

# OpenAtom Manual:

Modern Simulation Methods Applied to Chemistry, Physics and Biology

# Introduction

There are five types of files from which the OpenAtom script-language interface reads commands, the simulation setup file, the system setup file, molecular parameter/topology files, the potential energy/pseudopotential parameter files and the parallel decomposition parameter file. Coordinate and electronic state input files do not contain commands but simply free format data.

In the simulation setup files, commands that drive a given simulation are stated. For example, run 300 time steps of Car-Parrinello *ab initio* molecular dynamics. In the system setup file, the system is described. For example, 300 water molecules, two peptides, three counter ions, thirty Kohn-Sham states etc. Topology files contain information about the molecular connectivity and potential energy/pseudopotential files contain information about the interactions. The parallel decomposition input file contains all the information about the parallel decomposition.

The idea behind the file division is that one often modifies the simulation commands, occasionally the system setup commands but seldom the topology, potential energy, pseudopotential or parallel decomposition information. The five file types help organization and transferability. For example, many simulation command files can drive the same system setup file, molecular parameter/topology files, potential energy/pseudopotential parameter and parallel decomposition files.

There are three levels of grouping for the OpenAtom commands, meta-keywords, keywords and key-arguments. The first level, the meta-keywords, sort keywords into naturally connected groups. The second level, the keywords, are specific commands to the computer program. The third level, key-arguments, are the arguments to the keywords. The syntax looks like:

~meta\_keyword1[ \keyword1{keyarg1} \keyword2{keyarg2} ].

~meta\_keyword2[ \keyword1{keyarg1} \keyword2{keyarg2} ].

The commands are case insensitive and can be specified in any order.

The present release of the code concentrates on the fine grained parallel Car-Parrinello molecular dynamics (CPA-IMD) computations and scaling results are given in IBM J. Res. Dev. **52** (2007). However, all the bio-widget input parameters are supported and biomolecules can be built. Some of the biomolecular functionality is not yet implemented in the source. The QM/MM extension is a work in progress.

In order to run the code type:

**OpenAtomMachine.x paraInfo.in simInput.in**

where machine is the machine-type, simInput.in is the simulation input file and paraInfo.in is the parallel decomposition input file. All file names are arbitrary.

**Warning:** The code will warn the user and stop the run if it isn't happy with the input. The designers felt that **not** running a simulation was better than taking potentially inappropriate input and forging ahead. Also, the code doesn't like to overwrite files because the designers have overwritten one too many useful files themselves and thought,

A file that big?!  
It might be very useful,  
But now it is gone.

Finally, many of the error messages are sometimes written in colloquial American English, a product of too many late nights writing code. A language option has not yet been implemented. The advisor may have to explain what "Dude" means. However, the code does have a lot of error checking because there is nothing worse than

Wind catches lily,  
Scatt'ring petals to the wind:  
Segmentation fault.

which leads one to believe

Errors have occurred.  
I can't tell where or why.  
Lazy programmers.

This manual was, of course, also a late night accomplishment.

# Simulation Keyword Dictionary:

The following commands maybe specified in the simulation setup file:

1. **~sim\_gen\_def** [ 16 keywords]
2. **~sim\_run\_def** [ 16 keywords]
3. **~sim\_nhc\_def** [ 28 keywords]
4. **~sim\_write\_def**[ 27 keywords]
5. **~sim\_list\_def** [ 14 keywords]
6. **~sim\_class\_PE\_def** [ 25 keywords]
7. **~sim\_vol\_def** [ 4 keywords]
8. **~sim\_cp\_def** [ 29 keywords]
9. **~sim\_pimd\_def** [ 10 keywords]

A complete list of all commands employed including default values are placed in the file: `~sim_write_def[ \sim_name_def{sim_input.out} ]`.

## ~sim\_gen\_def[ 16 keywords]

1. `\simulation_typ{md,minimize,debug ...}` :  
Perform a molecular dynamics, minimization, pimd, cp cp\_pimd, cp\_wave, cp\_wave\_pimd, cp\_min, cp\_wave\_min, cp\_wave\_min\_pimd, debug, debug\_cp\_pimd, debug\_cp, debug\_pimd. Here CP indicates Car-Parrinello and PIMD denotes path integral molecular dynamics.
2. `\ensemble_typ{nve,nvt,npt_i,npt_f}` :  
Use the statistical ensemble specified in the curly brackets.
3. `\minimize_typ{min_std,min_cg,min_diis}` :  
Perform a minimization run using the method specified in curly brackets:
  - *min\_std* – Steepest descent.
  - *min\_cg* – Conjugate gradient.
  - *min\_diis* – Direct inversion in the iterative subspace.
4. `\restart_type{initial,restart_pos,restart_posvel,restart_all}` :  
Option controlling how the coordinate input file is read in:
  - *initial* – Start using *initial* format with atomic positions in angstroms.
  - *restart\_pos* – Restart only the atomic positions. Velocities and thermostat velocities (if used) are sampled from a Maxwell distribution.
  - *restart\_posvel* – Restart both atomic position and atomic velocities. Thermostat velocities (if used) are sampled from a Maxwell distribution.
  - *restart\_all* – Restart atomic positions, velocities, and thermostat velocities (if used).
5. `\num_time_step{0}` :  
Total number of time steps for this run.
6. `\time_step{1}` :  
Fundamental or smallest time step. If no multiple time step integration is used, then this is *the* time step.
7. `\temperature{300}` :  
Atomic temperature. This is the temperature used for velocity rescaling, velocity resampling, thermostatting, etc.

8. `\pressure{0}` :

Pressure of system. Only used for simulations in the NPT ensembles.

## ~sim\_run\_def[ 16 keywords]

1. `\init_resmp_atm_vel{on,off}` :  
If turned on, atomic velocities are initially sampled/resampled from a Maxwell distribution.
2. `\resmpl_frq_atm_vel{0}` :  
Atomic velocities are resampled with a frequency equal to the number in the curly brackets. A zero indicates no resampling is to be done.
3. `\init_rescale_atm_vel{on,off}` :  
If turned on, atomic velocities are initially rescaled to preset temperature.
4. `\rescale_frq_atm_vel{0}` :  
Atomic velocities are rescaled to desired temperature with a frequency equal to the number in the curly brackets. A zero indicates no resampling is to be done.
5. `\init_rescale_atm_nhc{on,off}` :  
If turned on, atomic thermostat velocities are initially rescaled to preset temperature.
6. `\zero_com_vel{yes,no}` :  
If set to yes, the center of mass velocity is initially set to 0.
7. `\respa_steps_lrf{0}` :  
Number of short time steps to be taken between long range force updates. A zero indicates long range forces are updated every step.
8. `\respa_rheal{1}` :  
If `\respa_steps_lrf` is not zero, then the long range and short range forces are both switched off in space with a switching function of healing length given in the curly brackets.
9. `\respa_steps_torsion{0}` :  
Number of short time steps to be taken between updates of torsional forces. A zero indicates torsional forces are updated every step.

10. `\respa_steps_intra{0}` :  
Number of short time steps to be taken between updates of *intermolecular* forces. A zero indicates intermolecular forces are updated every step.
11. `\shake_tol{1.0e-6}` :  
Constraints not treated by the group constraint method are iterated to a tolerance given in curly brackets.
12. `\rattle_tol{1.0e-6}` :  
Time derivative of constraints not treated by the group constraint method are iterated to a tolerance given in curly brackets.
13. `\max_constrnt_iter{200}` :  
Maximum number of iterations to be performed on constraints before a warning that the tolerance has not yet been reached is printed out and iteration stops.
14. `\group_con_tol{1.0e-6}` :  
Group constraint method is iterated to a tolerance given in curly brackets.



## `\sim_nhc_def` [ 28 keywords ]

1. `\atm_nhc_tau_def{1000}` :  
Time scale (in femtoseconds) on which the thermostats should evolve. Generally set to some characteristic time scale in the system.
2. `\init_resmp_atm_nhc{on,off}` :  
If turned on, atomic thermostat velocities will be initially resampled from a Maxwell distribution.
3. `\atm_nhc_len{2}` :  
Number of elements in the thermostat chain. Generally 2-4 is adequate.
4. `\respa_steps_nhc{2}` :  
Number of individual Suzuki/Yoshida factorizations to be employed in integration of the thermostat variables. Only increase if energy conservation not satisfactory with default value.
5. `\yosh_steps_nhc{1,3,5,7}` :  
Order of the Suzuki/Yoshida integration scheme for the thermostat variables. Only increase if energy conservation not satisfactory with default value.
6. `\resmpl_atm_nhc{0}` :  
Atomic thermostat velocities will be resampled with a frequency specified in the curly brackets. A zero indicates no resampling of thermostat velocities.
7. `\respa_xi_opt{1,2,3,4}` :  
Depth of penetration of thermostat integration into multiple time step levels. Larger numbers indicate deeper penetration. A one indicates thermostat variables are updated at the beginning and end of every step (XO option).
8. `\atm_isokin_opt{on:on/off}` :  
Thermostat the atoms using isokinetic NHC (on) or plain NHC (off).
9. `\cp_thermstats{on:on/off}` :  
Thermostat the electrons (on) or run them without control (off). If “on”,

at least one isokinetic octopus NHC thermostat is placed on each g-space plane of each state.

10. `\cp_num_nhc_iso{2}`:

The number of tentacles in an isokinetic octopus NHC thermostat.

11. `\cp_nhc_chunk{1}`:

The number of thermostats per g-space electronic state plane.

## `\sim_write_def` [ 27 keywords ]

1. `\sim_name{sim_input.out}` :  
A complete list of all commands specified and defaults used.
2. `\write_screen_freq{1}` :  
Output information to screen will be written with a frequency specified in curly brackets.
3. `\write_dump_freq{1}` :  
The restart file of atomic coordinates and velocities, etc. will be written with a frequency specified in curly brackets.
4. `\write_inst_freq{1}` :  
Instantaneous averages of energy, temperature, pressure, etc. will be written to the instantaneous file with a frequency specified in curly brackets.
5. `\write_pos_freq{100}` :  
Atomic positions will be appended to the trajectory position file with a frequency specified in curly brackets.
6. `\write_vel_freq{100}` :  
Atomic velocities will be appended to the trajectory velocity file with a frequency specified in curly brackets.
7. `\sim_name{sim_input.out}` :  
Name of file containing all keywords, both user set a default.
8. `\out_restart_file{sim_restart.out}` :  
Name of the restart (dump) file containing final atomic coordinates and velocities.
9. `\in_restart_file{sim_restart.in}` :  
Name of the file containing initial atomic coordinates and velocities for this run.
10. `\instant_file{sim_instant.out}` :  
File to which instantaneous averages are to be written.

11. `\atm_pos_file{sim_atm_pos.out}` :  
Trajectory position file name.
12. `\atm_vel_file{sim_atm_vel.out}` :  
Trajectory force file name.
13. `\atm_force_file{sim_atm_force.out}` :  
Trajectory velocity file name.
14. `\conf_partial_file{sim_atm_pos_part.out}` :  
Partial trajectory position file name.
15. `\mol_set_file{sim_atm_mol_set.in}` :  
Name of file containing instructions on how to name and build molecules.  
Detailed instructions on contents of this file given elsewhere.
16. `\write_force_freq{1000000}` :  
Atomic forces are written to the trajectory force file with a frequency specified in the curly brackets.
17. `\screen_output_units{au,kcal_mol,kelvin}` :  
Output information is written to the screen in units specified in curly brackets.
18. `\conf_file_format{binary,formatted}` :  
Trajectory files are written either in binary or formatted form.
19. `\conf_partial_limits{1,0}` :  
Two numbers specifying the first and last atoms to be written to the partial trajectory position file.

## ~sim\_list\_def[ 14 keywords]

1. `\neighbor_list{no_list,ver_list,lnk_list}` :  
Type of neighbor list to use. Optimal scheme for most systems: `\ver_list` with a `\lnk_lst` update type.
2. `\update_type{lnk_lst,no_list}` :  
Update the verlet list using either no list or a link list.
3. `\verlist_skin{1}` :  
Skin depth added to verlet list cutoff. Needs to be optimized between extra neighbors added and average required update frequency.
4. `\lnk_cell_divs{7}` :  
Number of link cell divisions in each dimension. Needs to be optimized if used either as list type or update type.

## ~sim\_class\_PE\_def[ 25 keywords]

1. `\ewald_kmax{7}` :  
Maximum length of k-vectors used in evaluating Ewald summation for electrostatic interactions.
2. `\ewald_alpha{7}` :  
Size of real-space damping (screening) parameter in Ewald sum.
3. `\ewald_respa_kmax{0}` :  
Maximum length of k-vectors used in long range force RESPA integration.
4. `\ewald_pme_opt{on,off}` :  
If turned on, then electrostatic interactions are evaluated using the smooth particle mesh method. Its use is recommended.
5. `\ewald_kmax_pme{7}` :  
Maximum length of k-vectors used in evaluating Ewald summation for electrostatic interactions via the smooth particle mesh method.
6. `\ewald_interp_pme{4}` :  
Order of mesh interpolation in the smooth particle mesh Ewald method.
7. `\ewald_respa_pme_opt{on,off}` :  
If turned on, then long range force RESPA is used in conjunction with the smooth particle mesh method.
8. `\ewald_respa_interp_pme{4}` :  
Order of mesh interpolation in the smooth particle mesh Ewald method used with RESPA.
9. `\sep_VanderWaals{on,off}` :  
If turned on, then the VanderWaals component of the *intermolecular* interaction energy is printed separately to screen.
10. `\inter_spline_pts{2000}` :  
Number of spline points used *intermolecular* interaction potential and derivative.

## ~sim\_vol\_def[ 4 keywords]

1. `\volume_tau{1000}` :  
Time scale of volume evolution under constant pressure (NPT\_I or NPT\_F)  
in femtoseconds.
2. `\volume_nhc_tau{1000}` :  
Time scale of volume heat bath evolution under constant pressure in  
femtoseconds.

## ~sim\_cp\_def[ 29 keywords]

1. `\cp_e_e_interact{on,off}` :  
Electron-electron interactions can be turned off for 1e problems.
2. `\cp_dft_typ{lda,lsda,gga_lda,gga_lsda}` :  
Density function type where gga mean gradient corrections are on.
3. `\cp_vxc_typ{pz_lda,pw_lda,pz_lsda}` :  
Exchange correlation function type.
4. `\cp_ggax_typ{becke,pw91x,fla_1x,fl_2x,off}` :  
Gradient corrected exchange function type.
5. `\cp_ggac_typ{lyp,lypm1,pw91c,off}` :  
Gradient corrected correlation function type.
6. `\cp_norb{full_ortho,norm_only,off}` :  
Non-orthogonal orbitals option (see Tuckerman-Hutter-Parr. papers).
7. `\cp_minimize_typ{min_std,min_cg}` :  
Minimization type, steepest descent, conjugate gradient
8. `\cp_mass_tau_def{25}` :  
CP fictitious dynamics time scale in femtoseconds.
9. `\cp_energy_cut_def{2}` :  
Plane wave expansion cutoff  $E_g \leq \hbar^2 g^2 / 2m_e$
10. `\cp_mass_cut_def{2}` :  
Renormalize CP masses for  $E_g \leq \hbar^2 g^2 / 2m_e$  Rhydborg.
11. `\cp_fict_KE{1000}` :  
Energy give to the plane waves to create the Born-Oppenheimer surface with there fake dynamics
12. `\cp_ptens{on,off}` :  
Evaluate the pressure tensor.



13. `\cp_init_orthog{on,off}` :  
Orthogonalize the states at the start.
14. `\cp_orth_meth{gram_schmidt,lowdin}` :  
Orthogonalize using gram-schmidt or lowdin.
15. `\cp_restart_type{gen_wave,initial, restart_pos,restart_posvel,restart_a`  
:  
Start the run by generating sum guess to the states, ...
16. `\cp_nonloc_ees_opt{on:on/off }`:  
Compute the non-local pseudopotential energy and forces using Euler exponential spline interpolation (EES).
17. `\cp_eext_ees_opt{on:on/off }`:  
Compute the local pseudopotential energy and forces as well as the reciprocal space part of the Ewald sum using EES.
18. `\cp_pseudo_ees_order{6 }`:  
Use a EES interpolation order of 6.
19. `\cp_pseudo_ees_scale{1.4 }`:  
Use a g-space expanded 1.4x to perform the EES interpolation.

## ~sim\_pimd\_def[ 10 keywords]

1. `\path_int_beads{1}` :  
Number of path integral beads.
2. `\path_int_md_typ{staging,centroid}` :  
Path integral molecular dynamics type, staging or centroid/normal mode.  
Staging gives the fastest equilibration.
3. `\path_int_gamma_adb{1}` :  
Path integral molecular dynamics type adiabaticity parameter. Employed with the centroid option to give approx. to quantum dynamics.
4. `\respa_steps_pimd{1}` :  
Path integral bead respa steps.
5. `\initial_spread_size{1}` :  
In growing cyclic initial paths, what is the how large do you want their diameter or spread in Angstroms.
6. `\initial_spread_opt{on,off}` :  
Do you want initial paths grown for you?

# Molecule and Wave function

## Keyword Dictionary:

The following commands maybe specified in the system setup file:

1. `~molecule_def []`
2. `~wavefunc_def []`
3. `~bond_free_def []`
4. `~data_base_def []`

## ~molecule\_def

1. `\mol_name{ }` :  
The name of the molecule type.
2. `\num_mol{ }` :  
The number of this molecule type you want in your system.
3. `\num_residue{ }` :  
The number of residues in in this molecule type.
4. `\mol_index{2}` :  
This is the “2nd” molecule type defined in the system.
5. `\mol_parm_file{ }` :  
The topology of the molecule type is described in this file.
6. `\mol_text_nhc{ }` :  
The temperature of this molecule type. It may be different than the external temperature for fancy simulation studies in the adiabatic limit.
7. `\mol_freeze_opt{none,all,backbone}` :  
Freeze this molecule to equilibrate the system.
8. `\hydrog_mass_opt{A,B}` :  
Increase the mass of type A hydrogens where A is **off**,all,backbone or sidechain to B amu. This allows selective deuteration for example.
9. `\hydrog_con_opt{off,all,polar}` :  
Constrain all bonds to this type of hydrogen in the molecule.
10. `\mol_nhc_opt{none,global,glob_mol,ind_mol,  
res_mol,atm_mol,mass_mol}` :  
Nose-Hoover Chain option: Couple the atoms in this molecule to:
  - none: no thermostats.
  - global: the global thermostat.
  - glob\_mol: a thermostat for this molecule type.
  - ind\_mol: a thermostat for each molecule of this type.

- res\_mol: a thermostat for each residue in each molecule.
- atm\_mol: a thermostat for each atom in each molecule.
- mass\_mol: a thermostat for each degree of freedom.

11. \mol\_tau\_nhc{ } :

Nose-Hoover Chain time scale in femtoseconds for this molecule type.

## $\tilde{\text{wavefunc\_def}}$

1.  $\backslash\text{nstate\_up}\{1\}$  :  
Number of spin up states in the spin up electron density.
2.  $\backslash\text{nstate\_dn}\{1\}$  :  
Number of spin down states in the spin down electron density.
3.  $\backslash\text{cp\_tau\_nhc}\{25\}$  :  
Nose-Hoover Chain coupling time scale.

## \bond\_free\_def

1. `\atom1_moltyp_ind{ }` :  
Index of molecule type to which atom 1 belongs.
2. `\atom2_moltyp_ind{ }` :  
Index of molecule type to which atom 2 belongs.
3. `\atom1_mol_ind{ }` :  
Index of the molecule of the specified molecule type to which atom 1 belongs.
4. `\atom2_mol_ind{ }` :  
Index of the molecule of the specified molecule type to which atom 2 belongs.
5. `\atom1_residue_ind{ }` :  
Index of the residue in the molecule to which atom 1 belongs.
6. `\atom2_residue_ind{ }` :  
Index of the residue in the molecule to which atom 2 belongs.
7. `\atom1_atm_ind{ }` :  
Index of the atom 1 in the residue.
8. `\atom2_atm_ind{ }` :  
Index of the atom 2 in the residue.
9. `\eq{ }` :  
Equilibrium bond length in Angstrom.
10. `\fk{ }` :  
Umbrella sampling force constant in K/Angstrom<sup>2</sup>.
11. `\rmin_hist{ }` :  
Min Histogram distance in Angstrom.
12. `\rmax_hist{ }` :  
Max Histogram distance in Angstrom.

13. `\num_hist{ }` :  
Number of points in the histogram.
14. `\hist_file{ }` :  
File to which the histogram is printed.



## ~data\_base\_def

1. `\inter_file{ }` :  
File containing intermolecular interaction parameters.
2. `\vps_file{pi_md.inter}` :  
File containing pseudopotential interaction parameters.
3. `\bond_file{pi_md.bond}` :  
File containing bond interaction parameters.
4. `\bend_file{pi_md.bend}` :  
File containing bend interaction parameters.
5. `\tors_file{pi_md.tors}` :  
File containing torsion interaction parameters.
6. `\onefour_file{pi_md.onfo}` :  
File containing onefour interaction parameters.

# Topology Keyword Dictionary:

The following commands maybe specified in the molecular topology and parameter files:

1. `~molecule_name_def []`
2. `~residue_def []`
3. `~residue_bond_def []`
4. `~residue_name_def []`
5. `~atom_def []`
6. `~bond_def []`
7. `~grp_bond_def []`
8. `~bend_def []`
9. `~bend_bnd_def []`
10. `~tors_def []`
11. `~onfo_def []`
12. `~residue_morph []`
13. `~atom_destroy []`
14. `~atom_create []`
15. `~atom_morph []`

## **`\molecule_name_def []`**

1. `\molecule_name{}` :  
Molecule name in characters.
2. `\nresidue{}` :  
Number of residues in the molecule.
3. `\natom{}` :  
Number of atoms in the molecule.

## **~residue\_def []**

1. `\residue_name{}` :  
Residue name in characters.
2. `\residue_index{}` :  
Residue index number (this is the third residue in the molecule).
3. `\natom{}` :  
Number of atoms in the residue (after morphing).
4. `\residue_parm_file{}` :  
Residue parameter file.
5. `\residue_fix_file{}` :  
File containing morphing instructions for this residue if any.

## **~residue\_bond\_def []**

1. `\res1_typ{}` :  
Residue name in characters.
2. `\res2_typ{}` :  
Residue name in characters.
3. `\res1_index{}` :  
Numerical index of first residue.
4. `\res2_index{}` :  
Numerical index of second residue.
5. `\res1_bond_site{}` :  
Connection point of residue bond in residue 1.
6. `\res2_bond_site{}` :  
Connection point of residue bond in residue 2.
7. `\res1_bondfile{}` :  
Morph file for residue 1 (lose a hydrogen, for example).
8. `\res2_bondfile{}` :  
Morph file for residue 2 (lose an halogen atom, for example).

## **`\residue_name_def []`**

1. `\res_name{}` :  
Name of the residue in characters.
2. `\natom{}` :  
Number of atoms in the residue

## `~atom_def []`

1. `\atom_typ{}` :  
Type of atom in characters.
2. `\atom_ind{}` :  
This is the nth atom in the molecule. The number is used to define bonds, bends, tors, etc involving this atom.
3. `\mass{}` :  
The mass of the atom in amu.
4. `\charge{}` :  
The charge on the atom in “e”.
5. `\valence{}` :  
The valence of the atom.
6. `\improper_def{0,1,2,3}` :  
How does this atom like its improper torsion constructed (if any).
7. `\bond_site_1{site,prim-branch,sec-branch}` :  
To what bond-site(s), character string, does this atom belong and where is it in the topology tree structure relative to the root (the atom that will bonded to some incoming atom).
  - Atom to be bonded =root atom (0,0).
  - 1st atom bonded to root atom (1,0).
  - 2nd atom bonded to root atom (2,0).
  - 1st atom bonded to 1st branch (1,1).
  - 2nd atom bonded to 1st branch (1,2).
8. `\def_ghost1{index,coeff}` :  
If the atom is a ghost (these funky sites that TIP4P type models have), its spatial position is constructed by taking linear combinations of the other atoms in the molecule specified by the index and the coef. A ghost can be composed of up to six other atoms (ghost\_1 ... ghost\_6).

## `\bond_def []`

1. `\atom1{}` :  
Numerical index of atom 1.
2. `\atom2{}` :  
Numerical index of atom 2.
3. `\modifier{con,on,off}` :  
The bond is active=`on`, inactive=`off`, or constrained=`con`.



## **~residue\_morph []**

- Used to define a file which contains modifications to a given residue.
- It has the same arguments as ~residue\_name\_def[].

## **~atom\_destroy []**

- Used to destroy an atom in a residue morph file.
- Uses the same key words as ~atom\_def[]

## **~atom\_create []**

- Used to create an atom in a residue morph file.
- Uses the same key words as ~atom\_def[]

## **~atom\_morph []**

- Used to morph an atom in a residue morph file.
- Uses the same key words as ~atom\_def[]

# Potential Parameter Keyword Dictionary:

The following commands maybe specified in the potential parameter files:

1. `~inter_parm []`
2. `~bond_parm []`
3. `~bend_parm []`
4. `~tors_parm []`
5. `~onfo_parm []`
6. `~pseudo_parm []`
7. `~bend_bnd_parm []`

## ~inter\_parm

1. `\atom1{}` :  
Atom type 1 (character data).
2. `\atom2{}` :  
Atom type 2 (character data).
3. `\pot_type{lennard-jones,williams,aziz-chen,null}` :  
Potential type: Williams is an exponential c6-c8-c10. Aziz-chen has a short range switching function on the vanderwaals part.
4. `\min_dist{}` :  
Minimum interaction distance.
5. `\max_dist{}` :  
Spherical cutoff interaction distance.
6. `\res_dist{}` :  
Respa Spherical cutoff interaction distance.
7. `\sig{}` :  
Lennard-Jones parameter.
8. `\eps{}` :  
Lennard-Jones parameter.
9. `\c6{}` :  
Williams/Aziz-Chen Vdw parameter.
10. `\c8{}` :  
Williams/Aziz-Chen Vdw parameter.
11. `\c9{}` :  
Williams/Aziz-Chen Vdw parameter.
12. `\c10{}` :  
Williams/Aziz-Chen Vdw parameter.

13.  $\backslash Awill\{\}$  :  
Williams/Aziz-Chen parameter ( $A \exp(-Br - Cr^2)$ ).
14.  $\backslash Bwill\{\}$  :  
Williams/Aziz-Chen parameter ( $A \exp(-Br - Cr^2)$ ).
15.  $\backslash Cwill\{\}$  :  
Williams/Aziz-Chen parameter ( $A \exp(-Br - Cr^2)$ ).
16.  $\backslash rm\_swit\{\}$  :  
Williams/Aziz-Chen parameter controlling Vdw switching ( $f(r, r_m) =$ ).

## ~bond\_parm

1. `\atom1{}` :  
Atom type 1 (character data).
2. `\atom2{}` :  
Atom type 2 (character data).
3. `\pot_type{harmonic,power-series,morse,null}` :  
Potential type of bond.
4. `\fk{}` :  
Force constant of bond in K/Angstrom<sup>2</sup>.
5. `\eq{}` :  
Equilibrium bond length in Angstrom.
6. `\eq_res{}` :  
Respa Equilibrium bond length in Angstrom.
7. `\alpha{}` :  
Morse parameter alpha in inverse Angstrom  
( $\phi(r) = d_0[\exp(-\alpha(r - r_0)) - 1]^2$ ).
8. `\d0{}` :  
Morse d0 in Kelvin ( $\phi(r) = d_0[\exp(-\alpha(r - r_0)) - 1]^2$ ).

## **$\sim$ pseudo\_parm**

1. `\atom1{}` :  
Atom type in character data.
2. `\vps_typ{local, kb, vdb, null}` :  
Pseudopotential type: local, Kleinman-Bylander, Vanderbilt or null.
3. `\vps_file{}` :  
File containing the numerical generated pseudopotentials.
4. `\n_ang{}` :  
Number of angular momentum projection operators required.
5. `\loc_opt{}` :  
Which angular momentum pseudopotential is taken to be the local.

# Coordinate Input Files:

At present the code will build topologies for the user. However, it will not build coordinates. Therefore, the user must provide an initial input coordinate file( see `\restart_type{initial}` and `\in_restart_file{sim_restart.in}`) The first line of the restart file must contain the number of atoms, followed by a one, followed by the number of path integral beads (usually 1). The code will grow beads and only  $P=1$  need be provided initially. The atoms positions then follow in the order specified by the set file and the topology files. Finally, at the bottom of the code the 3x3 simulation cell matrix must be specified. The unit is Angstrom.

Example:

The molecular set file specifies 25 water molecules as molecule type 1 and 3 bromine atom as molecule type 2. The water parameter file is written as OHH, i.e. oxygen is atom 1, hydrogen1 is atom 2, hydrogen2 is atom 3. Therefore, the input file should have 25 OHH coordinates followed 3 bromines. If the box is a square 25 angstrom on edge then the last three lines of the file should be

```
25 0 0
0 25 0
0 0 25
```

# Parallel Decomposition Keyword Dictionary:

The following commands maybe specified in the parallel decomposition file:

1. `~charm_conf_gen_def[ ]`
2. `~charm_conf_rho_def[ ]`
3. `~charm_conf_state_def[ ]`
4. `~charm_conf_PC_def[ ]`
5. `~charm_conf_NL_def[ ]`
6. `~charm_conf_map_def[ ]`

If no commands are set, the charm++ driver will decide values based on system size and processor number and architecture. Below, the name `nstate` refers to the number of KS states and the name `nproc` refers to the number of processors to be used.



## **`~charm_conf_gen_def`**

1. `\useCommLib{on:on,off }` :  
Turn on/off Charm communication library use. Default on
2. `\useCommLibMulticast{ }` :  
Turn on/off Charm multicast communication library use. Default on
3. `\atmOutput{on:on,off }` :  
Turn on/off atom output. Default on

## `~charm_conf_rho_def`

1. `\gExpandFactRho{1 }` :  
Expands the g-space parallelization of the electron density beyond the number of planes by the specified non-integer multiplicative factor.
2. `\rhoGHelpers{1 }` :  
Expands the g-space parallelization of the local pseudopotential evaluation by the integer increment.
3. `\rhoRsubplanes{1 }` :  
Expands the r-space parallelization of the exchange correlation and local pseudopotential energies by the integer increment. The latter only matters if EES is on.
4. `\rhoLineOrder{skip:skip,none,random }` :  
Static Load balance scheme for density g-space parallelization.
5. `\nchareHartAtmT{1 : 1 ≤ ≤ natmTyp}` :  
Decomposition for the local pseudopotential energy for use with the EES method.
6. `\rhoSubPlaneBalance{off:on/off }` :  
When `rhoRsubplanes > 1`, balance the communication.
7. `\rhoGToRhoRMsgCombine{off:on/off }` :  
When `rhoRsubplanes > 1`, combine messages.

## **~charm\_conf\_state\_def**

1. `\dataPath{./STATES }` :

The directory in which the electronic state input files are stored. If the “gen\_wave” option is selected, the dataPath command is ignored.

2. `\dataPathOut{./STATES_OUT }` :

The directory in which the electronic state output files are stored.

3. `\gExpandFact{1.0 }` :

Expands the g-space parallelization of the electronic states beyond the number of planes by the specified non-integer multiplicative factor. If the torus map option is employed, the product must be a power of 2, for example (gexpandfact=2)x(nplane\_state=4)=8.

4. `\stateOutput{on: on/off }` :

Turn the electronic state input on and off.

# ~charm\_conf\_PC\_def

1. \sGrainSize{ nstate} :

Integer smatrix decomposition parameter. The default value is number of electron states, e.g. the matrix is not decomposed.

2. \orthoGrainSize{ nstate} :

Integer lowdix decomposition parameter. The default value is number of electron states, e.g. the matrix is not decomposed. This parameter must be  $\leq$  sGrainSize and  $\text{mod}(sGrainSize, oGrainSize) = 0$ .

3. \numChunks{ 1 } :

Increase the g-space decomposition by the integer factor.

4. \phantomSym{ on:on/off} :

Add some extra parallelization for Smatrix computations.

5. \useOrthoHelpers{ off:on/off} :

Add some extra parallelization for Lowdin orthogonalization. Use only if  $(nstates/orthograinsize)^2 < nproc$ .

6. \invsqr\_tolerance{1e-15 } :

Tolerance on the iterative matrix square root method.

7. \invsqr\_max\_iter{10 } :

Maximum number of iteration for the matrix square root method.

## **`~charm_conf_NL_def`**

1. `\numSfGrps{ 1}` :  
Decompose the  $N^3$  non-local computation into the specified number of groups.
2. `\numSfDups{ }` :  
Duplicate the  $N^2$  evaluation of the structure factor for the  $N^3$  non-local computation the specified number of times.
3. `\launchNLeesFromRho{rs:rs,rhor,rhog }` :  
Specify the launch point for the Non-local EES computation.

# `~charm_conf_map_def`

1. `\Gstates_per_pe{nstates }` :  
If torusMap is off, specify the g-space state decomposition.
2. `\Rstates_per_pe{nstates }` :  
If torusMap is off, specify the r-space state decomposition.
3. `\torusMap{on: on/off }` :  
If your machine is a torus, this mapping scheme gives optimal performance.
4. `\loadMapFiles{off:on/off }` :  
Load pregenerated map files.
5. `\dumpMapFiles{off:on/off }` :  
Create map files.
6. `\fakeTorus{off:on/off }` :  
If your machine is a NOT torus, you can still use torus mapping.
7. `\torusDimX{ nproc }` :  
Fake Torus dimension along x in processors/node
8. `\torusDimY{1 }` :  
Fake Torus dimension along y in processors/node
9. `\torusDimZ{1 }` :  
Fake Torus dimension along z in processors/node
10. `\torusDimNX{1 }` :  
Fake Torus dimension along x in nodes
11. `\torusDimNY{1 }` :  
Fake Torus dimension along y in nodes

12. \torusDimNZ{ 1} :  
Fake Torus dimension along z in nodes