**­­­­Limitations/To do:**

* Overbonding may not work right when multiple atom types are used, or when multiple “to” overbonding atom types are requested
* Charge enforcement/conservation is hard coded and will only work for systems containing O and H.
* Units have not been annotated in all necessary locations within code/input files.
* Update the 3-body Chebyshev functionality. Currently this part is not working.
* Make the updated C++ files compatible with the MD code

**Compiling/running the code:**

* Compile by navigating to the SRC directory and typing make
* Once compiled, .o files can be removed with make clean, while the executable itself can be removed with make realclean
* The code can be run with: /path/to/executable

**Running the test suite**

* Navigate to the TEST\_SUITE folder, and open up the run\_test\_suite.sh file
* Ensure the “PATH\_TO\_LSQ\_PY\_CODE variable is set properly
* Run from TEST\_SUITE with ./run\_test\_suite.sh

**Main Control Variables**

|  |  |  |
| --- | --- | --- |
| Keyword | Allowed Values | Usage |
| # TRJFILE # | any string | Provides the name of the simulation trajectory file. Files use a .xyzf format, which is like the standard .xyz format, with two exceptions: (1) after the line containing the number of atoms, the x, y, and z box lengths are given, and (2) each coordinate line has x, y, and z forces on the corresponding atom appended. |
| # WRAPTRJ # | “true” or “false” | Defines whether coordinates should be wrapped (i.e. application of post-simulation periodic boundary conditions). |
| # NFRAMES # | Any integer > 0 | Number of frames in the .xyzf file |
| # NLAYERS # | Any integer > 0 | Number of supercells to create from simulation box (i.e. replicate images). |
| # FITCOUL # | “true” or “false” | Defines whether charges should be fit, or held fixed at user-defined values. |
| # CNSCOUL # | “true” or “false” | Will constraints (conservation) be enforced on charges? Only used if # FITCOUL # is true. |
| # FITPOVR # | “true” or “false” | Defines whether a ReaxFF type over-coordination force should be applied. |
| # PAIRTYP # | “SPLINE”, “CHEBYSHEV”, “DFTBPOLY”, or “INVRSE\_R” | The form of the inter-molecular potential to be used for fitting. |
| # SUBCRDS # | “true” or “false” | Defines whether over-coordination force should be subtracted prior to force field fitting. Only used if  # FITPOVR # is false. |
| # CHBTYPE # | “DEFAULT”, “INVRSE\_R”, “MORSE” | Determines how distance is transformed for a Chebyshev-type fit. Default means no transformation will be applied. Only used if # PAIRTYP # is CHEBYSHEV. |
| # POLORDR # | Any integer > 0 | Determines the order of polynomials used for fitting. Only used if # PAIRTYP # is “CHEBYSHEV” or “DFTBPOLY”. |

**­­­­Topology Variables**

|  |  |  |
| --- | --- | --- |
| Keyword | Allowed Values | Usage |
| # NATMTYP # | Any integer > 0 | Number of unique atom types in trajectory |
| # TYPEIDX # | Integers > 0 | Ascending integers, ranging from 1 to # NATMTYP#. Index for each unique atom type. Values form a column below  # TYPEIDX #. |
| # ATM\_TYP # | Any chemical symbol  (i.e. C or Si) | Chemical symbol for each unique atom type. Values form a column below # ATM\_TYP #. |
| # ATMCHRG # | Any float | User-defined partial atomic charge for each unique atom type. Values form a column below # ATMCHRG #. Only used if # FITCOUL # is false. |
| # ATMMASS # | Any float > 0 | User-defined atomic mass for each unique atom type. Values form a column below # ATMMASS #. Only used for MD. |
| # PAIRIDX # | Integers > 0 | Ascending integers, ranging from 1 to the total number of unique atom pair types. Values form a column below  # PAIRIDX #. |
| # ATM\_TYX # | Any chemical symbol  (i.e. C or Si) | # ATM\_TY1 # or # ATM\_TY2 #. Used to define interaction pair types. Order does not matter. |
| # S\_MINIM # | Any float > 0 | Inner cutoff for pair potential in Angstroms. |
| # S\_MAXIM # | Any float > 0 | Outer cutoff for pair potential in Angstroms. |
| # S\_DELTA # | Any float > 0 | Grid spacing for splines. Number of splines for a given pair type is (# S\_MAXIM # – # S\_MINIM #)/# S\_DELTA #. Only used if # PAIRTYP # is SPLINE . |
| # MORSE\_LAMBDA # | Any float > 0 | Morse-type lambda to use when a Morse transformation is used on pair distance for a CHEBYSHEV type pair. Only used if # PAIRTYP # is CHEBYSHEV. |
| # USEOVRP # | “true” or “false” | Determines whether overbonding should be included for pair type. |
| # TO\_ATOM # | Any chemical symbol  (i.e. C or Si) | The atom that overbonding is considered for. For example, “O” for water-type systems. Only used if # USEOVRP # is true. |
| # P\_OVERB # | Any float > 0 | *p*over from the ReaxFF overbonding equation of order 1. Only used if # USEOVRP # is true. |
| # R\_0\_VAL # | Any float > 0 | *r*0 from the ReaxFF overbonding equation of order 1. Only used if # USEOVRP # is true. |
| # P\_1\_VAL # | Any float > 0 | *p*bX,1 from the ReaxFF overbonding equation of order 1. “X” refers to the “TO\_ATOM.” Only used if # USEOVRP # is true. |
| # P\_2\_VAL # | Any float > 0 | *p*bX,2 from the ReaxFF overbonding equation of order 1. “X” refers to the “TO\_ATOM.” Only used if # USEOVRP # is true. |
| # LAMBDA6 # | Any float > 0 | *λ*6 from the ReaxFF overbonding equation of order 1. Only used if # USEOVRP # is true. |