

The array of rescaling factors

Definition at line 249 of file forcefield.py.

8.14.4.24 forcebalance.forcefield.FF.tinkerprm

Definition at line 402 of file forcefield.py.

8.14.4.25 forcebalance.forcefield.FF.tm

The transformation matrix for mathematical -> physical parameters.

Definition at line 251 of file forcefield.py.

8.14.4.26 forcebalance.forcefield.FF.tml

The transpose of the transformation matrix.

Definition at line 253 of file forcefield.py.

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

- [forcefield.py](#)

8.15 forcebalance.fitsim.FittingSimulation Class Reference

Base class for all fitting simulations.

Inheritance diagram for forcebalance.fitsim.FittingSimulation:

Collaboration diagram for forcebalance.fitsim.FittingSimulation:

Public Member Functions

- [def __init__](#)
Instantiation of a fitting simulation.
- [def get_X](#)
Computes the objective function contribution without any parametric derivatives.
- [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 fitting simulation must be able to return a contribution to the objective function - however, this must be implemented in the specific subclass.
- def [sget](#)
Stages the directory for the fitting simulation, and then calls 'get'.

Public Attributes

- [tempdir](#)
Root directory of the whole project.
- [rundir](#)
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.
- [wq](#)

8.15.1 Detailed Description

Base class for all fitting simulations.

In ForceBalance a 'fitting simulation' is defined as a simulation which computes a quantity that we can compare to a reference. The force field parameters are tuned to reproduce the reference value as closely as possible.

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 [FittingSimulation](#) as a base class. Thus, the contents of [FittingSimulation](#) itself are meant to be as general as possible, because the pertinent variables apply to all types of fitting simulations.

An important note: [FittingSimulation](#) 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 `FitSim` 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': numpy.array(np), 'H': numpy.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 [FittingSimulation](#). Obviously 'get' itself is not defined here, because its calculation will depend entirely on specifically which simulation we wish to run. However, this should give us a unified framework which will facilitate rapid implementation of FittingSimulations.

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 77 of file fitsim.py.

8.15.2 Constructor & Destructor Documentation

8.15.2.1 def forcebalance.fitsim.FittingSimulation.__init__(self, options, sim_opts, forcefield)

Instantiation of a fitting simulation.

All options here are intended to be usable by every conceivable type of fitting simulation (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 Ablntio that subclasses [FittingSimulation](#).

Definition at line 96 of file fitsim.py.

Here is the call graph for this function:

8.15.3 Member Function Documentation

8.15.3.1 def forcebalance.fitsim.FittingSimulation.get(self, mvals, AGrad=False, AHess=False)

Every fitting simulation 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 261 of file fitsim.py.

Here is the call graph for this function:

8.15.3.2 def forcebalance.fitsim.FittingSimulation.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.

Definition at line 179 of file fitsim.py.

Here is the call graph for this function:

8.15.3.3 def forcebalance.fitsim.FittingSimulation.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 202 of file `fitsim.py`.

Here is the call graph for this function:

8.15.3.4 `def forcebalance.fitsim.FittingSimulation.get_X (self, mvals = None)`

Computes the objective function contribution without any parametric derivatives.

Definition at line 162 of file `fitsim.py`.

Here is the call graph for this function:

8.15.3.5 `def forcebalance.fitsim.FittingSimulation.link_from_tempdir (self, absdestdir)`

Definition at line 220 of file `fitsim.py`.

8.15.3.6 `def forcebalance.fitsim.FittingSimulation.refresh_temp_directory (self)`

Back up the temporary directory if desired, delete it and then create a new one.

Definition at line 226 of file `fitsim.py`.

Here is the call graph for this function:

8.15.3.7 `def forcebalance.fitsim.FittingSimulation.sget (self, mvals, AGrad=False, AHess=False, customdir=None)`

Stages the directory for the fitting simulation, and then calls 'get'.

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

Definition at line 273 of file `fitsim.py`.

Here is the call graph for this function:

8.15.4 Member Data Documentation

8.15.4.1 forcebalance.fitsim.FittingSimulation.FF

Need the forcefield (here for now)

Definition at line 140 of file `fitsim.py`.

8.15.4.2 forcebalance.fitsim.FittingSimulation.gct

Counts how often the gradient was computed.

Definition at line 144 of file `fitsim.py`.

8.15.4.3 forcebalance.fitsim.FittingSimulation.htc

Counts how often the Hessian was computed.

Definition at line 146 of file `fitsim.py`.

8.15.4.4 forcebalance.fitsim.FittingSimulation.rundir

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/simulation_name/iteration_number
The 'customdir' is customizable and can go below anything.

Definition at line 138 of file fitsim.py.

8.15.4.5 forcebalance.fitsim.FittingSimulation.tempdir

Root directory of the whole project.

Name of the fitting simulation Type of fitting simulation Relative weight of the fitting simulation Switch for finite difference gradients Switch for finite difference Hessians Switch for FD gradients + Hessian diagonals Parameter types that trigger FD gradient elements Parameter types that trigger FD Hessian elements Finite difference step size Work Queue Port (The specific simulation itself may or may not actually use this.) Manual override: bypass the parameter transformation and use physical parameters directly. For power users only! :) Whether to make backup files Relative directory of fitting simulation Temporary (working) directory; it is temp/(simulation_name) Used for storing temporary variables that don't change through the course of the optimization

Definition at line 136 of file fitsim.py.

8.15.4.6 forcebalance.fitsim.FittingSimulation.wq

Definition at line 156 of file fitsim.py.

8.15.4.7 forcebalance.fitsim.FittingSimulation.xct

Counts how often the objective function was computed.

Definition at line 142 of file fitsim.py.

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

- [fitsim.py](#)

8.16 forcebalance.baseclass.ForceBalanceBaseClass Class Reference

Provides some nifty functions that are common to all ForceBalance classes.

Inheritance diagram for forcebalance.baseclass.ForceBalanceBaseClass:

Collaboration diagram for forcebalance.baseclass.ForceBalanceBaseClass:

Public Member Functions

- `def __init__`
- `def set_option`

Public Attributes

- `PrintOptionDict`
- `verbose_options`

8.16.1 Detailed Description

Provides some nifty functions that are common to all ForceBalance classes.

Definition at line 6 of file baseclass.py.

8.16.2 Constructor & Destructor Documentation

8.16.2.1 `def forcebalance.baseclass.ForceBalanceBaseClass.__init__(self, options)`

Definition at line 8 of file baseclass.py.

8.16.3 Member Function Documentation

8.16.3.1 `def forcebalance.baseclass.ForceBalanceBaseClass.set_option(self, in_dict, src_key, dest_key=None, val=None, default=None, forceprint=False)`

Definition at line 12 of file baseclass.py.

8.16.4 Member Data Documentation

8.16.4.1 `forcebalance.baseclass.ForceBalanceBaseClass.PrintOptionDict`

Definition at line 9 of file baseclass.py.

8.16.4.2 `forcebalance.baseclass.ForceBalanceBaseClass.verbose_options`

Definition at line 10 of file baseclass.py.

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

- [baseclass.py](#)

8.17 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`

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](#)

8.17.1 Detailed Description

Finite state machine for parsing FrcMod force field file.

Definition at line 96 of file amberio.py.

8.17.2 Constructor & Destructor Documentation

8.17.2.1 `def forcebalance.amberio.FrcMod_Reader.__init__(self, fnm)`

Definition at line 98 of file amberio.py.

8.17.3 Member Function Documentation

8.17.3.1 `def forcebalance.amberio.FrcMod_Reader.feed(self, line)`

Definition at line 116 of file amberio.py.

8.17.3.2 `def forcebalance.amberio.FrcMod_Reader.Split(self, line)`

Definition at line 110 of file amberio.py.

Here is the call graph for this function:

8.17.3.3 `def forcebalance.amberio.FrcMod_Reader.Whites(self, line)`

Definition at line 113 of file amberio.py.

Here is the call graph for this function:

8.17.4 Member Data Documentation

8.17.4.1 `forcebalance.amberio.FrcMod_Reader.adict`

The frcmod file never has any atoms in it.

Definition at line 108 of file amberio.py.

8.17.4.2 `forcebalance.amberio.FrcMod_Reader.atom`

The atom numbers in the interaction (stored in the parser)

Definition at line 104 of file amberio.py.

8.17.4.3 `forcebalance.amberio.FrcMod_Reader.dihe`

Whether we're inside the dihedral section.

Definition at line 106 of file amberio.py.

8.17.4.4 forcebalance.amberio.FrcMod_Reader.itype

Definition at line 127 of file amberio.py.

8.17.4.5 forcebalance.amberio.FrcMod_Reader.pdict

The parameter dictionary (defined in this file)

Definition at line 102 of file amberio.py.

8.17.4.6 forcebalance.amberio.FrcMod_Reader.suffix

Definition at line 162 of file amberio.py.

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

- [amberio.py](#)

8.18 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.*

Public Attributes

- [element](#)
- [amom](#)
- [last_amom](#)
- [basis_number](#)
- [contraction_number](#)
- [adict](#)
- [isdata](#)
- [destroy](#)

8.18.1 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 32 of file psi4io.py.

8.18.2 Constructor & Destructor Documentation

8.18.2.1 def forcebalance.psi4io.GBS_Reader.__init__(self, fnm = None)

Definition at line 34 of file psi4io.py.

8.18.3 Member Function Documentation

8.18.3.1 def forcebalance.psi4io.GBS_Reader.build_pid(self, pfld)

Definition at line 45 of file psi4io.py.

Here is the call graph for this function:

8.18.3.2 def forcebalance.psi4io.GBS_Reader.feed(self, line, linindep = False)

Feed in a line.

Parameters

| | | |
|-----------|-------------|------------------|
| <i>in</i> | <i>line</i> | The line of data |
|-----------|-------------|------------------|

Definition at line 58 of file psi4io.py.

Here is the call graph for this function:

8.18.4 Member Data Documentation

8.18.4.1 forcebalance.psi4io.GBS_Reader.adict

Definition at line 41 of file psi4io.py.

8.18.4.2 forcebalance.psi4io.GBS_Reader.amom

Definition at line 37 of file psi4io.py.

8.18.4.3 forcebalance.psi4io.GBS_Reader.basis_number

Definition at line 39 of file psi4io.py.

8.18.4.4 forcebalance.psi4io.GBS_Reader.contraction_number

Definition at line 40 of file psi4io.py.

8.18.4.5 forcebalance.psi4io.GBS_Reader.destroy

Definition at line 43 of file psi4io.py.

8.18.4.6 forcebalance.psi4io.GBS_Reader.element

Definition at line 36 of file psi4io.py.

8.18.4.7 forcebalance.psi4io.GBS_Reader.isdata

Definition at line 42 of file psi4io.py.

8.18.4.8 forcebalance.psi4io.GBS_Reader.last_amom

Definition at line 38 of file psi4io.py.

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

- [psi4io.py](#)

8.19 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.

Public Attributes

- `sec`
The current section that we're in.
- `pdict`
The parameter dictionary (defined in this file)
- `itype`
- `suffix`

8.19.1 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.

8.19.2 Constructor & Destructor Documentation

8.19.2.1 `def forcebalance.custom_io.Gen_Reader.__init__(self, fnm)`

Definition at line 43 of file custom_io.py.

8.19.3 Member Function Documentation

8.19.3.1 `def forcebalance.custom_io.Gen_Reader.feed(self, line)`

Feed in a line.

Parameters

| | | |
|-----------------|-------------------|------------------|
| <code>in</code> | <code>line</code> | The line of data |
|-----------------|-------------------|------------------|

Definition at line 57 of file custom_io.py.

8.19.4 Member Data Documentation

8.19.4.1 forcebalance.custom_io.Gen_Reader.itype

Definition at line 60 of file custom_io.py.

8.19.4.2 forcebalance.custom_io.Gen_Reader.pdict

The parameter dictionary (defined in this file)

Definition at line 49 of file custom_io.py.

8.19.4.3 forcebalance.custom_io.Gen_Reader.sec

The current section that we're in.

Definition at line 47 of file custom_io.py.

8.19.4.4 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](#)

8.20 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.*

Public Attributes

- [element](#)
- [point](#)
- [radii](#)
- [isdata](#)

8.20.1 Detailed Description

Finite state machine for parsing DVR grid files.

Definition at line 246 of file psi4io.py.

8.20.2 Constructor & Destructor Documentation

8.20.2.1 `def forcebalance.psi4io.Grid_Reader.__init__(self, fnm = None)`

Definition at line 248 of file psi4io.py.

8.20.3 Member Function Documentation

8.20.3.1 `def forcebalance.psi4io.Grid_Reader.build_pid(self, pfld)`

Definition at line 254 of file psi4io.py.

Here is the call graph for this function:

8.20.3.2 `def forcebalance.psi4io.Grid_Reader.feed(self, line, lin indep = False)`

Feed in a line.

Parameters

| | | |
|-----------|-------------|------------------|
| <i>in</i> | <i>line</i> | The line of data |
|-----------|-------------|------------------|

Definition at line 269 of file psi4io.py.

Here is the call graph for this function:

8.20.4 Member Data Documentation

8.20.4.1 `forcebalance.psi4io.Grid_Reader.element`

Definition at line 250 of file psi4io.py.

8.20.4.2 `forcebalance.psi4io.Grid_Reader.isdata`

Definition at line 280 of file psi4io.py.

8.20.4.3 `forcebalance.psi4io.Grid_Reader.point`

Definition at line 251 of file psi4io.py.

8.20.4.4 `forcebalance.psi4io.Grid_Reader.radii`

Definition at line 252 of file psi4io.py.

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

- [psi4io.py](#)

8.21 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 prepare_temp_directory`
Prepare the temporary directory, by default does nothing.
- `def indicate`
- `def get`
Evaluate objective function.

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`
Qualitative Indicator: average energy error (in kJ/mol)
- `e_err_pct`
- `ns`
Read in the trajectory file.
- `traj`
- `divisor`
Read in the reference data.
- `prefactor`
- `weight`
- `emm`
- `objective`

8.21.1 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 32 of file interaction.py.

8.21.2 Constructor & Destructor Documentation

8.21.2.1 def forcebalance.interaction.Interaction.__init__(self, options, tgt_opts, forcefield)

Definition at line 35 of file interaction.py.

Here is the call graph for this function:

8.21.3 Member Function Documentation

8.21.3.1 def forcebalance.interaction.Interaction.get(self, mvals, AGrad=False, AHess=False)

Evaluate objective function.

Definition at line 160 of file interaction.py.

8.21.3.2 def forcebalance.interaction.Interaction.indicate(self)

Definition at line 144 of file interaction.py.

Here is the call graph for this function:

8.21.3.3 def forcebalance.interaction.Interaction.prepare_temp_directory(self, options, tgt_opts)

Prepare the temporary directory, by default does nothing.

Definition at line 141 of file interaction.py.

8.21.3.4 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 the GROMACS/OpenMM units (kJ/mol for energy, kJ/mol/nm force).

Definition at line 122 of file interaction.py.

Here is the call graph for this function:

8.21.4 Member Data Documentation

8.21.4.1 forcebalance.interaction.Interaction.divisor

Read in the reference data.

Prepare the temporary directory

Definition at line 93 of file interaction.py.

8.21.4.2 forcebalance.interaction.Interaction.e_err

Qualitative Indicator: average energy error (in kJ/mol)

Definition at line 75 of file interaction.py.

8.21.4.3 forcebalance.interaction.Interaction.e_err_pct

Definition at line 76 of file interaction.py.

8.21.4.4 forcebalance.interaction.Interaction.emm

Definition at line 197 of file interaction.py.

8.21.4.5 forcebalance.interaction.Interaction.eqm

Set upper cutoff energy.

Reference (QM) interaction energies

Definition at line 69 of file interaction.py.

8.21.4.6 forcebalance.interaction.Interaction.label

Snapshot label, useful for graphing.

Definition at line 71 of file interaction.py.

8.21.4.7 forcebalance.interaction.Interaction.ns

Read in the trajectory file.

Definition at line 78 of file interaction.py.

8.21.4.8 forcebalance.interaction.Interaction.objective

Definition at line 198 of file interaction.py.

8.21.4.9 forcebalance.interaction.Interaction.prefactor

Definition at line 111 of file interaction.py.

8.21.4.10 forcebalance.interaction.Interaction.qfnm

The qdata.txt file that contains the QM energies and forces.

Definition at line 73 of file interaction.py.

8.21.4.11 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 57 of file interaction.py.

8.21.4.12 forcebalance.interaction.Interaction.select2

Set fragment 2.

Definition at line 62 of file interaction.py.

8.21.4.13 forcebalance.interaction.Interaction.traj

Definition at line 79 of file interaction.py.

8.21.4.14 forcebalance.interaction.Interaction.weight

Definition at line 164 of file interaction.py.

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

- [interaction.py](#)

8.22 forcebalance.gmxio.Interaction_GMX Class Reference

Subclass of Interaction for 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 prepare_temp_directory](#)
- [def interaction_driver](#)
Computes the energy and force using GROMACS for a single snapshot.
- [def interaction_driver_all](#)
Computes the energy and force using GROMACS for a trajectory.

Public Attributes

- [trajfnm](#)
Name of the trajectory.
- [topfnm](#)
- [Dielectric](#)
- [Diel_B](#)

8.22.1 Detailed Description

Subclass of Interaction for interaction energy matching using GROMACS.

Definition at line 618 of file gmxio.py.

8.22.2 Constructor & Destructor Documentation

8.22.2.1 `def forcebalance.gmxio.Interaction_GMX.__init__(self, options, tgt_opts, forcefield)`

Definition at line 620 of file gmxio.py.

Here is the call graph for this function:

8.22.3 Member Function Documentation

8.22.3.1 `def forcebalance.gmxio.Interaction_GMX.interaction_driver(self, shot)`

Computes the energy and force using GROMACS for a single snapshot.

This does not require GROMACS-X2.

Definition at line 651 of file gmxio.py.

8.22.3.2 `def forcebalance.gmxio.Interaction_GMX.interaction_driver_all(self, dielectric = False)`

Computes the energy and force using GROMACS for a trajectory.

This does not require GROMACS-X2.

Definition at line 656 of file gmxio.py.

Here is the call graph for this function:

8.22.3.3 `def forcebalance.gmxio.Interaction_GMX.prepare_temp_directory(self, options, tgt_opts)`

Definition at line 628 of file gmxio.py.

Here is the call graph for this function:

8.22.4 Member Data Documentation

8.22.4.1 `forcebalance.gmxio.Interaction_GMX.Diel_B`

Definition at line 696 of file gmxio.py.

8.22.4.2 `forcebalance.gmxio.Interaction_GMX.Dielectric`

Definition at line 625 of file gmxio.py.

8.22.4.3 `forcebalance.gmxio.Interaction_GMX.topfnm`

Definition at line 623 of file gmxio.py.

8.22.4.4 `forcebalance.gmxio.Interaction_GMX.trafnm`

Name of the trajectory.

Definition at line 622 of file gmxio.py.

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

- [gmxio.py](#)

8.23 forcebalance.openmmio.Interaction_OpenMM Class Reference

Subclass of Target for interaction matching using OpenMM.

Inheritance diagram for forcebalance.openmmio.Interaction_OpenMM:

Collaboration diagram for forcebalance.openmmio.Interaction_OpenMM:

Public Member Functions

- `def __init__`
- `def prepare_temp_directory`
- `def energy_driver_all`
- `def interaction_driver_all`

Public Attributes

- `trajfnm`
Name of the trajectory file containing snapshots.
- `simulations`
Dictionary of simulation objects (dimer, fraga, fragb)
- `platform`
Set up three OpenMM System objects.

8.23.1 Detailed Description

Subclass of Target for interaction matching using OpenMM.

Definition at line 534 of file openmmio.py.

8.23.2 Constructor & Destructor Documentation

8.23.2.1 `def forcebalance.openmmio.Interaction_OpenMM.__init__(self, options, tgt_opts, forcefield)`

Definition at line 537 of file openmmio.py.

8.23.3 Member Function Documentation

8.23.3.1 `def forcebalance.openmmio.Interaction_OpenMM.energy_driver_all(self, mode)`

Definition at line 598 of file openmmio.py.

Here is the call graph for this function:

8.23.3.2 `def forcebalance.openmmio.Interaction_OpenMM.interaction_driver_all(self, dielectric = False)`

Definition at line 651 of file openmmio.py.

8.23.3.3 `def forcebalance.openmmio.Interaction_OpenMM.prepare_temp_directory(self, options, tgt_opts)`

Definition at line 545 of file openmmio.py.

8.23.4 Member Data Documentation

8.23.4.1 forcebalance.openmmio.Interaction_OpenMM.platform

Set up three OpenMM System objects.

Set the device to the environment variable or zero otherwise.

TODO: The following code should not be repeated everywhere. Set the simulation platform

Definition at line 563 of file openmmio.py.

8.23.4.2 forcebalance.openmmio.Interaction_OpenMM.simulations

Dictionary of simulation objects (dimer, fraga, fragb)

Definition at line 541 of file openmmio.py.

8.23.4.3 forcebalance.openmmio.Interaction_OpenMM.trajfnm

Name of the trajectory file containing snapshots.

Definition at line 539 of file openmmio.py.

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

- [openmmio.py](#)

8.24 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 prepare_temp_directory](#)
- [def energy_driver_all](#)
- [def interaction_driver_all](#)

Public Attributes

- [trajfnm](#)
Name of the trajectory.

8.24.1 Detailed Description

Subclass of Target for interaction matching using TINKER.

Definition at line 582 of file tinkerio.py.

8.24.2 Constructor & Destructor Documentation

8.24.2.1 `def forcebalance.tinkerio.Interaction_TINKER.__init__(self, options, tgt_opts, forcefield)`

Definition at line 585 of file `tinkerio.py`.

Here is the call graph for this function:

8.24.3 Member Function Documentation

8.24.3.1 `def forcebalance.tinkerio.Interaction_TINKER.energy_driver_all(self, select=None)`

Definition at line 598 of file `tinkerio.py`.

Here is the call graph for this function:

8.24.3.2 `def forcebalance.tinkerio.Interaction_TINKER.interaction_driver_all(self, dielectric=False)`

Definition at line 615 of file `tinkerio.py`.

8.24.3.3 `def forcebalance.tinkerio.Interaction_TINKER.prepare_temp_directory(self, options, tgt_opts)`

Definition at line 590 of file `tinkerio.py`.

8.24.4 Member Data Documentation

8.24.4.1 `forcebalance.tinkerio.Interaction_TINKER.trajfnm`

Name of the trajectory.

Definition at line 587 of file `tinkerio.py`.

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

- [tinkerio.py](#)

8.25 forcebalance.interactions.Interactions Class Reference

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

Inheritance diagram for `forcebalance.interactions.Interactions`:

Collaboration diagram for `forcebalance.interactions.Interactions`:

Public Member Functions

- `def __init__`
- `def indicate`
- `def get`

Public Attributes

- `inter_opts`
- `PrintDict`

- [RMSDDict](#)
- [rmsd_part](#)
- [energy_part](#)
- [objective](#)

8.25.1 Detailed Description

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

Definition at line 120 of file interactions.py.

8.25.2 Constructor & Destructor Documentation

8.25.2.1 `def forcebalance.interactions.Interactions.__init__(self, options, tgt_opts, forcefield)`

Definition at line 123 of file interactions.py.

Here is the call graph for this function:

8.25.3 Member Function Documentation

8.25.3.1 `def forcebalance.interactions.Interactions.get(self, mvals, AGrad=False, AHess=False)`

Definition at line 154 of file interactions.py.

8.25.3.2 `def forcebalance.interactions.Interactions.indicate(self)`

Definition at line 148 of file interactions.py.

Here is the call graph for this function:

8.25.4 Member Data Documentation

8.25.4.1 `forcebalance.interactions.Interactions.energy_part`

Definition at line 190 of file interactions.py.

8.25.4.2 `forcebalance.interactions.Interactions.inter_opts`

Definition at line 126 of file interactions.py.

8.25.4.3 `forcebalance.interactions.Interactions.objective`

Definition at line 214 of file interactions.py.

8.25.4.4 `forcebalance.interactions.Interactions.PrintDict`

Definition at line 156 of file interactions.py.

8.25.4.5 `forcebalance.interactions.Interactions.rmsd_part`

Definition at line 188 of file interactions.py.

8.25.4.6 forcebalance.interactions.Interactions.RMSDDict

Definition at line 157 of file interactions.py.

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

- [interactions.py](#)

8.26 forcebalance.gmxio.OTP_Reader Class Reference

Finite state machine for parsing GROMACS force field files.

Inheritance diagram for forcebalance.gmxio.OTP_Reader:

Collaboration diagram for forcebalance.gmxio.OTP_Reader:

Public Member Functions

- `def __init__`
- `def feed`

Given a line, determine the interaction type and the atoms involved (the suffix).

Public Attributes

- `sec`
The current section that we're in.
- `nbtype`
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`

8.26.1 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 'PARM' or 'RPT' keywords.

As we go through the file, we figure out the atoms involved in the interaction described on each line.

When a 'PARM' 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 ; PARM 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 'ANGLE-SKCACBO'.

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_ANGLESKCACAH /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 272 of file `gmxio.py`.

8.26.2 Constructor & Destructor Documentation

8.26.2.1 def forcebalance.gmxio.ITP_Reader.__init__(self, fnm)

Definition at line 275 of file `gmxio.py`.

8.26.3 Member Function Documentation

8.26.3.1 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
; PARM 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 313 of file `gmxio.py`.

8.26.4 Member Data Documentation

8.26.4.1 forcebalance.gmxio.OTP_Reader.atomnames

Listing of all atom names in the file, (probably unnecessary)

Definition at line 287 of file `gmxio.py`.

8.26.4.2 forcebalance.gmxio.OTP_Reader.atomtype_to_mass

A dictionary of atomic masses.

Definition at line 291 of file `gmxio.py`.

8.26.4.3 forcebalance.gmxio.OTP_Reader.atomtypes

Listing of all atom types in the file, (probably unnecessary)

Definition at line 289 of file `gmxio.py`.

8.26.4.4 forcebalance.gmxio.OTP_Reader.itype

Definition at line 316 of file `gmxio.py`.

8.26.4.5 forcebalance.gmxio.OTP_Reader.mol

The current molecule (set by the `moleculetype` keyword)

Definition at line 283 of file `gmxio.py`.

8.26.4.6 forcebalance.gmxio.OTP_Reader.molatom

Definition at line 423 of file `gmxio.py`.

8.26.4.7 forcebalance.gmxio.OTP_Reader.nbtype

Nonbonded type.

Definition at line 281 of file `gmxio.py`.

8.26.4.8 forcebalance.gmxio.OTP_Reader.pdict

The parameter dictionary (defined in this file)

Definition at line 285 of file `gmxio.py`.

8.26.4.9 forcebalance.gmxio.OTP_Reader.sec

The current section that we're in.

Definition at line 279 of file `gmxio.py`.

8.26.4.10 forcebalance.gmxio.ITP_Reader.suffix

Definition at line 418 of file gmxio.py.

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

- [gmxio.py](#)

8.27 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.

Public Attributes

- [call_derivatives](#)
Number of snapshots.
- [MAQ](#)
Dictionary for derivative terms.
- [D](#)
- [objective](#)

8.27.1 Detailed Description

Subclass of Target for general least squares fitting.

Definition at line 32 of file leastsq.py.

8.27.2 Constructor & Destructor Documentation

8.27.2.1 def forcebalance.leastsq.LeastSquares.__init__(self, options, tgt_opts, forcefield)

Definition at line 35 of file leastsq.py.

Here is the call graph for this function:

8.27.3 Member Function Documentation

8.27.3.1 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 72 of file leastsq.py.

Here is the call graph for this function:

8.27.3.2 `def forcebalance.leastsq.LeastSquares.indicate (self)`

Definition at line 50 of file leastsq.py.

Here is the call graph for this function:

8.27.4 Member Data Documentation

8.27.4.1 `forcebalance.leastsq.LeastSquares.call_derivatives`

Number of snapshots.

Which parameters are differentiated?

Definition at line 48 of file leastsq.py.

8.27.4.2 `forcebalance.leastsq.LeastSquares.D`

Definition at line 135 of file leastsq.py.

8.27.4.3 `forcebalance.leastsq.LeastSquares.MAQ`

Dictionary for derivative terms.

Definition at line 98 of file leastsq.py.

8.27.4.4 `forcebalance.leastsq.LeastSquares.objective`

Definition at line 136 of file leastsq.py.

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

- [leastsq.py](#)

8.28 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__](#)
Instantiation of the subclass.
- def [read_data](#)
- def [npt_simulation](#)
Submit a NPT simulation to the Work Queue.
- def [indicate](#)
- def [objective_term](#)
- def [submit_jobs](#)
- def [get](#)
Fitting of liquid bulk properties.
- def [polarization_correction](#)
Return the self-polarization correction as described in Berendsen et al., JPC 1987.

Public Attributes

- [do_self_pol](#)
- [SavedMVal](#)
Read the reference data.
- [SavedTraj](#)
Saved trajectories for all iterations and all temperatures :)
- [MBarEnergy](#)
Evaluated energies for all trajectories (i.e.
- [nptpfx](#)
- [nptfiles](#)
- [nptsfx](#)
- [RefData](#)
- [PhasePoints](#)
- [Labels](#)
- [w_rho](#)
Density.
- [w_hvap](#)
- [w_alpha](#)
- [w_kappa](#)
- [w_cp](#)
- [w_eps0](#)

8.28.1 Detailed Description

Subclass of Target for liquid property matching.

Definition at line 48 of file liquid.py.

8.28.2 Constructor & Destructor Documentation

8.28.2.1 `def forcebalance.liquid.Liquid.__init__(self, options, tgt_opts, forcefield)`

Instantiation of the subclass.

We begin by instantiating the superclass here and also defining a number of core concepts for energy / force matching.

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

Definition at line 61 of file liquid.py.

Here is the call graph for this function:

8.28.3 Member Function Documentation

8.28.3.1 `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 (Hvap) of liquid 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 | <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 392 of file liquid.py.

Here is the call graph for this function:

8.28.3.2 `def forcebalance.liquid.Liquid.indicate(self)`

Definition at line 252 of file liquid.py.

8.28.3.3 `def forcebalance.liquid.Liquid.npt_simulation(self, temperature, pressure, simnum)`

Submit a NPT simulation to the Work Queue.

Definition at line 232 of file liquid.py.

Here is the call graph for this function:

```
8.28.3.4 def forcebalance.liquid.Liquid.objective_term ( self, points, expname, calc, err, grad, name = "Quantity",  
SubAverage = False )
```

Definition at line 256 of file liquid.py.

Here is the call graph for this function:

```
8.28.3.5 def forcebalance.liquid.Liquid.polarization_correction ( self, mvals )
```

Return the self-polarization correction as described in Berendsen et al., JPC 1987.

Definition at line 724 of file liquid.py.

```
8.28.3.6 def forcebalance.liquid.Liquid.read_data ( self )
```

Definition at line 140 of file liquid.py.

```
8.28.3.7 def forcebalance.liquid.Liquid.submit_jobs ( self, mvals, AGrad = True, AHess = True )
```

Definition at line 334 of file liquid.py.

Here is the call graph for this function:

8.28.4 Member Data Documentation

8.28.4.1 forcebalance.liquid.Liquid.do_self_pol

Definition at line 104 of file liquid.py.

8.28.4.2 forcebalance.liquid.Liquid.Labels

Definition at line 220 of file liquid.py.

8.28.4.3 forcebalance.liquid.Liquid.MBarEnergy

Evaluated energies for all trajectories (i.e.
all iterations and all temperatures), using all mvals

Definition at line 127 of file liquid.py.

8.28.4.4 forcebalance.liquid.Liquid.nptfiles

Definition at line 131 of file liquid.py.

8.28.4.5 forcebalance.liquid.Liquid.nptpfx

Definition at line 129 of file liquid.py.

8.28.4.6 forcebalance.liquid.Liquid.nptsfx

Definition at line 133 of file liquid.py.

8.28.4.7 forcebalance.liquid.Liquid.PhasePoints

Definition at line 216 of file liquid.py.

8.28.4.8 forcebalance.liquid.Liquid.RefData

Definition at line 150 of file liquid.py.

8.28.4.9 forcebalance.liquid.Liquid.SavedMVal

Read the reference data.

Prepare the temporary directory Saved force field mvals for all iterations

Definition at line 123 of file liquid.py.

8.28.4.10 forcebalance.liquid.Liquid.SavedTraj

Saved trajectories for all iterations and all temperatures :)

Definition at line 125 of file liquid.py.

8.28.4.11 forcebalance.liquid.Liquid.w_alpha

Definition at line 641 of file liquid.py.

8.28.4.12 forcebalance.liquid.Liquid.w_cp

Definition at line 643 of file liquid.py.

8.28.4.13 forcebalance.liquid.Liquid.w_eps0

Definition at line 644 of file liquid.py.

8.28.4.14 forcebalance.liquid.Liquid.w_hvap

Definition at line 640 of file liquid.py.

8.28.4.15 forcebalance.liquid.Liquid.w_kappa

Definition at line 642 of file liquid.py.

8.28.4.16 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 639 of file liquid.py.

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

- [liquid.py](#)

8.29 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 prepare_temp_directory](#)
Prepare the temporary directory by copying in important files.
- [def polarization_correction](#)

Public Attributes

- [liquid_fnm](#)
- [liquid_conf](#)
- [liquid_traj](#)
- [gas_fnm](#)
- [nptpfx](#)
- [engine](#)

8.29.1 Detailed Description

Definition at line 570 of file gmxio.py.

8.29.2 Constructor & Destructor Documentation

8.29.2.1 `def forcebalance.gmxio.Liquid_GMX.__init__(self, options, tgt_opts, forcefield)`

Definition at line 571 of file gmxio.py.

Here is the call graph for this function:

8.29.3 Member Function Documentation

8.29.3.1 `def forcebalance.gmxio.Liquid_GMX.polarization_correction(self, mvals)`

Definition at line 612 of file gmxio.py.

Here is the call graph for this function:

8.29.3.2 `def forcebalance.gmxio.Liquid_GMX.prepare_temp_directory(self, options, tgt_opts)`

Prepare the temporary directory by copying in important files.

Definition at line 595 of file gmxio.py.

Here is the call graph for this function:

8.29.4 Member Data Documentation

8.29.4.1 `forcebalance.gmxio.Liquid_GMX.engine`

Definition at line 591 of file gmxio.py.

8.29.4.2 forcebalance.gmxio.Liquid_GMX.gas_fnm

Definition at line 578 of file gmxio.py.

8.29.4.3 forcebalance.gmxio.Liquid_GMX.liquid_conf

Definition at line 576 of file gmxio.py.

8.29.4.4 forcebalance.gmxio.Liquid_GMX.liquid_fnm

Definition at line 575 of file gmxio.py.

8.29.4.5 forcebalance.gmxio.Liquid_GMX.liquid_traj

Definition at line 577 of file gmxio.py.

8.29.4.6 forcebalance.gmxio.Liquid_GMX.nptpfx

Definition at line 585 of file gmxio.py.

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

- [gmxio.py](#)

8.30 forcebalance.openmmio.Liquid_OpenMM Class Reference

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 [polarization_correction](#)

Public Attributes

- [mpdb](#)
- [platform](#)
- [msim](#)
- [liquid_fnm](#)
- [liquid_conf](#)
- [liquid_traj](#)
- [gas_fnm](#)
- [engine](#)

8.30.1 Detailed Description

Definition at line 327 of file openmmio.py.

8.30.2 Constructor & Destructor Documentation

8.30.2.1 `def forcebalance.openmmio.Liquid_OpenMM.__init__(self, options, tgt_opts, forcefield)`

Definition at line 328 of file openmmio.py.

8.30.3 Member Function Documentation

8.30.3.1 `def forcebalance.openmmio.Liquid_OpenMM.polarization_correction (self, mvals)`

Definition at line 375 of file openmmio.py.

Here is the call graph for this function:

8.30.3.2 `def forcebalance.openmmio.Liquid_OpenMM.prepare_temp_directory (self, options, tgt_opts)`

Prepare the temporary directory by copying in important files.

Definition at line 368 of file openmmio.py.

Here is the call graph for this function:

8.30.4 Member Data Documentation

8.30.4.1 `forcebalance.openmmio.Liquid_OpenMM.engine`

Definition at line 364 of file openmmio.py.

8.30.4.2 `forcebalance.openmmio.Liquid_OpenMM.gas_fnm`

Definition at line 351 of file openmmio.py.

8.30.4.3 `forcebalance.openmmio.Liquid_OpenMM.liquid_conf`

Definition at line 349 of file openmmio.py.

8.30.4.4 `forcebalance.openmmio.Liquid_OpenMM.liquid_fnm`

Definition at line 348 of file openmmio.py.

8.30.4.5 `forcebalance.openmmio.Liquid_OpenMM.liquid_traj`

Definition at line 350 of file openmmio.py.

8.30.4.6 `forcebalance.openmmio.Liquid_OpenMM.mpdb`

Definition at line 336 of file openmmio.py.

8.30.4.7 `forcebalance.openmmio.Liquid_OpenMM.msim`

Definition at line 346 of file openmmio.py.

8.30.4.8 `forcebalance.openmmio.Liquid_OpenMM.platform`

Definition at line 344 of file openmmio.py.

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

- [openmmio.py](#)

8.31 forcebalance.tinkerio.Liquid_TINKER Class Reference

Inheritance diagram for forcebalance.tinkerio.Liquid_TINKER:

Collaboration diagram for forcebalance.tinkerio.Liquid_TINKER:

Public Member Functions

- [def __init__](#)
- [def prepare_temp_directory](#)
Prepare the temporary directory by copying in important files.
- [def npt_simulation](#)
Submit a NPT simulation to the Work Queue.

Public Attributes

- [DynDict](#)
- [DynDict_New](#)

8.31.1 Detailed Description

Definition at line 232 of file tinkerio.py.

8.31.2 Constructor & Destructor Documentation

8.31.2.1 `def forcebalance.tinkerio.Liquid_TINKER.__init__(self, options, tgt_opts, forcefield)`

Definition at line 233 of file tinkerio.py.

Here is the call graph for this function:

8.31.3 Member Function Documentation

8.31.3.1 `def forcebalance.tinkerio.Liquid_TINKER.npt_simulation(self, temperature, pressure, simnum)`

Submit a NPT simulation to the Work Queue.

Definition at line 260 of file tinkerio.py.

Here is the call graph for this function:

8.31.3.2 `def forcebalance.tinkerio.Liquid_TINKER.prepare_temp_directory(self, options, tgt_opts)`

Prepare the temporary directory by copying in important files.

Definition at line 242 of file tinkerio.py.

Here is the call graph for this function:

8.31.4 Member Data Documentation

8.31.4.1 forcebalance.tinkerio.Liquid_TINKER.DynDict

Definition at line 235 of file tinkerio.py.

8.31.4.2 forcebalance.tinkerio.Liquid_TINKER.DynDict_New

Definition at line 236 of file tinkerio.py.

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

- [tinkerio.py](#)

8.32 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](#)
number of sets (integer)
- 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](#)

8.32.1 Detailed Description

This is to manage one [mol2](#) series of lines on the form:

```
@<TRIPOS>MOLECULE
CDK2.xray.inh1.1E9H
 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.

8.32.2 Constructor & Destructor Documentation

8.32.2.1 `def forcebalance.Mol2.mol2.__init__(self, data)`

Definition at line 289 of file Mol2.py.

8.32.3 Member Function Documentation

8.32.3.1 `def forcebalance.Mol2.mol2.__repr__(self)`

Definition at line 305 of file Mol2.py.

Here is the call graph for this function:

8.32.3.2 `def forcebalance.Mol2.mol2.get_atom(self, id)`

return the atom instance given its atom identifier

Definition at line 461 of file Mol2.py.

Here is the call graph for this function:

8.32.3.3 `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.

8.32.3.4 `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:

8.32.3.5 `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:

8.32.3.6 `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.

Here is the call graph for this function:

8.32.3.7 `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:

8.32.3.8 `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.

Here is the call graph for this function:

8.32.3.9 `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.

Here is the call graph for this function:

8.32.3.10 `def forcebalance.Mol2.mol2.set_num_atoms (self, num_atoms=None)`

number of atoms (integer)

Definition at line 341 of file Mol2.py.

Here is the call graph for this function:

8.32.3.11 `def forcebalance.Mol2.mol2.set_num_bonds (self, num_bonds=None)`

number of bonds (integer)

Definition at line 350 of file Mol2.py.

Here is the call graph for this function:

8.32.3.12 `def forcebalance.Mol2.mol2.set_num_feat (self, num_feat = None)`

number of features (integer)

Definition at line 368 of file Mol2.py.

Here is the call graph for this function:

8.32.3.13 `def forcebalance.Mol2.mol2.set_num_sets (self, num_sets = None)`

number of sets (integer)

Definition at line 377 of file Mol2.py.

Here is the call graph for this function:

8.32.3.14 `def forcebalance.Mol2.mol2.set_num_subst (self, num_subst = None)`

number of substructures (integer)

Definition at line 359 of file Mol2.py.

Here is the call graph for this function:

8.32.4 Member Data Documentation

8.32.4.1 forcebalance.Mol2.mol2.atoms

Definition at line 300 of file Mol2.py.

8.32.4.2 forcebalance.Mol2.mol2.bonds

Definition at line 301 of file Mol2.py.

8.32.4.3 forcebalance.Mol2.mol2.charge_type

Definition at line 297 of file Mol2.py.

8.32.4.4 forcebalance.Mol2.mol2.comments

Definition at line 298 of file Mol2.py.

8.32.4.5 forcebalance.Mol2.mol2.mol_name

Definition at line 290 of file Mol2.py.

8.32.4.6 forcebalance.Mol2.mol2.mol_type

Definition at line 296 of file Mol2.py.

8.32.4.7 forcebalance.Mol2.mol2.num_atoms

Definition at line 291 of file Mol2.py.

8.32.4.8 forcebalance.Mol2.mol2.num_bonds

Definition at line 292 of file Mol2.py.

8.32.4.9 forcebalance.Mol2.mol2.num_feat

Definition at line 294 of file Mol2.py.

8.32.4.10 forcebalance.Mol2.mol2.num_sets

Definition at line 295 of file Mol2.py.

8.32.4.11 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](#)

8.33 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](#)

8.33.1 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.

8.33.2 Constructor & Destructor Documentation

8.33.2.1 `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.

8.33.3 Member Function Documentation

8.33.3.1 `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.

Here is the call graph for this function:

8.33.3.2 `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:

8.33.3.3 `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.

Here is the call graph for this function:

8.33.3.4 `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.

Here is the call graph for this function:

8.33.3.5 `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.

Here is the call graph for this function:

8.33.3.6 `def forcebalance.Mol2.mol2_atom.set_charge (self, charge = None)`

atomic charge

Definition at line 146 of file Mol2.py.

8.33.3.7 `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.

Here is the call graph for this function:

8.33.3.8 `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.

Here is the call graph for this function:

8.33.3.9 `def forcebalance.Mol2.mol2_atom.set_subst_id (self, subst_id = None)`

substructure identifier

Definition at line 128 of file Mol2.py.

Here is the call graph for this function:

8.33.3.10 `def forcebalance.Mol2.mol2_atom.set_subst_name (self, subst_name = None)`

substructure name

Definition at line 137 of file Mol2.py.

Here is the call graph for this function:

8.33.4 Member Data Documentation

8.33.4.1 `forcebalance.Mol2.mol2_atom.atom_id`

Definition at line 38 of file Mol2.py.

8.33.4.2 forcebalance.Mol2.mol2_atom.atom_name

Definition at line 39 of file Mol2.py.

8.33.4.3 forcebalance.Mol2.mol2_atom.atom_type

Definition at line 43 of file Mol2.py.

8.33.4.4 forcebalance.Mol2.mol2_atom.charge

Definition at line 46 of file Mol2.py.

8.33.4.5 forcebalance.Mol2.mol2_atom.status_bit

Definition at line 47 of file Mol2.py.

8.33.4.6 forcebalance.Mol2.mol2_atom.subst_id

Definition at line 44 of file Mol2.py.

8.33.4.7 forcebalance.Mol2.mol2_atom.subst_name

Definition at line 45 of file Mol2.py.

8.33.4.8 forcebalance.Mol2.mol2_atom.x

Definition at line 40 of file Mol2.py.

8.33.4.9 forcebalance.Mol2.mol2_atom.y

Definition at line 41 of file Mol2.py.

8.33.4.10 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](#)

8.34 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](#)

8.34.1 Detailed Description

This is to manage [mol2](#) bond lines on the form: 1 1 2 ar.

Definition at line 172 of file Mol2.py.

8.34.2 Constructor & Destructor Documentation

8.34.2.1 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.

8.34.3 Member Function Documentation

8.34.3.1 def forcebalance.Mol2.mol2_bond.__repr__(self)

Definition at line 186 of file Mol2.py.

Here is the call graph for this function:

8.34.3.2 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:

8.34.3.3 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.

Here is the call graph for this function:

8.34.3.4 `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.

8.34.3.5 `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.

8.34.3.6 `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.

Here is the call graph for this function:

8.34.3.7 `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.

Here is the call graph for this function:

8.34.4 Member Data Documentation

8.34.4.1 `forcebalance.Mol2.mol2_bond.bond_id`

Definition at line 178 of file Mol2.py.

8.34.4.2 `forcebalance.Mol2.mol2_bond.bond_type`

Definition at line 181 of file Mol2.py.

8.34.4.3 `forcebalance.Mol2.mol2_bond.origin_atom_id`

Definition at line 179 of file Mol2.py.

8.34.4.4 `forcebalance.Mol2.mol2_bond.status_bit`

Definition at line 206 of file Mol2.py.

8.34.4.5 `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](#)

8.35 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`

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`

8.35.1 Detailed Description

Finite state machine for parsing `Mol2` force field file.

(just for parameterizing the charges)

Definition at line 40 of file `amberio.py`.

8.35.2 Constructor & Destructor Documentation

8.35.2.1 `def forcebalance.amberio.Mol2_Reader.__init__(self, fnm)`

Definition at line 42 of file `amberio.py`.

8.35.3 Member Function Documentation

8.35.3.1 `def forcebalance.amberio.Mol2_Reader.feed(self, line)`

Definition at line 56 of file `amberio.py`.

8.35.4 Member Data Documentation

8.35.4.1 `forcebalance.amberio.Mol2_Reader.atom`

The atom numbers in the interaction (stored in the parser)

Definition at line 48 of file `amberio.py`.

8.35.4.2 forcebalance.amberio.Mol2_Reader.atomnames

The mol2 file provides a list of atom names.

Definition at line 50 of file amberio.py.

8.35.4.3 forcebalance.amberio.Mol2_Reader.itype

Definition at line 61 of file amberio.py.

8.35.4.4 forcebalance.amberio.Mol2_Reader.mol

Definition at line 54 of file amberio.py.

8.35.4.5 forcebalance.amberio.Mol2_Reader.molatom

Definition at line 92 of file amberio.py.

8.35.4.6 forcebalance.amberio.Mol2_Reader.pdict

The parameter dictionary (defined in this file)

Definition at line 46 of file amberio.py.

8.35.4.7 forcebalance.amberio.Mol2_Reader.section

The section that we're in.

Definition at line 52 of file amberio.py.

8.35.4.8 forcebalance.amberio.Mol2_Reader.suffix

Definition at line 90 of file amberio.py.

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

- [amberio.py](#)

8.36 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](#)

Public Attributes

- [pdict](#)
The parameter dictionary (defined in this file)
- [atom](#)

The atom numbers in the interaction (stored in the parser)

- [itype](#)
- [suffix](#)

8.36.1 Detailed Description

Finite state machine for parsing [Mol2](#) force field file.

(just for parameterizing the charges)

Definition at line 22 of file mol2io.py.

8.36.2 Constructor & Destructor Documentation

8.36.2.1 `def forcebalance.mol2io.Mol2_Reader.__init__(self, fnm)`

Definition at line 24 of file mol2io.py.

8.36.3 Member Function Documentation

8.36.3.1 `def forcebalance.mol2io.Mol2_Reader.feed(self, line)`

Definition at line 32 of file mol2io.py.

8.36.4 Member Data Documentation

8.36.4.1 `forcebalance.mol2io.Mol2_Reader.atom`

The atom numbers in the interaction (stored in the parser)

Definition at line 30 of file mol2io.py.

8.36.4.2 `forcebalance.mol2io.Mol2_Reader.itype`

Definition at line 36 of file mol2io.py.

8.36.4.3 `forcebalance.mol2io.Mol2_Reader.pdict`

The parameter dictionary (defined in this file)

Definition at line 28 of file mol2io.py.

8.36.4.4 `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](#)

8.37 forcebalance.Mol2.mol2_set Class Reference

Public Member Functions

- def `__init__`

A collection is organized as a dictionary of compounds self.num_compounds : the number of compounds self.-compounds : the dictionary 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`

8.37.1 Detailed Description

Definition at line 568 of file Mol2.py.

8.37.2 Constructor & Destructor Documentation

8.37.2.1 `def forcebalance.Mol2.mol2_set.__init__(self, data=None, subset=None)`

A collection is organized as a dictionary of compounds self.num_compounds : the number of compounds self.-compounds : the dictionary 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.

8.37.3 Member Function Documentation

8.37.3.1 `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.

8.37.4 Member Data Documentation

8.37.4.1 `forcebalance.Mol2.mol2_set.comments`

Definition at line 579 of file Mol2.py.

8.37.4.2 `forcebalance.Mol2.mol2_set.compounds`

Definition at line 580 of file Mol2.py.

8.37.4.3 `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](#)

8.38 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 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 load_frames](#)
- [def edit_qcrems](#)
- [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." Note that we're following the MSMBuild convention of using all ones for the masses.
- def [align](#)
Align molecules.
- def [build_topology](#)
A bare-bones implementation of the bond graph capability in the nanoreactor code.
- 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 MSMBuild.)
- 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](#)
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.
- [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](#)

8.38.1 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 2 through 10.

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']`. `ns` = The number of snapshots. You'll get this if you use `MyMol.ns` or `MyMol['ns']`.

Unit system: Angstroms.

Definition at line 647 of file `molecule.py`.

8.38.2 Constructor & Destructor Documentation

8.38.2.1 `def forcebalance.molecule.Molecule.__init__(self, fnm = None, ftype = None, positive_resid = True, build_topology = True)`

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 817 of file `molecule.py`.

8.38.3 Member Function Documentation

8.38.3.1 `def forcebalance.molecule.Molecule.__add__(self, other)`

Add method for [Molecule](#) objects.

Definition at line 756 of file `molecule.py`.

Here is the call graph for this function:

8.38.3.2 `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 736 of file `molecule.py`.

Here is the call graph for this function:

8.38.3.3 `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 667 of file `molecule.py`.

Here is the call graph for this function:

8.38.3.4 `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 715 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.5 def forcebalance.molecule.Molecule.__iadd__( self, other )
```

Add method for [Molecule](#) objects.

Definition at line 786 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.6 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 745 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.7 def forcebalance.molecule.Molecule.__len__( self )
```

Return the number of frames in the trajectory.

Definition at line 651 of file molecule.py.

```
8.38.3.8 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 703 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.9 def forcebalance.molecule.Molecule.add_quantum( self, other )
```

Definition at line 997 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.10 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 1009 of file molecule.py.

```
8.38.3.11 def forcebalance.molecule.Molecule.align( self, smooth = True, center = True )
```

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.

Definition at line 1145 of file molecule.py.

Here is the call graph for this function:

8.38.3.12 `def forcebalance.molecule.Molecule.align_by_moments (self)`

Align molecules using the "moment of inertia." Note that we're following the MSMBuild convention of using all ones for the masses.

Definition at line 1126 of file molecule.py.

8.38.3.13 `def forcebalance.molecule.Molecule.align_center (self)`

Definition at line 1249 of file molecule.py.

8.38.3.14 `def forcebalance.molecule.Molecule.all_pairwise_rmsd (self)`

Find pairwise RMSD (super slow, not like the one in MSMBuild.)

Definition at line 1233 of file molecule.py.

Here is the call graph for this function:

8.38.3.15 `def forcebalance.molecule.Molecule.append (self, other)`

Definition at line 810 of file molecule.py.

Here is the call graph for this function:

8.38.3.16 `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 1047 of file molecule.py.

8.38.3.17 `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 1082 of file molecule.py.

Here is the call graph for this function:

8.38.3.18 `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 1164 of file molecule.py.

Here is the call graph for this function:

8.38.3.19 `def forcebalance.molecule.Molecule.center_of_mass (self)`

Definition at line 954 of file molecule.py.

Here is the call graph for this function:

8.38.3.20 `def forcebalance.molecule.Molecule.edit_qcrems (self, in_dict, subcalc=None)`

Definition at line 988 of file molecule.py.

Here is the call graph for this function:

8.38.3.21 `def forcebalance.molecule.Molecule.load_frames (self, fnm)`

Definition at line 981 of file molecule.py.

8.38.3.22 `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 1206 of file molecule.py.

Here is the call graph for this function:

8.38.3.23 `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 1275 of file molecule.py.

8.38.3.24 `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 1258 of file molecule.py.

Here is the call graph for this function:

8.38.3.25 `def forcebalance.molecule.Molecule.radius_of_gyration (self)`

Definition at line 958 of file molecule.py.

Here is the call graph for this function:

8.38.3.26 `def forcebalance.molecule.Molecule.read_arc (self, fnm)`

Read a TINKER .arc file.

Parameters

| | | |
|-----------|------------|---------------------|
| <i>in</i> | <i>fnm</i> | The input file name |
|-----------|------------|---------------------|

Returns

xyzs A list for the XYZ coordinates.

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 1552 of file molecule.py.

Here is the call graph for this function:

8.38.3.27 `def forcebalance.molecule.Molecule.read_charmm (self, fnm)`

Read a CHARMM .cor (or .crd) file.

Definition at line 1679 of file molecule.py.

Here is the call graph for this function:

8.38.3.28 `def forcebalance.molecule.Molecule.read_com (self, fnm)`

Parse a Gaussian .com file and return a SINGLE-ELEMENT list of xyz coordinates (no multiple file support)

Parameters

| | | |
|-----------|------------|---------------------|
| <i>in</i> | <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 1509 of file molecule.py.

Here is the call graph for this function:

8.38.3.29 `def forcebalance.molecule.Molecule.read_dcd (self, fnm)`

Definition at line 1470 of file molecule.py.

Here is the call graph for this function:

8.38.3.30 `def forcebalance.molecule.Molecule.read_gro (self, fnm)`

Read a GROMACS .gro file.

Definition at line 1615 of file molecule.py.

Here is the call graph for this function:

8.38.3.31 `def forcebalance.molecule.Molecule.read_mdcrd (self, fnm)`

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

| | | |
|-----------|------------|---------------------|
| <i>in</i> | <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 1361 of file molecule.py.

Here is the call graph for this function:

8.38.3.32 `def forcebalance.molecule.Molecule.read_mol2 (self, fnm)`

Definition at line 1421 of file molecule.py.

Here is the call graph for this function:

8.38.3.33 `def forcebalance.molecule.Molecule.read_pdb(self, fnm)`

Loads a PDB and returns a dictionary containing its data.

Definition at line 1859 of file molecule.py.

Here is the call graph for this function:

8.38.3.34 `def forcebalance.molecule.Molecule.read_qcesp(self, fnm)`

Definition at line 1934 of file molecule.py.

8.38.3.35 `def forcebalance.molecule.Molecule.read_qcin(self, fnm)`

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 1747 of file molecule.py.

Here is the call graph for this function:

8.38.3.36 `def forcebalance.molecule.Molecule.read_qcout(self, fnm)`

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

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 1963 of file molecule.py.

Here is the call graph for this function:

8.38.3.37 `def forcebalance.molecule.Molecule.read_qdata(self, fnm)`

Definition at line 1386 of file molecule.py.

8.38.3.38 `def forcebalance.molecule.Molecule.read_xyz(self, fnm)`

Parse a .xyz file which contains several xyz coordinates, and return their elements.

Parameters

| | | |
|-----------|------------|---------------------|
| <i>in</i> | <i>fnm</i> | 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 1316 of file molecule.py.

Here is the call graph for this function:

8.38.3.39 `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 1026 of file molecule.py.

8.38.3.40 `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 rename is SOL.

Definition at line 1037 of file molecule.py.

Here is the call graph for this function:

8.38.3.41 `def forcebalance.molecule.Molecule.require (self, args)`

Definition at line 905 of file molecule.py.

8.38.3.42 `def forcebalance.molecule.Molecule.require_boxes (self)`

Definition at line 2436 of file molecule.py.

Here is the call graph for this function:

8.38.3.43 `def forcebalance.molecule.Molecule.require_resid (self)`

Definition at line 2423 of file molecule.py.

8.38.3.44 `def forcebalance.molecule.Molecule.require_resname (self)`

Definition at line 2431 of file molecule.py.

Here is the call graph for this function:

8.38.3.45 `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 1298 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.46 def forcebalance.molecule.Molecule.write ( self, fnm=None, ftype=None, append=False, select=None )
```

Definition at line 920 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.47 def forcebalance.molecule.Molecule.write_arc ( self, select )
```

Definition at line 2220 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.48 def forcebalance.molecule.Molecule.write_dcd ( self, select )
```

Definition at line 2256 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.49 def forcebalance.molecule.Molecule.write_gro ( self, select )
```

Definition at line 2232 of file molecule.py.

```
8.38.3.50 def forcebalance.molecule.Molecule.write_mdcrd ( self, select )
```

Definition at line 2209 of file molecule.py.

```
8.38.3.51 def forcebalance.molecule.Molecule.write_molproq ( self, select )
```

Definition at line 2197 of file molecule.py.

Here is the call graph for this function:

```
8.38.3.52 def forcebalance.molecule.Molecule.write_pdb ( self, select )
```

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 2312 of file molecule.py.

Here is the call graph for this function:

8.38.3.53 `def forcebalance.molecule.Molecule.write_qcin (self, select)`

Definition at line 2140 of file molecule.py.

Here is the call graph for this function:

8.38.3.54 `def forcebalance.molecule.Molecule.write_qdata (self, select)`

Text quantum data format.

Definition at line 2402 of file molecule.py.

Here is the call graph for this function:

8.38.3.55 `def forcebalance.molecule.Molecule.write_xyz (self, select)`

Definition at line 2186 of file molecule.py.

Here is the call graph for this function:

8.38.4 Member Data Documentation

8.38.4.1 forcebalance.molecule.Molecule.bboxes

Definition at line 2484 of file molecule.py.

8.38.4.2 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 884 of file molecule.py.

8.38.4.3 forcebalance.molecule.Molecule.Data

Definition at line 867 of file molecule.py.

8.38.4.4 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 931 of file molecule.py.

8.38.4.5 forcebalance.molecule.Molecule.Funnel

A funnel dictionary that takes redundant file types and maps them down to a few.

Definition at line 849 of file molecule.py.

8.38.4.6 forcebalance.molecule.Molecule.molecules

Definition at line 895 of file molecule.py.

8.38.4.7 forcebalance.molecule.Molecule.positive_resid

Creates entries like 'gromacs' : 'gromacs' and 'xyz' : 'xyz' in the Funnel.

Definition at line 863 of file molecule.py.

8.38.4.8 forcebalance.molecule.Molecule.Read_Tab

The table of file readers.

Definition at line 824 of file molecule.py.

8.38.4.9 forcebalance.molecule.Molecule.resid

Definition at line 2427 of file molecule.py.

8.38.4.10 forcebalance.molecule.Molecule.resname

Definition at line 2434 of file molecule.py.

8.38.4.11 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 894 of file molecule.py.

8.38.4.12 forcebalance.molecule.Molecule.Write_Tab

The table of file writers.

Definition at line 838 of file molecule.py.

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

- [molecule.py](#)

8.39 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:

8.39.1 Detailed Description

Wrapper for the timestep C structure used in molfile plugins.

Definition at line 471 of file molecule.py.

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

- [molecule.py](#)

8.40 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 [prepare_temp_directory](#)
Prepare the temporary directory.
- def [indicate](#)
Print qualitative indicator.
- def [unpack_moments](#)
- def [get](#)
Evaluate objective function.

Public Attributes

- [denoms](#)
- [mfnm](#)
The mdata.txt file that contains the moments.
- [ref_moments](#)
- [na](#)
Number of atoms.
- [ref_eigvals](#)
- [ref_eigvecs](#)
- [calc_moments](#)
- [objective](#)

8.40.1 Detailed Description

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

Currently Tinker is supported.

Definition at line 27 of file moments.py.

8.40.2 Constructor & Destructor Documentation

8.40.2.1 `def forcebalance.moments.Moments.__init__(self, options, tgt_opts, forcefield)`

Initialization.

Definition at line 32 of file moments.py.

Here is the call graph for this function:

8.40.3 Member Function Documentation

8.40.3.1 `def forcebalance.moments.Moments.get(self, mvals, AGrad=False, AHess=False)`

Evaluate objective function.

Definition at line 170 of file moments.py.

Here is the call graph for this function:

8.40.3.2 `def forcebalance.moments.Moments.indicate(self)`

Print qualitative indicator.

Definition at line 138 of file moments.py.

Here is the call graph for this function:

8.40.3.3 `def forcebalance.moments.Moments.prepare_temp_directory(self, options, tgt_opts)`

Prepare the temporary directory.

Definition at line 133 of file moments.py.

8.40.3.4 `def forcebalance.moments.Moments.read_reference_data(self)`

Read the reference data from a file.

Definition at line 64 of file moments.py.

8.40.3.5 `def forcebalance.moments.Moments.unpack_moments(self, moment_dict)`

Definition at line 164 of file moments.py.

Here is the call graph for this function:

8.40.4 Member Data Documentation

8.40.4.1 `forcebalance.moments.Moments.calc_moments`

Definition at line 198 of file moments.py.

8.40.4.2 `forcebalance.moments.Moments.denoms`

Definition at line 45 of file moments.py.

8.40.4.3 `forcebalance.moments.Moments.mfnm`

The mdata.txt file that contains the moments.

Definition at line 54 of file moments.py.

8.40.4.4 forcebalance.moments.Moments.na

Number of atoms.

Definition at line 66 of file moments.py.

8.40.4.5 forcebalance.moments.Moments.objective

Definition at line 199 of file moments.py.

8.40.4.6 forcebalance.moments.Moments.ref_eigvals

Definition at line 67 of file moments.py.

8.40.4.7 forcebalance.moments.Moments.ref_eigvecs

Definition at line 68 of file moments.py.

8.40.4.8 forcebalance.moments.Moments.ref_moments

Definition at line 55 of file moments.py.

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

- [moments.py](#)

8.41 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 prepare_temp_directory](#)
- [def moments_driver](#)

Additional Inherited Members

8.41.1 Detailed Description

Subclass of Target for multipole moment matching using TINKER.

Definition at line 402 of file tinkerio.py.

8.41.2 Constructor & Destructor Documentation

8.41.2.1 `def forcebalance.tinkerio.Moments_TINKER.__init__(self, options, tgt_opts, forcefield)`

Definition at line 405 of file tinkerio.py.

Here is the call graph for this function:

8.41.3 Member Function Documentation

8.41.3.1 `def forcebalance.tinkerio.Moments_TINKER.moments_driver (self)`

Definition at line 421 of file `tinkerio.py`.

Here is the call graph for this function:

8.41.3.2 `def forcebalance.tinkerio.Moments_TINKER.prepare_temp_directory (self, options, tgt_opts)`

Definition at line 410 of file `tinkerio.py`.

Here is the call graph for this function:

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

- [tinkerio.py](#)

8.42 forcebalance.gmxqpio.Monomer_QTPIE Class Reference

Subclass of Target for monomer properties of QTPIE (implemented within gromacs WCV branch).

Inheritance diagram for `forcebalance.gmxqpio.Monomer_QTPIE`:

Collaboration diagram for `forcebalance.gmxqpio.Monomer_QTPIE`:

Public Member Functions

- `def __init__`
- `def indicate`
Print qualitative indicator.
- `def prepare_temp_directory`
- `def unpack_moments`
- `def get`

Public Attributes

- `ref_moments`
- `weights`
- `calc_moments`
- `objective`

8.42.1 Detailed Description

Subclass of Target for monomer properties of QTPIE (implemented within gromacs WCV branch).

Definition at line 127 of file `gmxqpio.py`.

8.42.2 Constructor & Destructor Documentation

8.42.2.1 `def forcebalance.gmxqpio.Monomer_QTPIE.__init__(self, options, tgt_opts, forcefield)`

Definition at line 129 of file gmxqpio.py.

Here is the call graph for this function:

8.42.3 Member Function Documentation

8.42.3.1 `def forcebalance.gmxqpio.Monomer_QTPIE.get(self, mvals, AGrad=False, AHess=False)`

Definition at line 218 of file gmxqpio.py.

Here is the call graph for this function:

8.42.3.2 `def forcebalance.gmxqpio.Monomer_QTPIE.indicate(self)`

Print qualitative indicator.

Definition at line 176 of file gmxqpio.py.

Here is the call graph for this function:

8.42.3.3 `def forcebalance.gmxqpio.Monomer_QTPIE.prepare_temp_directory(self, options, tgt_opts)`

Definition at line 197 of file gmxqpio.py.

Here is the call graph for this function:

8.42.3.4 `def forcebalance.gmxqpio.Monomer_QTPIE.unpack_moments(self, moment_dict)`

Definition at line 214 of file gmxqpio.py.

Here is the call graph for this function:

8.42.4 Member Data Documentation

8.42.4.1 `forcebalance.gmxqpio.Monomer_QTPIE.calc_moments`

Definition at line 255 of file gmxqpio.py.

8.42.4.2 `forcebalance.gmxqpio.Monomer_QTPIE.objective`

Definition at line 256 of file gmxqpio.py.

8.42.4.3 `forcebalance.gmxqpio.Monomer_QTPIE.ref_moments`

Definition at line 148 of file gmxqpio.py.

8.42.4.4 `forcebalance.gmxqpio.Monomer_QTPIE.weights`

Definition at line 162 of file gmxqpio.py.

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

- [gmxqpio.py](#)

8.43 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](#)

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](#)

8.43.1 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 106 of file objective.py.

8.43.2 Constructor & Destructor Documentation

8.43.2.1 def forcebalance.objective.Objective.__init__(self, options, tgt_opts, forcefield)

Definition at line 107 of file objective.py.

Here is the call graph for this function:

8.43.3 Member Function Documentation

8.43.3.1 `def forcebalance.objective.Objective.Full (self, mvals, Order = 0, verbose = False)`

Definition at line 250 of file objective.py.

Here is the call graph for this function:

8.43.3.2 `def forcebalance.objective.Objective.Indicate (self)`

Print objective function contributions.

Definition at line 213 of file objective.py.

Here is the call graph for this function:

8.43.3.3 `def forcebalance.objective.Objective.Target_Terms (self, mvals, Order = 0, verbose = False)`

Definition at line 153 of file objective.py.

Here is the call graph for this function:

8.43.4 Member Data Documentation

8.43.4.1 `forcebalance.objective.Objective.FF`

The force field (it seems to be everywhere)

Definition at line 132 of file objective.py.

8.43.4.2 `forcebalance.objective.Objective.ObjDict`

Definition at line 142 of file objective.py.

8.43.4.3 `forcebalance.objective.Objective.ObjDict_Last`

Definition at line 143 of file objective.py.

8.43.4.4 `forcebalance.objective.Objective.Penalty`

Initialize the penalty function.

Definition at line 134 of file objective.py.

8.43.4.5 `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 122 of file objective.py.

8.43.4.6 `forcebalance.objective.Objective.WTot`

Obtain the denominator.

Definition at line 139 of file objective.py.

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

- [objective.py](#)

8.44 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)

Public Attributes

- [pdict](#)

Initialize the superclass.

8.44.1 Detailed Description

Class for parsing OpenMM force field files.

Definition at line 302 of file openmmio.py.

8.44.2 Constructor & Destructor Documentation

8.44.2.1 `def forcebalance.openmmio.OpenMM_Reader.__init__(self, fnm)`

Definition at line 303 of file openmmio.py.

Here is the call graph for this function:

8.44.3 Member Function Documentation

8.44.3.1 `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 312 of file openmmio.py.

Here is the call graph for this function:

8.44.4 Member Data Documentation

8.44.4.1 forcebalance.openmmio.OpenMM_Reader.pdict

Initialize the superclass.

:) The parameter dictionary (defined in this file)

Definition at line 307 of file openmmio.py.

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

- [openmmio.py](#)

8.45 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 [Run](#)
Call the appropriate optimizer.
- 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 simulated annealing 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.

Public Attributes

- [OptTab](#)
A list of all the things we can ask the optimizer to do.
- [Objective](#)
The root directory.
- [bhyp](#)
Whether the penalty function is hyperbolic.
- [FF](#)
The force field itself.
- [excision](#)
The indices to be excluded from the Hessian update.
- [np](#)
Number of parameters.
- [mvals0](#)
The original parameter values.
- [chk](#)
Put data into the checkpoint file.
- [H](#)
- [dx](#)
- [Val](#)
- [Grad](#)
- [Hess](#)
- [Penalty](#)

8.45.1 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 42 of file optimizer.py.

8.45.2 Constructor & Destructor Documentation

8.45.2.1 `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 55 of file optimizer.py.

Here is the call graph for this function:

8.45.3 Member Function Documentation

8.45.3.1 `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 780 of file optimizer.py.

8.45.3.2 `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 600 of file optimizer.py.

8.45.3.3 `def forcebalance.optimizer.Optimizer.ConjugateGradient (self)`

Use SciPy's built-in simulated annealing algorithm to optimize the parameters.

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 785 of file optimizer.py.

8.45.3.4 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 881 of file optimizer.py.

Here is the call graph for this function:

8.45.3.5 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 913 of file optimizer.py.

Here is the call graph for this function:

8.45.3.6 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 677 of file optimizer.py.

Here is the call graph for this function:

8.45.3.7 def forcebalance.optimizer.Optimizer.Gradient (self)

A single-point gradient computation.

Definition at line 859 of file optimizer.py.

Here is the call graph for this function:

8.45.3.8 def forcebalance.optimizer.Optimizer.Hessian (self)

A single-point Hessian computation.

Definition at line 867 of file optimizer.py.

Here is the call graph for this function:

8.45.3.9 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 is vestigial and currently does not work.

BFGS is a pseudo-Newton method in the sense that it builds an approximate Hessian matrix from the gradient information in previous steps; Newton-Raphson requires the actual Hessian matrix. However, the algorithms are similar in that they both compute the step by inverting the Hessian and multiplying by the gradient.

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 228 of file optimizer.py.

Here is the call graph for this function:

8.45.3.10 `def forcebalance.optimizer.Optimizer.NewtonRaphson (self)`

Optimize the force field parameters using the Newton-Raphson method (.

See Also

[MainOptimizer](#))

Definition at line 595 of file optimizer.py.

Here is the call graph for this function:

8.45.3.11 `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 775 of file optimizer.py.

8.45.3.12 `def forcebalance.optimizer.Optimizer.readchk (self)`

Read the checkpoint file for the main optimizer.

Definition at line 941 of file optimizer.py.

8.45.3.13 `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 166 of file optimizer.py.

Here is the call graph for this function:

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

Definition at line 811 of file optimizer.py.

Here is the call graph for this function:

8.45.3.15 `def forcebalance.optimizer.Optimizer.ScanMVals (self)`

Scan through the mathematical parameter space.

See Also

Optimizer::ScanValues

Definition at line 843 of file optimizer.py.

Here is the call graph for this function:

8.45.3.16 `def forcebalance.optimizer.Optimizer.ScanPVals (self)`

Scan through the physical parameter space.

See Also

Optimizer::ScanValues

Definition at line 848 of file optimizer.py.

8.45.3.17 `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

| | | |
|-----------------|------------------|--|
| <code>in</code> | <i>Algorithm</i> | The optimization algorithm to use, for example 'powell', 'simplex' or 'anneal' |
|-----------------|------------------|--|

Definition at line 613 of file optimizer.py.

Here is the call graph for this function:

8.45.3.18 `def forcebalance.optimizer.Optimizer.Simplex (self)`

Use SciPy's built-in simplex algorithm to optimize the parameters.

See Also

[Optimizer::ScipyOptimizer](#)

Definition at line 770 of file optimizer.py.

Here is the call graph for this function:

8.45.3.19 `def forcebalance.optimizer.Optimizer.SinglePoint (self)`

A single-point objective function computation.

Definition at line 853 of file optimizer.py.

Here is the call graph for this function:

8.45.3.20 `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 420 of file optimizer.py.

Here is the call graph for this function:

8.45.3.21 `def forcebalance.optimizer.Optimizer.writechk (self)`

Write the checkpoint file for the main optimizer.

Definition at line 953 of file optimizer.py.

8.45.4 Member Data Documentation

8.45.4.1 `forcebalance.optimizer.Optimizer.bhyp`

Whether the penalty function is hyperbolic.

Definition at line 139 of file optimizer.py.

8.45.4.2 `forcebalance.optimizer.Optimizer.chk`

Put data into the checkpoint file.

Definition at line 271 of file optimizer.py.

8.45.4.3 forcebalance.optimizer.Optimizer.dx

Definition at line 449 of file optimizer.py.

8.45.4.4 forcebalance.optimizer.Optimizer.excision

The indices to be excluded from the Hessian update.

Definition at line 147 of file optimizer.py.

8.45.4.5 forcebalance.optimizer.Optimizer.FF

The force field itself.

Definition at line 141 of file optimizer.py.

8.45.4.6 forcebalance.optimizer.Optimizer.Grad

Definition at line 451 of file optimizer.py.

8.45.4.7 forcebalance.optimizer.Optimizer.H

Definition at line 448 of file optimizer.py.

8.45.4.8 forcebalance.optimizer.Optimizer.Hess

Definition at line 452 of file optimizer.py.

8.45.4.9 forcebalance.optimizer.Optimizer.mvals0

The original parameter values.

Sometimes the optimizer doesn't return anything (i.e.

in the case of a single point calculation) In these situations, don't do anything Check derivatives by finite difference after the optimization is over (for good measure)

Definition at line 153 of file optimizer.py.

8.45.4.10 forcebalance.optimizer.Optimizer.np

Number of parameters.

Definition at line 150 of file optimizer.py.

8.45.4.11 forcebalance.optimizer.Optimizer.Objective

The root directory.

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) Guess value for Brent Step size for numerical finite difference Number of steps to average over Function value convergence threshold Step size convergence threshold Gradient convergence threshold 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 nonlinear search will stop if the change is below this threshold) The objective function (needs to pass in when I instantiate)

Definition at line 137 of file optimizer.py.

8.45.4.12 forcebalance.optimizer.Optimizer.OptTab

A list of all the things we can ask the optimizer to do.

Definition at line 59 of file optimizer.py.

8.45.4.13 forcebalance.optimizer.Optimizer.Penalty

Definition at line 453 of file optimizer.py.

8.45.4.14 forcebalance.optimizer.Optimizer.Val

Definition at line 450 of file optimizer.py.

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

- [optimizer.py](#)

8.46 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](#)

8.46.1 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 'rmsake' method.

Definition at line 307 of file objective.py.

8.46.2 Constructor & Destructor Documentation

8.46.2.1 `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 313 of file objective.py.

8.46.3 Member Function Documentation

8.46.3.1 `def forcebalance.objective.Penalty.compute(self, mvals, Objective)`

Definition at line 339 of file objective.py.

Here is the call graph for this function:

8.46.3.2 `def forcebalance.objective.Penalty.FUSE(self, mvals)`

Definition at line 399 of file objective.py.

Here is the call graph for this function:

8.46.3.3 `def forcebalance.objective.Penalty.FUSE_BARRIER(self, mvals)`

Definition at line 440 of file objective.py.

Here is the call graph for this function:

8.46.3.4 def forcebalance.objective.Penalty.FUSE_L0 (*self*, *mvals*)

Definition at line 482 of file objective.py.

Here is the call graph for this function:

8.46.3.5 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

| | | |
|-----------|--------------|----------------------|
| <i>in</i> | <i>mvals</i> | The parameter vector |
|-----------|--------------|----------------------|

Returns

DC0 The hyperbolic penalty
 DC1 The gradient
 DC2 The Hessian

Definition at line 391 of file objective.py.

Here is the call graph for this function:

8.46.3.6 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

| | | |
|-----------|--------------|----------------------|
| <i>in</i> | <i>mvals</i> | 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 371 of file objective.py.

Here is the call graph for this function:

8.46.4 Member Data Documentation

8.46.4.1 forcebalance.objective.Penalty.a

Definition at line 316 of file objective.py.

8.46.4.2 forcebalance.objective.Penalty.b

Definition at line 317 of file objective.py.

8.46.4.3 forcebalance.objective.Penalty.fadd

Definition at line 314 of file objective.py.

8.46.4.4 forcebalance.objective.Penalty.FF

Definition at line 318 of file objective.py.

8.46.4.5 forcebalance.objective.Penalty.fmul

Definition at line 315 of file objective.py.

8.46.4.6 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, '
3   QUADRATIC' : 2, 'FUSE' : 3, 'FUSION' : 3, 'FUSE_L0' : 4, 'FUSION_L0' : 4,
4   'FUSION-L0' : 4, 'FUSE-BARRIER' : 5, 'FUSE-BARRIER' : 5, 'FUSE_BARRIER' :
5   5, 'FUSION_BARRIER' : 5}
```

Definition at line 308 of file objective.py.

8.46.4.7 forcebalance.objective.Penalty.Pen_Tab

Definition at line 320 of file objective.py.

8.46.4.8 forcebalance.objective.Penalty.ptyp

Definition at line 319 of file objective.py.

8.46.4.9 forcebalance.objective.Penalty.spacings

Find exponential spacings.

Definition at line 336 of file objective.py.

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

- [objective.py](#)

8.47 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__](#)

8.47.1 Detailed Description

A subclass of the python Pickler that implements pickling of _ElementTree types.

Definition at line 496 of file nifty.py.

8.47.2 Constructor & Destructor Documentation

8.47.2.1 `def forcebalance.nifty.Pickler_LP.__init__(self, file, protocol=None)`

Definition at line 497 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](#)

8.48 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.

Public Attributes

- `atom`
- `snum`
- `cnum`
- `shell`
- `pdict`
- `sec`
- `itype`
- `suffix`

8.48.1 Detailed Description

Finite state machine for parsing Q-Chem input files.

Definition at line 28 of file qchemio.py.

8.48.2 Constructor & Destructor Documentation

8.48.2.1 def forcebalance.qchemio.QCIn_Reader.__init__(self, fnm)

Definition at line 30 of file qchemio.py.

8.48.3 Member Function Documentation

8.48.3.1 def forcebalance.qchemio.QCIn_Reader.feed(self, line)

Feed in a line.

Parameters

| | | |
|-----------|-------------|------------------|
| <i>in</i> | <i>line</i> | The line of data |
|-----------|-------------|------------------|

Definition at line 45 of file qchemio.py.

8.48.4 Member Data Documentation

8.48.4.1 forcebalance.qchemio.QCIn_Reader.atom

Definition at line 33 of file qchemio.py.

8.48.4.2 forcebalance.qchemio.QCIn_Reader.cnum

Definition at line 35 of file qchemio.py.

8.48.4.3 forcebalance.qchemio.QCIn_Reader.itype

Definition at line 64 of file qchemio.py.

8.48.4.4 forcebalance.qchemio.QCIn_Reader.pdict

Definition at line 37 of file qchemio.py.

8.48.4.5 forcebalance.qchemio.QCIn_Reader.sec

Definition at line 55 of file qchemio.py.

8.48.4.6 forcebalance.qchemio.QCIn_Reader.shell

Definition at line 36 of file qchemio.py.

8.48.4.7 forcebalance.qchemio.QCIn_Reader.snum

Definition at line 34 of file qchemio.py.

8.48.4.8 forcebalance.qchemio.QCIn_Reader.suffix

Definition at line 69 of file qchemio.py.

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

- [qchemio.py](#)

8.49 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](#)

8.49.1 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 27 of file output.py.

8.49.2 Member Function Documentation

8.49.2.1 def forcebalance.output.RawFileHandler.emit (*self*, *record*)

Definition at line 28 of file output.py.

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

- [output.py](#)

8.50 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](#)

8.50.1 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 14 of file output.py.

8.50.2 Constructor & Destructor Documentation

8.50.2.1 `def forcebalance.output.RawStreamHandler.__init__(self, stream = sys.stdout)`

Definition at line 15 of file output.py.

Here is the call graph for this function:

8.50.3 Member Function Documentation

8.50.3.1 `def forcebalance.output.RawStreamHandler.emit(self, record)`

Definition at line 18 of file output.py.

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

- [output.py](#)

8.51 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 driver`
- `def get`

LPW 04-17-2013.

Public Attributes

- `objfiles`

Which parameters are differentiated?

- `objvals`
- `elements`
- `molecules`
- `calldervs`
- `factor`
- `tdir`
- `objd`
- `gradd`
- `hdiagd`
- `objective`

8.51.1 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 295 of file psi4io.py.

8.51.2 Constructor & Destructor Documentation

8.51.2.1 `def forcebalance.psi4io.RDVR3_Psi4.__init__(self, options, tgt_opts, forcefield)`

Definition at line 298 of file psi4io.py.

8.51.3 Member Function Documentation

8.51.3.1 `def forcebalance.psi4io.RDVR3_Psi4.driver (self, mvals, d)`

Definition at line 346 of file psi4io.py.

Here is the call graph for this function:

8.51.3.2 `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 | <i>AHess</i> | Switch to turn on analytic Hessian |

Returns

Answer Contribution to the objective function

Definition at line 382 of file psi4io.py.

8.51.3.3 `def forcebalance.psi4io.RDVR3_Psi4.indicate (self)`

Definition at line 337 of file psi4io.py.

Here is the call graph for this function:

8.51.4 Member Data Documentation

8.51.4.1 forcebalance.psi4io.RDVR3_Psi4.callderivs

Definition at line 308 of file psi4io.py.

8.51.4.2 forcebalance.psi4io.RDVR3_Psi4.elements

Definition at line 306 of file psi4io.py.

8.51.4.3 forcebalance.psi4io.RDVR3_Psi4.factor

Definition at line 309 of file psi4io.py.

8.51.4.4 forcebalance.psi4io.RDVR3_Psi4.gradd

Definition at line 392 of file psi4io.py.

8.51.4.5 forcebalance.psi4io.RDVR3_Psi4.hdiagd

Definition at line 393 of file psi4io.py.

8.51.4.6 forcebalance.psi4io.RDVR3_Psi4.molecules

Definition at line 307 of file psi4io.py.

8.51.4.7 forcebalance.psi4io.RDVR3_Psi4.objd

Definition at line 391 of file psi4io.py.

8.51.4.8 forcebalance.psi4io.RDVR3_Psi4.objective

Definition at line 454 of file psi4io.py.

8.51.4.9 forcebalance.psi4io.RDVR3_Psi4.objfiles

Which parameters are differentiated?

Definition at line 304 of file psi4io.py.

8.51.4.10 forcebalance.psi4io.RDVR3_Psi4.objvals

Definition at line 305 of file psi4io.py.

8.51.4.11 forcebalance.psi4io.RDVR3_Psi4.tdir

Definition at line 390 of file psi4io.py.

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

- [psi4io.py](#)

8.52 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 `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 `sget`
Stages the directory for the target, and then calls 'get'.
- 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.

Public Attributes

- `tempdir`
Root directory of the whole project.
- `rundir`
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.

8.52.1 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': `numpy.array(np)`, 'H': `numpy.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 72 of file `target.py`.

8.52.2 Constructor & Destructor Documentation

8.52.2.1 `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 `AbInitio` that inherits from [Target](#).

Definition at line 89 of file `target.py`.

Here is the call graph for this function:

8.52.3 Member Function Documentation

8.52.3.1 `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 251 of file target.py.

Here is the call graph for this function:

8.52.3.2 `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.

Definition at line 169 of file target.py.

Here is the call graph for this function:

8.52.3.3 `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 192 of file target.py.

Here is the call graph for this function:

8.52.3.4 `def forcebalance.target.Target.get_X (self, mvals=None)`

Computes the objective function contribution without any parametric derivatives.

Definition at line 152 of file target.py.

Here is the call graph for this function:

8.52.3.5 `def forcebalance.target.Target.link_from_tempdir (self, absdestdir)`

Definition at line 210 of file target.py.

8.52.3.6 `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 364 of file target.py.

Here is the call graph for this function:

8.52.3.7 `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 216 of file target.py.

Here is the call graph for this function:

8.52.3.8 `def forcebalance.target.Target.sget (self, mvals, AGrad=False, AHess=False, customdir=None)`

Stages the directory for the target, and then calls 'get'.

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

Definition at line 263 of file target.py.

Here is the call graph for this function:

8.52.3.9 `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 298 of file target.py.

Here is the call graph for this function:

8.52.3.10 `def forcebalance.target.Target.submit_jobs (self, mvals, AGrad=False, AHess=False)`

Definition at line 288 of file target.py.

8.52.3.11 `def forcebalance.target.Target.wq_complete (self)`

This method determines whether the Work Queue tasks for the current target have completed.

Definition at line 328 of file target.py.

Here is the call graph for this function:

8.52.4 Member Data Documentation

8.52.4.1 forcebalance.target.Target.FF

Need the forcefield (here for now)

Definition at line 136 of file target.py.

8.52.4.2 forcebalance.target.Target.gct

Counts how often the gradient was computed.

Definition at line 140 of file target.py.

8.52.4.3 forcebalance.target.Target.hct

Counts how often the Hessian was computed.

Definition at line 142 of file target.py.

8.52.4.4 forcebalance.target.Target.rundir

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.

Definition at line 134 of file target.py.

8.52.4.5 forcebalance.target.Target.tempdir

Root directory of the whole project.

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 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 132 of file target.py.

8.52.4.6 forcebalance.target.Target.xct

Counts how often the objective function was computed.

Definition at line 138 of file target.py.

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

- [target.py](#)

8.53 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](#)

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](#)

8.53.1 Detailed Description

Definition at line 94 of file psi4io.py.

8.53.2 Constructor & Destructor Documentation

8.53.2.1 `def forcebalance.psi4io.THCDF_Psi4.__init__(self, options, tgt_opts, forcefield)`

Definition at line 96 of file psi4io.py.

8.53.3 Member Function Documentation

8.53.3.1 `def forcebalance.psi4io.THCDF_Psi4.driver (self)`

Definition at line 171 of file psi4io.py.

Here is the call graph for this function:

8.53.3.2 `def forcebalance.psi4io.THCDF_Psi4.indicate (self)`

Definition at line 149 of file psi4io.py.

Here is the call graph for this function:

8.53.3.3 `def forcebalance.psi4io.THCDF_Psi4.prepare_temp_directory (self, options, tgt_opts)`

Definition at line 138 of file psi4io.py.

Here is the call graph for this function:

8.53.3.4 `def forcebalance.psi4io.THCDF_Psi4.write_nested_destroy (self, fnm, linedestroy)`

Definition at line 156 of file psi4io.py.

Here is the call graph for this function:

8.53.4 Member Data Documentation

8.53.4.1 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 134 of file psi4io.py.

8.53.4.2 forcebalance.psi4io.THCDF_Psi4.DF_Energy

Definition at line 237 of file psi4io.py.

8.53.4.3 forcebalance.psi4io.THCDF_Psi4.Elements

Definition at line 114 of file psi4io.py.

8.53.4.4 forcebalance.psi4io.THCDF_Psi4.GBSfnm

Psi4 basis set file.

Definition at line 127 of file psi4io.py.

8.53.4.5 forcebalance.psi4io.THCDF_Psi4.Molecules

Definition at line 102 of file psi4io.py.

8.53.4.6 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 235 of file psi4io.py.

8.53.4.7 forcebalance.psi4io.THCDF_Psi4.throw_outs

Definition at line 103 of file psi4io.py.

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

- [psi4io.py](#)

8.54 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).

Public Attributes

- [pdict](#)
The parameter dictionary (defined in this file)
- [atom](#)
The atom numbers in the interaction (stored in the TINKER parser)
- [itype](#)
- [suffix](#)

8.54.1 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 65 of file `tinkerio.py`.

8.54.2 Constructor & Destructor Documentation

8.54.2.1 `def forcebalance.tinkerio.Tinker_Reader.__init__(self, fnm)`

Definition at line 67 of file `tinkerio.py`.

8.54.3 Member Function Documentation

8.54.3.1 `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 # PARM 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 '#PARM 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 108 of file `tinkerio.py`.

8.54.4 Member Data Documentation

8.54.4.1 forcebalance.tinkerio.Tinker_Reader.atom

The atom numbers in the interaction (stored in the TINKER parser)

Definition at line 72 of file tinkerio.py.

8.54.4.2 forcebalance.tinkerio.Tinker_Reader.itype

Definition at line 116 of file tinkerio.py.

8.54.4.3 forcebalance.tinkerio.Tinker_Reader.pdict

The parameter dictionary (defined in this file)

Definition at line 70 of file tinkerio.py.

8.54.4.4 forcebalance.tinkerio.Tinker_Reader.suffix

Definition at line 138 of file tinkerio.py.

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

- [tinkerio.py](#)

8.55 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__](#)

8.55.1 Detailed Description

A subclass of the python Unpickler that implements unpickling of _ElementTree types.

Definition at line 520 of file nifty.py.

8.55.2 Constructor & Destructor Documentation

8.55.2.1 def forcebalance.nifty.Unpickler_LP.__init__(self, file)

Definition at line 521 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](#)

8.56 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 [prepare_temp_directory](#)
Prepare the temporary directory, by default does nothing.
- def [indicate](#)
Print qualitative indicator.
- def [get](#)
Evaluate objective function.

Public Attributes

- [vfnm](#)
The vdata.txt file that contains the vibrations.
- [na](#)
Number of atoms.
- [ref_eigvals](#)
- [ref_eigvecs](#)
- [calc_eigvals](#)
- [objective](#)

8.56.1 Detailed Description

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

Currently Tinker is supported.

Definition at line 27 of file vibration.py.

8.56.2 Constructor & Destructor Documentation

8.56.2.1 def forcebalance.vibration.Vibration.__init__(self, options, tgt_opts, forcefield)

Initialization.

Definition at line 32 of file vibration.py.

Here is the call graph for this function:

8.56.3 Member Function Documentation

8.56.3.1 `def forcebalance.vibration.Vibration.get (self, mvals, AGrad=False, AHess=False)`

Evaluate objective function.

Definition at line 108 of file vibration.py.

Here is the call graph for this function:

8.56.3.2 `def forcebalance.vibration.Vibration.indicate (self)`

Print qualitative indicator.

Definition at line 99 of file vibration.py.

Here is the call graph for this function:

8.56.3.3 `def forcebalance.vibration.Vibration.prepare_temp_directory (self, options, tgt_opts)`

Prepare the temporary directory, by default does nothing.

Definition at line 94 of file vibration.py.

8.56.3.4 `def forcebalance.vibration.Vibration.read_reference_data (self)`

Read the reference vibrational data from a file.

Definition at line 54 of file vibration.py.

8.56.4 Member Data Documentation

8.56.4.1 `forcebalance.vibration.Vibration.calc_eigvals`

Definition at line 137 of file vibration.py.

8.56.4.2 `forcebalance.vibration.Vibration.na`

Number of atoms.

Definition at line 56 of file vibration.py.

8.56.4.3 `forcebalance.vibration.Vibration.objective`

Definition at line 138 of file vibration.py.

8.56.4.4 `forcebalance.vibration.Vibration.ref_eigvals`

Definition at line 57 of file vibration.py.

8.56.4.5 `forcebalance.vibration.Vibration.ref_eigvecs`

Definition at line 58 of file vibration.py.

8.56.4.6 `forcebalance.vibration.Vibration.vfnm`

The vdata.txt file that contains the vibrations.

Definition at line 46 of file vibration.py.

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

- [vibration.py](#)

8.57 forcebalance.tinkerio.Vibration_TINKER Class Reference

Subclass of Target for 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 prepare_temp_directory](#)
- [def vibration_driver](#)

8.57.1 Detailed Description

Subclass of Target for vibrational frequency matching using TINKER.

Provides optimized geometry, vibrational frequencies (in cm-1), and eigenvectors.

Definition at line 352 of file tinkerio.py.

8.57.2 Constructor & Destructor Documentation

8.57.2.1 `def forcebalance.tinkerio.Vibration_TINKER.__init__(self, options, tgt_opts, forcefield)`

Definition at line 355 of file tinkerio.py.

Here is the call graph for this function:

8.57.3 Member Function Documentation

8.57.3.1 `def forcebalance.tinkerio.Vibration_TINKER.prepare_temp_directory(self, options, tgt_opts)`

Definition at line 360 of file tinkerio.py.

Here is the call graph for this function:

8.57.3.2 `def forcebalance.tinkerio.Vibration_TINKER.vibration_driver(self)`

Definition at line 370 of file tinkerio.py.

Here is the call graph for this function:

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

- [tinkerio.py](#)

9 File Documentation

9.1 `__init__.py` File Reference

Namespaces

- namespace `forcebalance`

Variables

- `forcebalance.WORK_QUEUE` None
- tuple `forcebalance.WQIDS` `defaultdict(list)`

9.2 `abinitio.py` File Reference

Classes

- class `forcebalance.abinitio.AbInitio`
Subclass of Target for fitting force fields to ab initio data.

Namespaces

- namespace `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.

9.3 `abinitio_gmxx2.py` File Reference

Classes

- class `forcebalance.abinitio_gmxx2.AbInitio_GMXX2`
ForceBalance class for force and energy matching with the modified GROMACS.

Namespaces

- namespace `forcebalance.abinitio_gmxx2`
- namespace `abinitio_gmxx2`
Force and energy matching with interface to modified GROMACS.

9.4 abinitio_internal.py File Reference

Classes

- class [forcebalance.abinitio_internal.AbInitio_Internal](#)
Subclass of Target for force and energy matching using an internal implementation.

Namespaces

- namespace [forcebalance.abinitio_internal](#)
Internal implementation of energy matching (for TIP3P water only)

9.5 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.AbInitio_AMBER](#)
Subclass of Target for force and energy matching using AMBER.

Namespaces

- namespace [forcebalance.amberio](#)
AMBER force field input/output.

Functions

- def [forcebalance.amberio.is_mol2_atom](#)

Variables

- dictionary [forcebalance.amberio.mol2_pdict](#) {'COUL': {'Atom': [1], 8: ''}}
- dictionary [forcebalance.amberio.frcmod_pdict](#)

9.6 api.dox File Reference

9.7 baseclass.py File Reference

Classes

- class [forcebalance.baseclass.ForceBalanceBaseClass](#)
Provides some nifty functions that are common to all ForceBalance classes.

Namespaces

- namespace [forcebalance.baseclass](#)

9.8 basereader.py File Reference

Classes

- class [forcebalance.basereader.BaseReader](#)
The 'reader' class.

Namespaces

- namespace [forcebalance.basereader](#)
Base class for force field line reader.

9.9 binding.py File Reference

Classes

- class [forcebalance.binding.BindingEnergy](#)
Improved subclass of Target for fitting force fields to binding energies.

Namespaces

- namespace [forcebalance.binding](#)
Binding energy fitting module.

Functions

- def [forcebalance.binding.parse_interactions](#)
Parse through the interactions input file.

9.10 chemistry.py File Reference

Namespaces

- namespace [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.
- dictionary `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])`

9.11 `contact.py` File Reference

Namespaces

- namespace `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.

9.12 `counterpoise.py` File Reference

Classes

- class `forcebalance.counterpoise.Counterpoise`
Target subclass for matching the counterpoise correction.

Namespaces

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

9.13 `custom_io.py` File Reference

Classes

- class `forcebalance.custom_io.Gen_Reader`
Finite state machine for parsing custom GROMACS force field files.

Namespaces

- namespace [forcebalance.custom_io](#)
Custom force field parser.

Variables

- list [forcebalance.custom_io.cptypes](#) [None, 'CPGAUSS', 'CPEXP', '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.

9.14 finite_difference.py File Reference

Namespaces

- namespace [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.in_fd](#)
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.

9.15 fitsim.py File Reference

Classes

- class [forcebalance.fitsim.FittingSimulation](#)
Base class for all fitting simulations.

Namespaces

- namespace [forcebalance.fitsim](#)

9.16 forcefield.py File Reference

Classes

- class [forcebalance.forcefield.BackedUpDict](#)
- class [forcebalance.forcefield.FF](#)
Force field class.

Namespaces

- namespace [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

- dictionary [forcebalance.forcefield.FF_Extensions](#)
- dictionary [forcebalance.forcefield.FF_IOModules](#)

9.17 gmxml.py File Reference

Classes

- class [forcebalance.gmxml.OTP_Reader](#)
Finite state machine for parsing GROMACS force field files.
- class [forcebalance.gmxml.AbInitio_GMX](#)
Subclass of AbInitio for force and energy matching using normal GROMACS.
- class [forcebalance.gmxml.Liquid_GMX](#)
- class [forcebalance.gmxml.Interaction_GMX](#)
Subclass of Interaction for interaction energy matching using GROMACS.

Namespaces

- namespace [forcebalance.gmxio](#)
GROMACS input/output.

Functions

- def [forcebalance.gmxio.edit_mdp](#)
Create or edit a Gromacs MDP file.
- def [forcebalance.gmxio.parse_atomtype_line](#)
Parses the 'atomtype' line.
- def [forcebalance.gmxio.rm_gmx_baks](#)

Variables

- 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.

9.18 gmxqpio.py File Reference

Classes

- class [forcebalance.gmxqpio.Monomer_QTPIE](#)
Subclass of Target for monomer properties of QTPIE (implemented within gromacs WCV branch).

Namespaces

- namespace [forcebalance.gmxqpio](#)
- namespace [forcebalance.gmxio](#)
GROMACS input/output.

Functions

- def [forcebalance.gmxqpio.get_monomer_properties](#)

9.19 implemented.py File Reference

Namespaces

- namespace [forcebalance.implemented](#)
Contains the dictionary of usable Target classes.

Variables

- dictionary [forcebalance.implemented.Implemented_Targets](#)
The table of implemented Targets.

9.20 interaction.py File Reference

Classes

- class [forcebalance.interaction.Interaction](#)
Subclass of Target for fitting force fields to interaction energies.

Namespaces

- namespace [forcebalance.interaction](#)
Interaction energy fitting module.

9.21 interactions.py File Reference

Classes

- class [forcebalance.interactions.Interactions](#)
Improved subclass of Target for fitting force fields to interaction energies.

Namespaces

- namespace [forcebalance.interactions](#)
- namespace [interaction](#)
Interaction energy fitting module.

Functions

- def [forcebalance.interactions.parse_interactions](#)
Parse through the interactions input file.

9.22 leastsq.py File Reference

Classes

- class [forcebalance.leastsq.LeastSquares](#)
Subclass of Target for general least squares fitting.

Namespaces

- namespace [forcebalance.leastsq](#)
- namespace [forcebalance.abinitio](#)
Ab-initio fitting module (energies, forces, resp).

Functions

- def [forcebalance.leastsq.CheckBasis](#)
- def [forcebalance.leastsq.LastMvals](#)

Variables

- [forcebalance.leastsq.CHECK_BASIS](#) False
- [forcebalance.leastsq.LAST_MVALS](#) None

9.23 liquid.py File Reference

Classes

- class [forcebalance.liquid.Liquid](#)
Subclass of Target for liquid property matching.

Namespaces

- namespace [forcebalance.liquid](#)
Matching of liquid bulk properties.

Functions

- def [forcebalance.liquid.weight_info](#)

9.24 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

- namespace [forcebalance.Mol2](#)

Variables

- tuple `forcebalance.Mol2.data` `mol2_set(sys.argv[1], subset=["RNAse.xray.inh8.1QHC"])`

9.25 mol2io.py File Reference

Classes

- class `forcebalance.mol2io.Mol2_Reader`
Finite state machine for parsing Mol2 force field file.

Namespaces

- namespace `forcebalance.mol2io`
Mol2 I/O.

Variables

- dictionary `forcebalance.mol2io.mol2_pdict` `{'COUL':{'Atom':[1], 6:''}}`

9.26 molecule.py File Reference

Classes

- 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

- namespace `forcebalance.molecule`

Functions

- def `forcebalance.molecule.getElement`
- 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.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.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', '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
- `forcebalance.molecule.Alive`

9.27 moments.py File Reference

Classes

- class `forcebalance.moments.Moments`
Subclass of Target for fitting force fields to multipole moments (from experiment or theory).

Namespaces

- namespace `forcebalance.moments`
Multipole moment fitting module.

9.28 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.

Namespaces

- namespace `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.pmat2d`
Printout of a 2-D matrix.
- def `forcebalance.nifty.encode`
- def `forcebalance.nifty.segments`
- def `forcebalance.nifty.commadash`
- def `forcebalance.nifty.uncommadash`
- def `forcebalance.nifty.printcool`
Cool-looking printout for slick formatting of output.
- def `forcebalance.nifty.printcool_dictionary`
See documentation for printcool; this is a nice way to print out keys/values in a dictionary.
- def `forcebalance.nifty.isint`

- 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.floatornan`

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.orthogonalize`

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

Invert a matrix using singular value decomposition.
- def `forcebalance.nifty.get_least_squares`
- def `forcebalance.nifty.statisticalinefficiency`

Compute the (cross) statistical inefficiency of (two) timeseries.
- def `forcebalance.nifty.lp_dump`

Use this instead of `pickle.dump` for pickling anything that contains `_ElementTree` types.
- def `forcebalance.nifty.lp_load`

Use this instead of `pickle.load` for unpickling anything that contains `_ElementTree` types.
- def `forcebalance.nifty.getWorkQueue`
- def `forcebalance.nifty.getWQIds`
- def `forcebalance.nifty.createWorkQueue`
- def `forcebalance.nifty.queue_up`

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.GoInto`
- def `forcebalance.nifty.allsplit`
- def `forcebalance.nifty.Leave`
- def `forcebalance.nifty.MissingFileInspection`
- 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().
- def [forcebalance.nifty.multiopen](#)
This function be given any of several variable types (single file name, file object, or list of lines, or a list of the above) and give a list of files:

Variables

- 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.
- 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))))

9.29 objective.py File Reference

Classes

- class [forcebalance.objective.Objective](#)
Objective function.
- class [forcebalance.objective.Penalty](#)
Penalty functions for regularizing the force field optimizer.

Namespaces

- namespace [forcebalance.objective](#)
ForceBalance objective function.

Variables

- 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.

9.30 openmmio.py File Reference

Classes

- class [forcebalance.openmmio.OpenMM_Reader](#)
Class for parsing OpenMM force field files.
- class [forcebalance.openmmio.Liquid_OpenMM](#)
- class [forcebalance.openmmio.Ablinitio_OpenMM](#)
Subclass of Ablinitio for force and energy matching using OpenMM.
- class [forcebalance.openmmio.Interaction_OpenMM](#)
Subclass of Target for interaction matching using OpenMM.

Namespaces

- namespace [forcebalance.openmmio](#)
OpenMM input/output.

Functions

- def [forcebalance.openmmio.get_dipole](#)
Return the current dipole moment in Debye.
- 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.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.MTSVVVRIntegrator](#)
Create a multiple timestep velocity verlet with velocity randomization (VVVR) integrator.

Variables

- dictionary [forcebalance.openmmio.suffix_dict](#)
- string [forcebalance.openmmio.pdict](#) "XML_Override"
pdict is a useless variable if the force field is XML.

9.31 optimizer.py File Reference

Classes

- class [forcebalance.optimizer.Optimizer](#)
Optimizer class.

Namespaces

- namespace [forcebalance.optimizer](#)
Optimization algorithms.

Functions

- def [forcebalance.optimizer.Counter](#)
- def [forcebalance.optimizer.GoodStep](#)

Variables

- int [forcebalance.optimizer.ITERATION_NUMBER](#) 0
- int [forcebalance.optimizer.GOODSTEP](#) 0

9.32 output.py File Reference

Classes

- 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.CleanFileHandler](#)
File handler that does not write terminal escape codes to files.

Namespaces

- namespace [forcebalance.output](#)

Variables

- tuple [forcebalance.output.logger](#) getLogger('forcebalance')

9.33 parser.py File Reference

Namespaces

- namespace [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

- dictionary [forcebalance.parser.gen_opts_types](#)
Default general options.
- dictionary [forcebalance.parser.tgt_opts_types](#)
Default fitting target options.
- dictionary [forcebalance.parser.gen_opts_defaults](#) {}
Default general options - basically a collapsed veresion 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](#) {"simtype" : "type"}
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.

9.34 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

- namespace [forcebalance.psi4io](#)
PSI4 force field input/output.

9.35 PT.py File Reference

Namespaces

- namespace [forcebalance.PT](#)

Variables

- dictionary [forcebalance.PT.PeriodicTable](#)
- list [forcebalance.PT.Elements](#)

9.36 qchemio.py File Reference

Classes

- class [forcebalance.qchemio.QCIn_Reader](#)
Finite state machine for parsing Q-Chem input files.

Namespaces

- namespace [forcebalance.qchemio](#)
Q-Chem input file parser.

Functions

- def [forcebalance.qchemio.QChem_Dielectric_Energy](#)

Variables

- 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.

9.37 simtab.py File Reference

Namespaces

- namespace [forcebalance.simtab](#)
- namespace [simtab](#)
Contains the dictionary of fitting simulation classes.

Variables

- dictionary [forcebalance.simtab.SimTab](#)
The table of fitting simulations.

9.38 target.py File Reference

Classes

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

Namespaces

- namespace [forcebalance.target](#)

9.39 tinkerio.py File Reference

Classes

- class [forcebalance.tinkerio.Tinker_Reader](#)
Finite state machine for parsing TINKER force field files.
- class [forcebalance.tinkerio.Liquid_TINKER](#)
- class [forcebalance.tinkerio.AbInitio_TINKER](#)
Subclass of Target for force and energy matching using TINKER.
- class [forcebalance.tinkerio.Vibration_TINKER](#)
Subclass of Target for vibrational frequency matching using TINKER.
- class [forcebalance.tinkerio.Moments_TINKER](#)
Subclass of Target for multipole moment matching using TINKER.
- class [forcebalance.tinkerio.BindingEnergy_TINKER](#)
Subclass of BindingEnergy for binding energy matching using TINKER.
- class [forcebalance.tinkerio.Interaction_TINKER](#)
Subclass of Target for interaction matching using TINKER.

Namespaces

- namespace [forcebalance.tinkerio](#)
TINKER input/output.

Functions

- def [forcebalance.tinkerio.write_key_with_prm](#)
Copies a TINKER .key file but changes the parameter keyword as necessary to reflect the ForceBalance settings.
- def [forcebalance.tinkerio.modify_key](#)
Performs in-place modification of a TINKER .key file.

Variables

- dictionary [forcebalance.tinkerio.pdict](#)

9.40 vibration.py File Reference

Classes

- class [forcebalance.vibration.Vibration](#)
Subclass of Target for fitting force fields to vibrational spectra (from experiment or theory).

Namespaces

- namespace [forcebalance.vibration](#)
Vibrational mode fitting module.

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