

GOMC

User Manual
Version 2.00

Distributed by the Potoff and Schwiebert Groups
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Contents

1 Tutorial Overview

This document will instruct a new user how to download, compile, and run the GOMC molecular simulation code. A basic understanding of statistical physics is recommended to complete this tutorial.

To demonstrate the capabilities of the code, the user is guided through the process of downloading and compiling a GOMC executable. That executable is then used to perform saturated vapor and liquid equilibria (VLE) studies on systems of pure isobutane (R600a), a branched alkane that whose application as a refrigerant/propellant is increasing.

<http://en.wikipedia.org/wiki/Isobutane>

The Transferable Potentials for Phase Equilibria (TraPPE) united atom (UA) force field is used to describe the molecular geometry constraints and the intermolecular interactions.

2 Introduction

Monte Carlo (MC) simulation is a type of simulation driven by stochastic processes. "GO" stands for GPU-Optimized; this code was intended to run optimally on modern graphics process hardware.

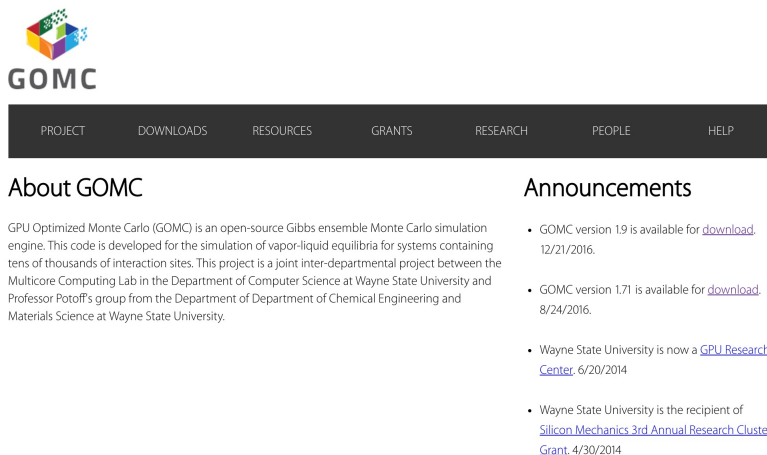
More specifically, this engine includes serial and GPU-Optimized (multi-threaded) codes designed to run Markov chain Boltzmann sampling of chemical systems – effectively sets of points defined by topological maps and interaction algorithms in a simulation box. From statistical mechanics, we know this is one way to sample phase space and model chemical systems.

GOMC currently supports canonical, isobaric-isothermal, Grand canonical, constant volume Gibbs ensemble, and constant pressure Gibbs ensemble simulations. GOMC employs widely-used simulation file types (PDB, CHARMM-style parameter file, PSF). GOMC includes configurational bias algorithms for both linear and branched charged, and none charged systems.

3 How to get the software

The latest public code builds, project logo, manual, and other resources can be obtained via the following website:

<http://gomc.eng.wayne.edu/>



GOMC

PROJECT DOWNLOADS RESOURCES GRANTS RESEARCH PEOPLE HELP

About GOMC

GPU Optimized Monte Carlo (GOMC) is an open-source Gibbs ensemble Monte Carlo simulation engine. This code is developed for the simulation of vapor-liquid equilibria for systems containing tens of thousands of interaction sites. This project is a joint inter-departmental project between the Multicore Computing Lab in the Department of Computer Science at Wayne State University and Professor Potoff's group from the Department of Chemical Engineering and Materials Science at Wayne State University.

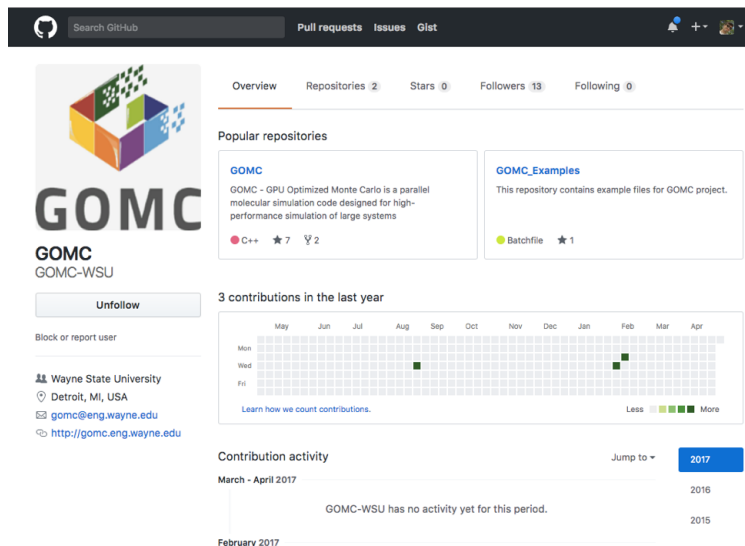
Announcements

- GOMC version 1.9 is available for [download](#). 12/21/2016.
- GOMC version 1.71 is available for [download](#). 8/24/2016.
- Wayne State University is now a [GPU Research Center](#). 6/20/2014
- Wayne State University is the recipient of [Silicon Mechanics 3rd Annual Research Cluster Grant](#). 4/30/2014

The code can be found under the download tab, below and to the right of the logo. When new betas (or release builds) are announced, they will replace the prior code under the downloads tab. An announcement will be posted on the front page to notify users.

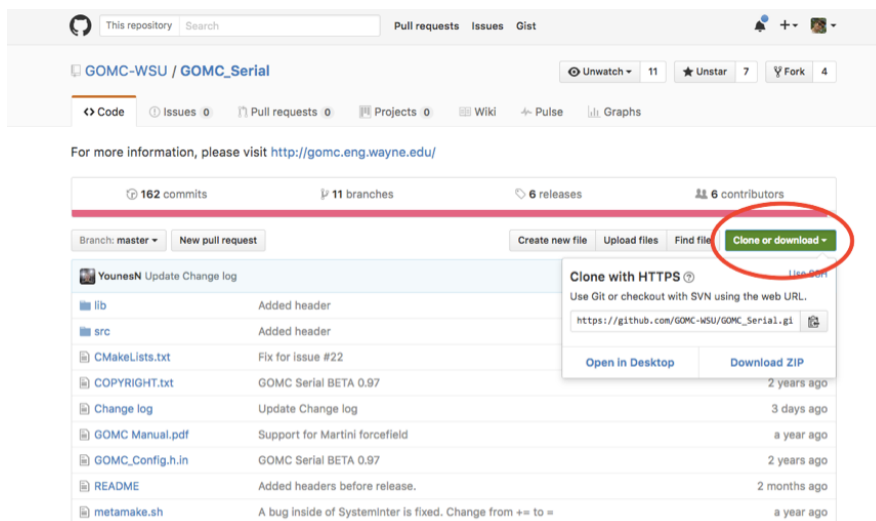
Currently, version control is handled through the GitHub repository. The posted builds in Master branch are “frozen” versions of the code that have been validated for a number of systems and ensembles. Other branches are created as a means of implementing new features. The latest updated code builds, project logo, manual, example files, and other resources can be obtained via the following GitHub repository:

<https://github.com/GOMC-WSU>



The CPU and GPU code are merged together under GOMC repository and can be found under the main page. In addition, Examples repository can be found under the main page. Under each repository, the code and manual can be downloaded by clicking on the Clone or download tab. For more information regarding GitHub, visit the following link:

<https://guides.github.com/activities/hello-world/>



4 Platform and Software Requirements

4.1 Supported Operating Systems

GOMC officially supports Windows 7, 8, and most modern distributions of Linux (see the next section). This software has the ability to compile on recent versions of OS X; however, such a platform is not officially supported.

4.2 Required Software Prerequisites

GOMC has some mild software requirements, which are widely available for Linux operating systems. Required software requirements are:

C++03 Compliant Compiler Linux/OS X icc (Intel C++)
Compiler)

Type the following command in a terminal:

```
$ icc --version
```

If gives a version number 4.4 or later, you're all set. If it's older than 4.4 (released in 2009), we recommend upgrading.

In Linux, the Intel compiler will generally produce the fastest serial executables (when running on Intel Core processors).

g++ (GNU GCC)

Type the following command in a terminal.

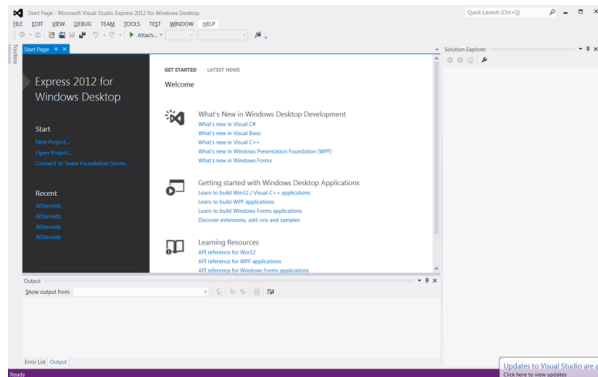
```
$ g++ --version
```

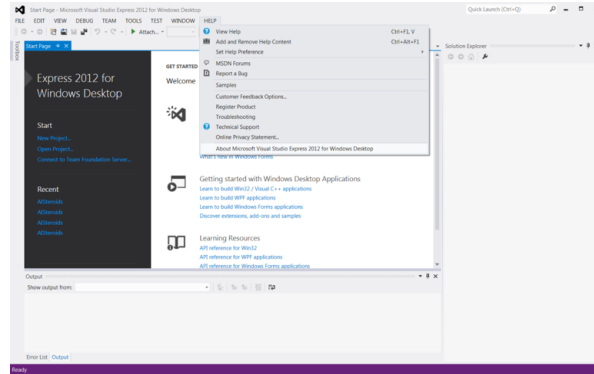
If gives a version number 4.4 or later, you're all set. If it's older than 4.4 (released in 2009), we recommend upgrading.

Windows Visual Studio
Microsoft's Visual Studio 2010 or later is recommended.

To check the version:

Help (top tab) → *About Microsoft Visual Studio*





cmake (if compiling on Linux)

To check if cmake is installed:

```
$ which cmake
```

To check the version number:

```
$ cmake --version
```

nvcc/CUDA libs

The GPU builds of the code requires NVIDIA's CUDA 6.0 or newer:

To check if nvcc is installed:

```
$ which nvcc
```

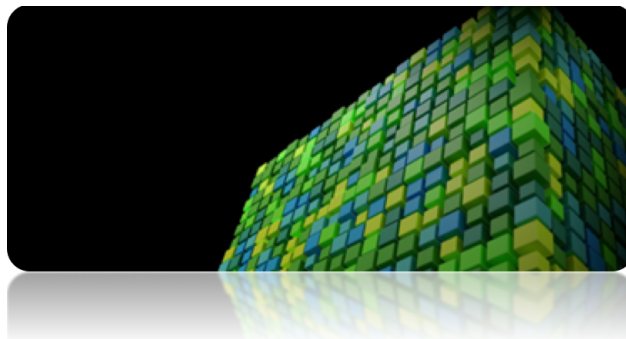
To check the version number:

```
$ nvcc --version
```

CUDA is viewed as an essential requirement, but is not used to compile the serial code, which can be compiled on systems without CUDA.

To download CUDA visit NVIDIA's webpage:

<https://developer.nvidia.com/cuda-downloads>



CUDA is required to compile the GPU executable in both Windows and Linux. Please refer to CUDA Developer webpages to select an appropriate version for the desired platform.

To install CUDA in Linux root/sudo, privileges are generally required. In Windows, administrative access

is required.

5 Highly Recommended Software Tools

NOTE: *The listed programs are used in this manual and are generally considered necessary.*

5.1 VMD

VMD (Visual Molecular Dynamics) is a 3-D visualization and manipulation engine for molecular systems written in C-language. VMD is distributed and maintained by the University of Illinois at Urbana-Champaign. Its sources and binaries are free to download. It comes with a robust scripting engine, which is capable of running python and tcl scripts. More info can be found here:

<http://www.ks.uiuc.edu/Research/vmd/>

Although GOMC uses the same fundamental file types ? PDB (coordinates) and PSF (topology) as VMD, it uses some special tricks to obey certain rules of those file formats.

One useful purpose of VMD is visualization of your systems.

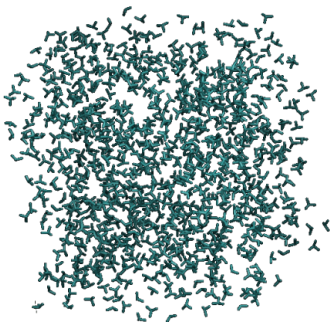


Figure 1: A system of united atom isobutane molecules

Nonetheless, the most critical part of VMD is a tool called PSFGen. PSFGen uses a tcl or python script to generate a PDB and PSF file for a system of one or more molecules. It is, perhaps, the most convenient way to generate a compliant PSF file.

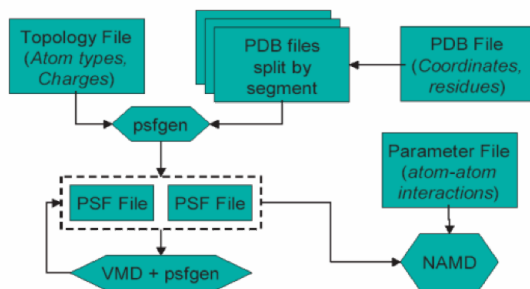


Figure 2: An overview of the PSFGen file generation process and its relationship to VMD/NAMD

To read more about PSFGen, reference:

Plugin homepage @ UIUC

<http://www.ks.uiuc.edu/Research/vmd/plugins/psfgen>

“Generating a Protein Structure File (PSF)”, part of the NAMD Tutorial from UIUC
<http://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-html/node6.html>

In-Depth Overview [PDF]
<http://www.ks.uiuc.edu/Research/vmd/plugins/psfgen/ug.pdf>

5.2 Packmol

Packmol is a molecule packing tool created by José Mario Martínez, a professor of mathematics at the State University of Campinas, Brazil. It is written in Fortran and is free to download. More information is available on their homepage:

<http://www.ime.unicamp.br/~martinez/packmol>

To compile it, a Fortran language compiler is needed, such as gfortran. Many Linux distributions no longer come with Fortran compilers automatically, so this may need to be installed additionally.

Packmol allows a specified number of molecules to be packed at defined separating distances within a certain region of space. One of Packmol's limitations is that it is unaware of topology; it treats each molecule or group of molecules as a rigid set of points.

WARNING: *Another more serious limitation is that it is not aware of periodic boundary conditions (PBC). As a result, when using Packmol to pack PDBs for GOMC, it is recommended to pack to a box 1 Angstroms smaller than the simulation box size. This prevents hard overlaps over the periodic boundary.*

6 Other Useful Software Tools

6.1 Grace

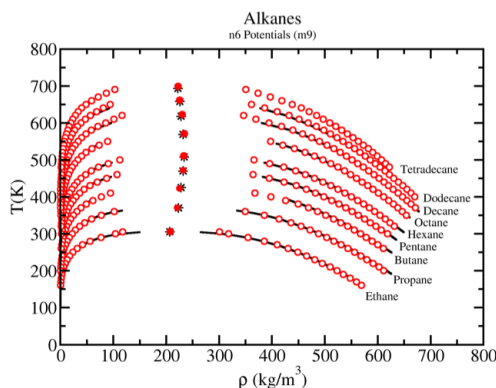
Grace is a piece of graphing software written and maintained by the Weizmann Institute of Science's Plasma Laboratory (Rehovot, Israel). Mostly used in Linux, it can also be compiled in Windows. The developers warn it may be missing some functionality.



In-depth information and the source can be found on the project page, here:

<http://plasma-gate.weizmann.ac.il/Grace>

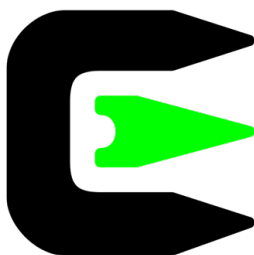
When compiled, Grace's executable in Linux is typically named “xmgrace”. This tool allows the production of high quality, precise line and dot graphs, ideal for visualizing much of the thermodynamic data from the GOMC engine. Below is an example of the results of simulations of saturated VLE densities of linear alkanes produced with Grace.



6.2 Cygwin

Cygwin is one option to assist in building and visualizing systems in Windows. It provides Microsoft Windows users with a Unix-like environment and command-line interface, and offers Windows-compatible ports of common Linux applications.

<https://cygwin.com>



The software is a free and open source, licensed under the GNU General Public License version 3. Its primary maintainers are Red Hat Inc. and NetApp. One of the most impressive abilities of Cygwin is its ability to launch a full Windows-compatible X-server Window, which allows convenient visualization of Linux app GUIs. It is compatible with the Grace graphing software. In practice, this package behaves most analogously to a Linux virtual machine in Windows.

7 Compiling GOMC

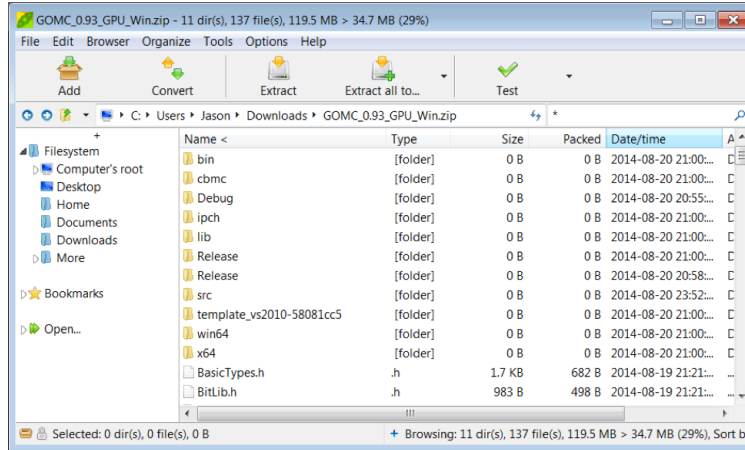
7.1 Extracting the code

GOMC is distributed as a compressed folder, containing the source and build system. To compile the code after downloading it, the first step is to extract the compressed build folder.

In Windows, the folder for the GPU code is compressed using a standard *.zip file format. To unzip simply use a utility like Peazip:

<http://peazip.sourceforge.net/>

Below is an example of what the downloaded code looks like when unzipping in Peazip.



In Linux, the GPU and Serial codes are compressed using gzip and tar (*.tar.gz). To extract, simply move to the desire folder and type in the command line:

```
$ tar -xzf <file name>.tar.gz
```

7.2 Compiling the code

7.2.1 GPU code

Compilation on Windows

Once the code is extracted, to compile it on Windows, you need to load the project into Visual Studio by opening the extracted folder and double clicking on the solution file of the desired Visual Studio version. After the solution is opened in Visual Studio, go to the “Build” menu and select “Build solution” to compile the code. You can compile either with release mode or with debug mode by selecting the desired mode from the “Solution Configuration” drop box. To run the project, simply click the run button or hit F5 on the keyboard.

Compilation on Linux

To compile the GPU code on Linux, go to the directory of the project, and type in the command line:

```
$ make
```

You can configure the “makefile” file to choose different C compilers, to select the desired compute capability, and to configure many more compilation flags.

The default compute capability is 3.0. To change the compute capability, go to the `GENCODE_FLAGS` option, and set it to one of the compute capability flags that are defined in the file. To run the program, run the executable “GOMC.out”. The system’s `LD_LIBRARY_PATH` will need to be configured to support CUDA (more on this later).

7.2.2 Serial Code

Compilation on Windows

See GPU “Compilation on Windows” section and follow an identical procedure for the released serial code. See README for instructions on how to use the CMake-GUI to build the configuration and solution files necessary for the Windows build.

Compilation on Linux

In Linux, the CPU code uses a simple makefile. Enter the directory and type in the command line:

```
$ make all
```

This will use the Makefile to compile a GPU-compatible executable called “GOMC.out”. To run, the system’s `LD_LIBRARY_PATH` will need to be configured to support CUDA (more on this later). For the serial code, which uses cmake for compilation, go to the base directory and type in the command line:

```
$ ./metamake.sh
```

This cmake script will create a directory named “bin”. Enter this directory:

```
$ cd bin
```

and type:

```
$ make
```

Four executables - `GOMC.Serial.GEMC` (Gibbs ensemble), `GOMC.Serial.NVT` (NVT ensemble), `GOMC.Serial.NPT` (isobaric-isothermal ensemble), and `GOMC.Serial.GCMC` (Grand canonical ensemble) - will be produced. By default, the distribution compiles in release mode. To compile in debug mode (if you’re using the code as a developer), open the file “`CMakeCache.txt`” while still in the “bin” folder. This file contains information used by cmake to build the executables. To compile in debug mode, change the value after “`CMAKE_BUILD_TYPE:STRING=`” from “Release” to “Debug”, and retype the command:

```
$ make
```

The output executables should now be compiled with debugger symbols. You can also swap the compiler by modifying the “`CMAKE_CXX_COMPILER`” variable. For more information, refer to the CMake documentation.

Running GOMC in parallel using OpenMP:

To run the parallel version of CPU code, it needs to be compiled with openmp library. Open the file “`CMakeCache.txt`”, while still in the “bin” folder, and change the value after “`CMAKE_CXX_FLAGS_RELEASE:STRING=`” from “`-O3 -DNDEBUG`” to “`-O3 -qopenmp -DNDEBUG`”.

And retype the command:

```
$ make
```

8 Input File Formats

In order to run simulation in GOMC, the following files need to be provided:

- GOMC executable
- Input file “NAME.conf” (proprietary control file)
- PDB file(s)
- PSF file(s)
- Parameter file

8.1 PDB File

The PDB file stores coordinates for the simulation. The file format is widely adopted.

- Protein Databank (PDB) Files (plural: PDB files)
- Open format, well-documented

- Fixed-width format (hence white space is significant)
- Up to 13.5m page views a month; up to 55.8m FTP requests per month
- Used by NAMD, GROMACS, CHARMM, ACEMD, Amber

An overview of the PDB standard can be found here:

<http://www.wwpdb.org/docs.html>

The advantage of PDB files is their ubiquity and thorough documentation. Disadvantages include limited fixed point floating precision for coordinates, unused space, and proprietary implementations creating inconsistencies.

One PDB file is required per box. For NVT ensemble simulations, one file is expected; for Gibbs and grand canonical ensemble, two files are required. GOMC recognizes the following keywords in PDB files:

◇ REMARK

◇ CRYST1

◇ ATOM


◇ END

Currently, REMARK is ignored. Formerly, it was used to store proprietary information in frames (e.g. step number). Packmol typically leaves the following remark:

REMARK	original	generated	coordinate	pdb	file
--------	----------	-----------	------------	-----	------

at the top of the file. Note that this is another example of an inconsistency with the spec. As of the PDB v3.30 specification the REMARK entry contains an identifying integer, which is supposed to occupy lines 8-10.

WORLDWIDE



PDB

PROTEIN DATA BANK

Atomic Coordinate Entry Format Version 3.3

Main Index

REMARK 3
REMARK 0, 1, 2, 4, 5 - 299
REMARK 300 - 999

REMARKS

Overview

REMARK records present experimental details, annotations, comments, and information not included in other records. In a number of cases, REMARKs are used to expand the contents of other record types. A new level of structure is being used for some REMARK records. This is expected to facilitate searching and will assist in the conversion to a relational database.

The very first line of every set of REMARK records is used as a spacer to aid in reading.

COLUMNS	DATA TYPE	FIELD	DEFINITION
1 - 6	Record name	"REMARK"	
8 - 10	Integer	remarkNum	Remark number. It is not an error for remark n to exist in an entry when remark n-1 does not.
12 - 79	LString	empty	Left as white space in first line of each new remark.

REMARK 3
REMARK 0,1,2,4,5-299
REMARK 300-999

© wwPDB

A file generated by Packmol has “ori” in this position. Hence you may see future codes that are incompatible with this legacy kind of remarks.

Note also that the spaces 7 and 11 are not reserved; hence, they may be used in proprietary specifications. CRYST1 can be used to store the cell dimensions, which can also be put as a tag in the proprietary control file.

<http://www.wwpdb.org/documentation/format33/sect8.html#CRYST1>

Crystallographic and Coordinate Transformation Section

This section describes the geometry of the crystallographic experiment and the coordinate system transformations.

CRYST1

Overview

The CRYST1 record presents the unit cell parameters, space group, and Z value. If the structure was not determined by crystallographic means, CRYST1 simply provides the unitary values, with an appropriate REMARK.

Record Format

COLUMNS	DATA TYPE	FIELD	DEFINITION
1 - 6	Record name	"CRYST1"	
7 - 15	Real (9.3)	a	a (Angstroms).
16 - 24	Real (9.3)	b	b (Angstroms).
25 - 33	Real (9.3)	c	c (Angstroms).
34 - 40	Real (7.2)	alpha	alpha (degrees).
41 - 47	Real (7.2)	beta	beta (degrees).
48 - 54	Real (7.2)	gamma	gamma (degrees).
56 - 66	LString	sGroup	Space group.
67 - 70	Integer	z	Z value.

Details

- If the entry describes a structure determined by a technique other than X-ray crystallography, CRYST1 contains $a = b = c = 1.0$, $\alpha = \beta = \gamma = 90$ degrees, space group = P 1, and $Z = 1$.
- The Hermann-Mauguin space group symbol is given without parenthesis, e.g., P 43 21 2. Please note that the screw axis is described as a two digit number.
- The full International Table's Hermann-Mauguin symbol is used, e.g., P 1 21 1 instead of P 21.
- For a rhombohedral space group in the hexagonal setting, the lattice type symbol used is H.
- The Z value is the number of polymeric chains in a unit cell. In the case of heteropolymers, Z is the number of occurrences of the most populous chain.

As an example, given two chains A and B, each with a different sequence, and the space group P 2 that has two equipoints in the standard unit cell, the following table gives the correct Z value.

NOTE: Only cubic and orthogonal cells are supported in this code. The main entry in the PDB file are ATOM entries. The keyword “ATOM” is always followed by two spaces. An entry has a number of fields.

Coordinate Section

The Coordinate Section contains the collection of atomic coordinates as well as the MODEL and ENDMDL records.

ATOM

Overview

The ATOM records present the atomic coordinates for standard amino acids and nucleotides. They also present the occupancy and temperature factor for each atom. Non-polymer chemical coordinates use the HETATM record type. The element symbol is always present on each ATOM record; charge is optional.

Changes in ATOM/HETATM records result from the standardization atom and residue nomenclature. This nomenclature is described in the Chemical Component Dictionary (<ftp://ftp.wwpdb.org/pub/pdb/data/monomers>).

Record Format

COLUMNS	DATA	TYPE	FIELD	DEFINITION
1 - 6	Record name	"ATOM "		
7 - 11	Integer	serial		Atom serial number.
13 - 16	Atom	name		Atom name.
17	Character	altLoc		Alternate location indicator.
18 - 20	Residue name	resName		Residue name.
22	Character	chainID		Chain identifier.
23 - 26	Integer	resSeq		Residue sequence number.
27	AChar	iCode		Code for insertion of residues.
31 - 38	Real(8.3)	x		Orthogonal coordinates for X in Angstroms.
39 - 46	Real(8.3)	y		Orthogonal coordinates for Y in Angstroms.
47 - 54	Real(8.3)	z		Orthogonal coordinates for Z in Angstroms.
55 - 60	Real(6.2)	occupancy		Occupancy.
61 - 66	Real(6.2)	tempFactor		Temperature factor.
77 - 78	LString(2)	element		Element symbol, right-justified.
79 - 80	LString(2)	charge		Charge on the atom.

Details

- ATOM records for proteins are listed from amino to carboxyl terminus.
- Nucleic acid residues are listed from the 5' to the 3' terminus.
- Alignment of one-letter atom name such as C starts at column 14, while two-letter atom name such as FE starts at column 13.
- Atom nomenclature begins with atom type.
- No ordering is specified for polysaccharides.
- Non-blank alphanumeric character is used for chain identifier.
- The list of ATOM records in a chain is terminated by a TER record.
- If more than one model is present in the entry, each model is delimited by MODEL and ENDMDL records.
- AltLoc is the place holder to indicate alternate conformation. The alternate conformation can be in the entire polymer chain, or several residues or partial residue (several atoms within one residue). If an atom is provided in more than one position, then a non-blank alternate location indicator must be used for each of the atomic positions. Within a residue, all atoms that are associated with each other in a given conformation are assigned the same alternate position indicator. There are two ways of representing alternate conformation- either at atom level or at residue level (see examples).
- For atoms that are in alternate sites indicated by the alternate site indicator, sorting of atoms in the ATOM/HETATM list uses the following general rules:
 - In the simple case that involves a few atoms or a few residues with alternate sites, the coordinates occur one after the other in the entry.
 - In the case of a large heterogen groups which are disordered, the atoms for each conformer are listed together.
- Alphabet letters are commonly used for insertion code. The insertion code is used when two residues have the same numbering. The combination of residue numbering and insertion code defines the unique residue.
- If the depositor provides the data, then the isotropic B value is given for the temperature factor.
- If there are neither isotropic B values from the depositor, nor anisotropic temperature factors in ANISOU, then the default value of 0.0 is used for the temperature factor.
- Columns 79 - 80 indicate any charge on the atom, e.g., 2+, 1-. In most cases, these are blank.
- For refinements with program REFMAC prior 5.5.0042 which use TLS refinement, the values of B may include only the TLS contribution to the isotropic temperature factor rather than the full isotropic value.

The key parameters are the coordinates x, y, and z. The precision is limited to eight whole decimal digits and three fractional decimal digits.

Other important entries are the residue name, atom name, and chain ID. Numbering is important primarily because it represents an inconvenience in packing/loading large systems. Revisiting the previous example,

the atom name is “C1” and residue name is “ISB”. The PSF file (next section) contains a lookup table of atoms. These contain the atom name from the PDB and the name of the atom kind in the parameter file it corresponds to. As multiple different atom names will all correspond to the same parameter, these can be viewed “atom aliases” of sorts. The chain letter (in this case ‘A’) is sometimes used when packing a number of PDBs into a single PDB file.

A few important **Notes** / **Warnings** on Undocumented PDB Format Conventions:

- While it is explicitly stated in some other sections of the PDB file, the general convention observed by most codes is to right align when padding with white space.
- Some codes (including PSFGen/VMD) use the 21st unused character to add a fourth letter to the residue (molecule name). This extension is currently supported, but is unofficial and, hence, may change in the future.
- VMD requires a constant number of ATOMS in a multi-frame PDB (multiple records terminated by “END” in a single file). To compensate for this, all atoms from all boxes in the system are written to the output PDBs of this code.
- For atoms not currently in a box, the coordinates are set to $< 0.00, 0.00, 0.00 >$
- The occupancy is commonly just set to “1.00” and is left unused by many codes. We recycle this legacy parameter by using it to denote, in our output PDBs, the box a particle is in (box 0 occupancy=0.00 ; box 1 occupancy=1.00)
- As the x, y, and z coordinates are fixed point with only three digits of precision, the energy values you get when restarting may be mildly different, particularly for bonded interactions due to roundoff in the coordinates. This will eventually be remedied by the implementation of a full-precision trajectory (e.g. DCD) file.
- The “ISB” entry in columns 73-75 is not an official part of the PDB standard. This is a proprietary entry called “Segname”, which has been embraced by NAMD and some other codes.


A frame in the PDB file is terminated with the keyword **END**.

With that overview of the format in mind, the following steps describe how a PDB file is typically built.

1. A single molecule PDB is obtained. In this example, the QM software package Gaussian was used to draw the molecule, which was then edited by hand to adhere to the PDB spec properly. The end result is a PDB for a single molecule:

```
REMARK 1 File created by GaussView 5.0.8
ATOM 1 C1 ISB 1 0.911 -0.313 0.000 C
ATOM 2 C2 ISB 1 1.424 -1.765 0.000 C
ATOM 3 C3 ISB 1 -0.629 -0.313 0.000 C
ATOM 4 C4 ISB 1 1.424 0.413 -1.257 C
END
```

2. Next, packings are calculated to place the simulation in a region of vapor-liquid coexistence. There are a couple of ways to do this in Gibbs ensemble:
 - Pack both boxes to a single “middle” density, which is an average of the liquid and vapor densities.
 - Same as 1, but add a modest amount to axis of one box (e.g. 10-30 Å). This technique can be handy in the constant pressure Gibbs ensemble.

- | | | | | | | | | | | | | | | | |
|--------------------|-------|---|---------|--|----------|---|-----|----------|---|---|---|---|---|---|---|
| T (K) | 407.7 | P (bar) | 36.5 | $\rho_{\text{liq}} (\text{g}/\text{cm}^3)$ | 223. |  | | | | | | | | | |
| μ_{HFE} | 262 | $\mu_{\text{HFE}} (\text{mJ}/\text{mol})$ | 58.1222 | $\Delta_{\text{vap}} (\text{kJ}/\text{mol})$ | 6.02E+23 | Conv. g/mol | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| T (K) | 140 | $\mu_{\text{HFE}} (\text{mJ}/\text{mol})$ | 63.2 | $\Delta_{\text{vap}} (\text{kJ}/\text{mol})$ | 1E+24 | N (mole) | 500 | 2.07E-08 | | | | | | | |
| FEOH1MS1 | | (click to browse) | | | | | | | | | | | | | |

SATURATED VLE																								
BOTH					VAPOR					LIQUID														
T(K)	P(bar)	$\rho_{\text{liq}} (\text{g}/\text{cm}^3)$	$\rho_{\text{vap}} (\text{g}/\text{cm}^3)$	U (kJ/mol)	S (kJ/mol)	C _p (J/mol·K)	C _v (J/mol·K)	C _∞ (J/mol·K)	α_{HFE} (m ² /s)	η (cP)	κ (Pa ⁻¹)	α (J/mol·K)	$\rho_{\text{liq}} (\text{g}/\text{cm}^3)$	$\rho_{\text{vap}} (\text{g}/\text{cm}^3)$	S (kJ/mol)	C _p (J/mol·K)	C _v (J/mol·K)	C _∞ (J/mol·K)	α_{HFE} (m ² /s)	η (cP)	κ (Pa ⁻¹)	α (J/mol·K)		
230	0.24387	0.0183	0.75223	1.3233	27.019	28.303	135.31	71.137	60.055	183.58	4.9534	5.8209	0.0104	627.33	0.0016	6.1547	6.157	36.415	83.344	120.95	-0.048	342.120	0.1863	
240	0.40218	0.017058	1.1963	0.58785	27.705	29.658	134.44	73.796	62.988	182.25	4.3661	6.0634	0.0101	618.95	0.0016	7.3758	7.3795	41.612	85.774	123.4	195.12	-0.045	238.320	0.1121
250	0.6335	0.015827	1.8253	0.34755	28.406	30.423	133.68	76.548	66.093	194.52	3.6843	6.3045	0.0122	608.28	0.0016	8.6216	8.6227	46.697	87.591	126	1093.4	-0.042	262.040	0.1079
260	0.95885	0.014608	2.6848	0.37247	29.12	31.396	133.58	79.396	69.439	196.32	3.4866	6.5453	0.0131	595.37	0.0017	9.8936	9.903	51.687	89.541	128.76	1036.1	-0.031	231.630	0.1039
270	1.4017	0.013404	3.8685	0.25162	29.846	31.974	133.5	82.398	72.394	197.53	3.1687	6.7673	0.014	584.17	0.0017	11.193	11.207	56.592	91.592	131.7	973.29	-0.036	205.670	0.0999
280	1.9876	0.012275	5.3164	0.1881	30.581	32.754	133.61	85.375	96.722	198.23	2.8823	7.0328	0.015	574.32	0.0017	12.522	12.543	61.427	93.728	134.98	922.77	-0.032	183.200	0.0986
290	2.74	0.011044	7.217	0.13856	31.326	33.535	133.67	88.503	103.75	199.35	2.5839	7.2844	0.016	560.71	0.0018	13.863	13.911	66.201	95.946	138.25	885.47	-0.027	164.800	0.0922
300	3.7	0.009817	9.6096	0.10406	32.076	34.314	134.26	91.721	105.2	197.74	2.4641	7.5457	0.017	548.32	0.0018	15.276	15.315	97.427	98.243	141.94	810.25	-0.022	148.220	0.0896
310	4.8858	0.0087166	12.589	0.07944	32.83	35.086	134.74	95.03	110.33	196.37	2.3074	7.8217	0.0182	535.33	0.0019	16.705	16.758	75.615	100.62	145.98	753.97	-0.016	133.640	0.0851
320	6.3335	0.0075559	16.263	0.05477																				

<http://webbook.nist.gov/chemistry/>

- ```
tolerance 3.0
filetype pdb
output STEP2_ISB_packed_BOX_0.pdb

structure isobutane.pdb
number 1000
inside box 0.1 0.1 0.1 70.20 70.20 70.20
end structure
```

Packmol scripts are typically saved with the extension `*.inp`, so this might be named `"pack_isobutane.inp"`. To run the script, we type the following line into the terminal:

```
$./packmol < pack_isobutane.inp
```

The PSF file stores the topology, mass, charges, and atom identities of molecules in the system.

- Protein Structure File (PSF)
- Space-separated file
- Used by NAMD, CHARMM, X-PLOR



The PSF file is not as robustly documented as the PDB format, but a basic description of it can be found here:

<http://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-win-html/node24.html>

The PSF file is generally composed of a series of sections. A line with a numeric value is typically at the top of each section. This value lists the number of entries in that section (lines can contain multiple entries; a dihedral, for example has two quadruplet entries of atom indices per line). Note that outside the remarks and atom section, this number is typically smaller than the number of lines by a factor of 2 to 4.

PSF files always start with the string “PSF” on their first line.

GOMC reuses PSF reading code from NAMD, hence it should have much of the same flexibility and limitations. By section, the segments of a PSF file are:

- TITLE: remarks on the file
- BONDS: the bonds (if applicable) in molecules
- ANGLE: the bonds (if applicable) in molecules
- DIHEDRAL: the bonds (if applicable) in molecules
- IMPROPER: the bonds (if applicable) in molecules
- (other sections such as cross terms)

The code currently skips the title section and reads the bonds, angles, dihedrals and impropers.

A few important **Notes** / **Warnings**:

- The PSF file format is a highly redundant file format. It repeats identical topology of thousands of molecules of a common kind in some cases. GOMC follows the same approach as NAMD, allowing this excess information externally and compiling it in the code.
- Other sections (e.g. cross terms) contain unsupported or legacy parameters and are ignored.
- Following the restrictions of VMD, the order of the PSF atoms must match the order in the PDB file.
- Improper entries are read and stored, but are not currently used. Support will eventually be added for this.

The PSF file is typically generated using PSFGen. It is convenient to make a script, such as the example below, to do this:

```
psfgen << ENDMOL
topology ./Top_branched_Alaknes.inp
segment ISB{
 pdb ./STEP2_ISB_packed_BOX_0.pdb
 first none
 last none
}

coordpdb ./STEP2_ISB_packed_BOX_0.pdb ISB

writepsf ./STEP3_START_ISB_sys_BOX_0.psf
writepdb ./STEP3_START_ISB_sys_BOX_0.pdb
```

Typically, one script is run per box to generate a finalized PDB/PSF for that box. The script requires one additional file, the NAMD-style topology file. While GOMC does not directly read or interact with this

file, it's typically used to generate the PSF and, hence, is considered one of the integral file types. It will be briefly discussed in the following section.

Here's a peek at how the generated PSF file looks for a packed isobutane system (abridged):

```

PSF
 3 !NTITLE
REMARKS original generated structure x-plor psf file
REMARKS topology ./Top_Branched_Alkanes.inp
REMARKS segment ISB { first NONE; last NONE; auto angles dihedrals }

 4000 !NATOM
 1 ISB 1 ISB C1 CH1 0.000000 13.0190 0
 2 ISB 1 ISB C2 CH3 0.000000 15.0350 0
 3 ISB 1 ISB C3 CH3 0.000000 15.0350 0
 4 ISB 1 ISB C4 CH3 0.000000 15.0350 0
 5 ISB 2 ISB C1 CH1 0.000000 13.0190 0
 6 ISB 2 ISB C2 CH3 0.000000 15.0350 0
 7 ISB 2 ISB C3 CH3 0.000000 15.0350 0
 8 ISB 2 ISB C4 CH3 0.000000 15.0350 0
.
.
.
 3997 ISB 1000 ISB C1 CH1 0.000000 13.0190 0
 3998 ISB 1000 ISB C2 CH3 0.000000 15.0350 0
 3999 ISB 1000 ISB C3 CH3 0.000000 15.0350 0
 4000 ISB 1000 ISB C4 CH3 0.000000 15.0350 0
 3000 !BOND: bonds
 1 2 1 3 1 4 5 6
 5 7 5 8
.
.
.
 3997 3998 3997 3998 3999 3997 4000
 3000 !NTHETA: angles
 2 1 4 2 1 3 3 1 4
 6 5 8 6 5 7 7 5 8
.
.
.
 3998 3997 4000 3998 3997 3999 3999 3997 4000

 0 !NPHI: dihedrals
 0 !NIMPHI: impropers
 0 !NDON: donors
 0 !NACC: acceptors
 0 !NNB
 0 0 0 0 0 0 0 0 0
 0 0 0 0 0 0 0 0 0
.
.
.

```

### 8.3 Topology File

The topology is a whitespace separated file format, which contains a list of atoms and their corresponding masses, and a list of residue information (charges, composition, and topology). Essentially, it is a non-redundant lookup table equivalent to the PSF file.

This is followed by a series of residues, which tell PSFGen what atoms are bonded to a given atom. Each residue is comprised of four key elements:

- A header beginning with the keyword RESI with the residue name and net charge
- A body with multiple ATOM entries (not to be confused with the PDB-style entries of the same name), which list the partial charge on the particle and what kind of atom each named atom in a specific molecule/residue is.
- A section of lines starting with the word BOND contains pairs of bonded atoms (typically 3 per line)
- A closing section with instructions for PSFGen.

Here's an example of a residue definition for isobutane:

```
RESI ISB 0.00 ! isobutane - TraPPE
GROUP
ATOM C1 CH1 0.00 ! C3
ATOM C2 CH3 0.00 ! C2-C1
ATOM C3 CH3 0.00 ! C4
ATOM C4 CH3 0.00 !
BOND C1 C2 C1 C3 C1 C4
PATCHING FIRS NONE LAST NONE
```

Here's a full parameter file prepared to pack a system of isobutane:

```
*
* Custom top file -- branched alkanes
*
1 1
!
MASS 1 CH3 15.035 C !
MASS 2 CH1 13.019 C !

RESI ISB 0.00 ! isobutane - TraPPE
GROUP
ATOM C1 CH1 0.00 ! C3
ATOM C2 CH3 0.00 ! C2-C1
ATOM C3 CH3 0.00 ! C4
ATOM C4 CH3 0.00 !
BOND C1 C2 C1 C3 C1 C4
PATCHING FIRS NONE LAST NONE

END
```

Note that the keyword END must be used to terminate this file and keywords related to the auto-generation process must be placed near the top of the file, after the MASS definitions.

More in-depth information can be found in the following links:

“Topology Tutorial” (PDF, in-depth)

<http://www.ks.uiuc.edu/Training/Tutorials/science/topology/topology-tutorial.pdf>

“NAMD Tutorial: 4. Examining the Topology File”

<http://www.ks.uiuc.edu/Training/Tutorials/science/topology/topology-html/node4.html>

“Developing Topology and Parameter Files”

<http://www.ks.uiuc.edu/Training/Tutorials/science/forcefield-tutorial/forcefield-html/node6.html>

“NAMD Tutorial: 25. Topology Files”

<http://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-win-html/node25.html>

**NOTE:** Links are courtesy of UIUC.

## 8.4 Parameter File(s):

Currently, GOMC uses a single parameter file and the user has the two kinds of parameter file choices:

- “CHARMM” (Chemistry at Harvard Molecular Mechanics) compatible parameter file
- “EXOTIC” parameter file

If the parameter file type is not specified or if the chosen file is missing, an error will result.

Both force field file options are whitespace separated files with sections preceded by a tag. When a known tag (representing a molecular interaction in the model) is encountered, reading of that section of the force field begins. Comments (anything after a \* or !) and whitespace are ignored. Reading concludes when the end of the file is reached or another section tag is encountered.

### CHARMM format parameter file

CHARMM contains a widely used model for describing energies in Monte Carlo and molecular dynamics simulations. It is intended to be compatible with other codes that use such a format, such as NAMD. For a general overview of the CHARMM force field, see:

[http://www.charmmtutorial.org/index.php/The\\_Energy\\_Function](http://www.charmmtutorial.org/index.php/The_Energy_Function)

Here’s the basic CHARMM contributions that are supported in GOMC:

$$\begin{aligned} U_{\text{bond}} &= \sum_{\text{bonds}} K_b (b - b_0)^2 & U_{\text{dihedral}} &= \sum_{\text{dihedrals}} K_\phi [1 + \cos(n\phi - \delta)] \\ U_{\text{angle}} &= \sum_{\text{angles}} K_\theta (\theta - \theta_0)^2 & U_{\text{LJ}} &= \sum_{\text{nonbonded}} \epsilon_{ij} \left[ \left( \frac{R_{\text{min}_{ij}}}{r_{ij}} \right)^{12} - 2 \left( \frac{R_{\text{min}_{ij}}}{r_{ij}} \right)^6 \right] + \frac{q_i q_j}{\epsilon r_{ij}} \end{aligned}$$

As seen above, the following are recognized, read and used:

- BONDS
  - Quadratic expression describing bond stretching based on bond length (b) in Angstrom
  - Typically, it is ignored as bonds are rigid for Monte Carlo simulations. To specify that it is to be ignored, put a very large value i.e. “999999999999” for  $K_b$ .

**NOTE:** GOMC does not sample bond stretch.

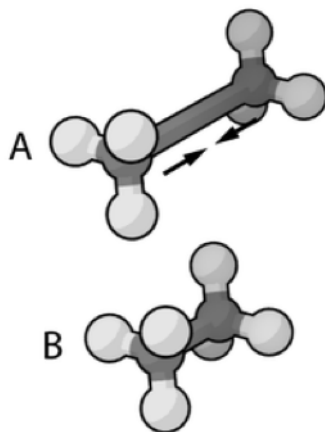


Figure 3: Image Courtesy of Wikimedia Commons

- ANGLES

- Describe the conformational behavior of an angle ( $\vartheta$ ) between three atoms, one of which is shared branch point to the other two. To fix any angle and ignore the related angle energy, put a very large value i.e. “999999999999” for  $K_\theta$ .

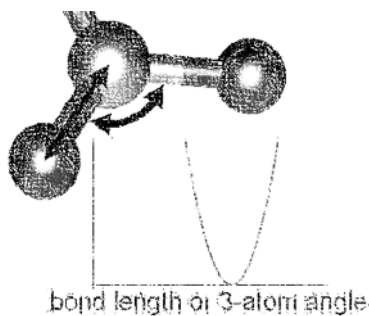


Figure 4: Image Courtesy of Wikimedia Commons

- DIHEDRALS

- Describes crankshaft-like rotation behavior about a central bond in a series of three consecutive bonds (rotation is given as  $\phi$ ).

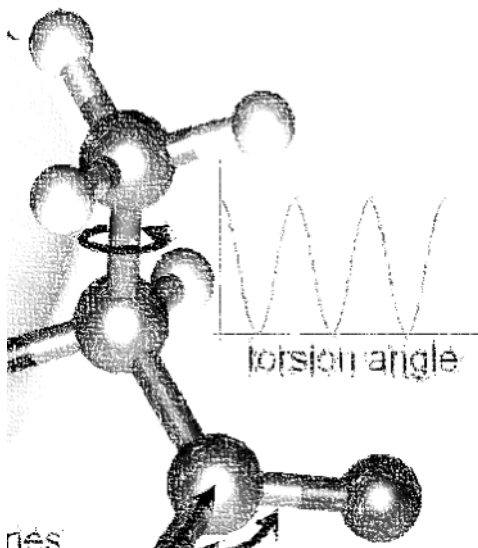


Figure 5: Image Courtesy of Wikimedia Commons

- **NONBONDED**

- This tag name only should be used if CHARMM force files are being used. This section describes 12-6 (Lennard-Jones) non-bonded interactions. Non-bonded parameters are assigned by specifying atom type name followed by polarizabilities (which will be ignored), minimum energy, and (minimum radius)/2. In order to modify 1-4 interaction, a second polarizability (again, will be ignored), minimum energy, and (minimum radius)/2 need to be defined; otherwise, the same parameter will be considered for 1-4 interaction.

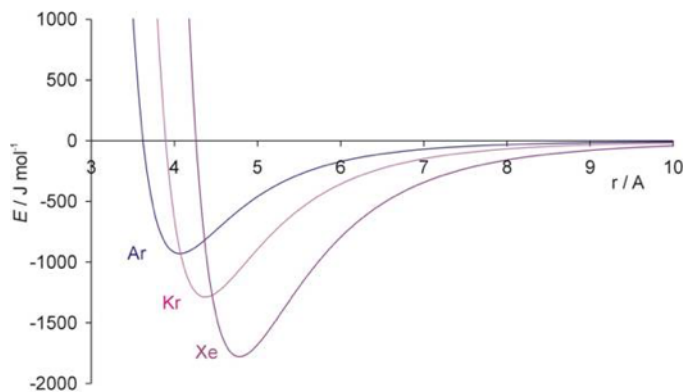


Figure 6: Image Courtesy of Wikimedia Commons

- **NBFIX**

- This tag name only should be used if CHARMM force field is being used. This section allows interaction between two pairs of atoms to be modified, done by specifying two atom type names followed by minimum energy and minimum radius. In order to modify 1-4 interaction, a second minimum energy and minimum radius need to be defined; otherwise, the same parameter will be considered for 1-4 interaction.

**NOTE:** Please pay attention that in this section we define minimum radius, not (minimum radius)/2 as it is defined in the NONBONDED section.

Currently, supported sections of the CHARMM compliant file include BONDS, ANGLES, DIHEDRALS, NONBONDED, NBFIX. Other sections such as CMAP are not currently read or supported.

### 8.4.1 BONDS

(“bond stretching”) is one key section of the CHARMM-compliant file. Units for the  $K_b$  variable in this section are in kcal/mol; the  $b_0$  section (which represents the equilibrium bond length for that kind of pair) is measured in Angstroms.

```
BONDS
!V(bond) = Kb(b - b0)**2
!
!Kb: kcal/mole/A**2
!b0: A
!
! Kb (kcal/mol) = Kb (K) * Boltz. const.;
!
!atom type Kb b0 description
CH3 CH1 9999999999 1.540 ! TraPPE 2
```

**NOTE:** The  $K_b$  value may appear odd, but this is because a larger value corresponds to a more rigid bond. As Monte Carlo force fields (e.g. TraPPE) typically treat molecules as rigid constructs,  $K_b$  is set to a large value - 9999999999. Sampling bond stretch is not supported in GOMC.

### 8.4.2 ANGLES

(“bond bending”), where  $\theta$  and  $\theta_0$  are commonly measured in degrees and  $K_\theta$  is measured in kcal/mol/K. These values, in literature, are often expressed in Kelvin (K). To convert Kelvin to kcal/mol/K, multiply by the Boltzmann constant –  $K_b$ , 0.0019872041 kcal/mol. In order to fix the angle, it requires to set a large value for  $K_\theta$ . By assigning a large value like 9999999999, specified angle will be fixed and energy of that angle will be considered to be zero.

Here is an example of what is necessary for isobutane:

```
ANGLES
!
!V(angle) = Ktheta(Theta - Theta0)**2
!
!V(Urey-Bradley) = Kub(S - S0)**2
!
!Ktheta: kcal/mole/rad**2
!Theta0: degrees
!S0: A
!
! Ktheta (kcal/mol) = Ktheta (K) * Boltz. const.
!
!atom types Ktheta Theta0 Kub(?) S0(?)
CH3 CH1 CH3 62.100125 112.00 ! TraPPE 2
```

Some CHARMM ANGLES section entries include Urey-Bradley potentials ( $K_{ub}$ ,  $b_{ub}$ ), in addition to the

standard quadratic angle potential. The constants related to this potential function are currently read, but the logic has not been added to calculate this potential function. Support for this potential function will be added in later versions of the code.

The final major bonded interactions section of the CHARMM compliant parameter file are the DIHEDRALS. Each dihedral is composed of a dihedral series of 1 or more terms. Often, there are 4 to 6 terms in a dihedral. Angles for the dihedrals' deltas are given in degrees.

Since isobutane has no dihedral, here are the parameters pertaining to 2,3-dimethylbutane:

```
DIHEDRALS
!
!V(dihedral) = Kchi(1 + cos(n(chi) - delta))
!
!Kchi: kcal/mole
!n: multiplicity
!delta: degrees
!
! Kchi (kcal/mol) = Kchi (K) * Boltz. const.
!
!atom types Kchi n delta description
X CH1 CH1 X -0.498907 0 0.0 ! TraPPE 2
X CH1 CH1 X 0.851974 1 0.0 ! TraPPE 2
X CH1 CH1 X -0.222269 2 180.0 ! TraPPE 2
X CH1 CH1 X 0.876894 3 0.0 ! TraPPE 2
```

**NOTE:** The code allows the use of 'X' to indicate ambiguous positions on the ends. This is useful because this kind is often determined solely by the two middle atoms in the middle of the dihedral, according to literature.

### 8.4.3 IMPROPER

Energy parameters used to describe out-of-plane rocking are currently read, but unused. The section is often blank. If it becomes necessary, algorithms to calculate the improper energy will need to be added.

The next section of the CHARMM style parameter file is the NONBONDED. In order to use TraPPE this section of the CHARMM compliant file is critical. Here's an example with our isobutane potential model:

```
NONBONDED
!
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!atom ignored epsilon Rmin/2 ignored eps,1-4 Rmin/2,1-4
!
CH3 0.0 -0.194745992 2.10461634058 0.0 0.0 0.0 ! TraPPE 1
CH1 0.0 -0.019872040 2.62656119304 0.0 0.0 0.0! TraPPE 2
End
```

**NOTE:** The  $R_{min}$  is different from  $\sigma$ .  $\sigma$  is the distance to the x-intercept (where interaction energy goes from being repulsive to positive).  $R_{min}$  is the potential well-depth, where the attraction is maximum. To convert  $\sigma$  to  $R_{min}$ , simply multiply  $\sigma$  by 0.56123102415, and flag it with a negative sign.

The last section of the CHARMM style parameter file is the NBFIX. In this section, individual pair interaction will be modified. First, pseudo non-bonded parameters have to be defined in NONBONDED and modified in NBFIX. Here's an example if it is required to modify interaction between CH3 and CH1 atoms:



```

NBFIX
!V(Lennard-Jones) = Eps,i,j[(Rmin,i,j/ri,j)**12 - 2(Rmin,i,j/ri,j)**6]
!
!atom atom epsilon Rmin eps,1-4 Rmin,1-4
CH3 CH1 -0.294745992 1.10461634058 !
End

```

## 8.5 Exotic Parameter file

The exotic file is intended for use with nonstandard/specialty models of molecular interaction, which are not included in CHARMM standard. Currently, two custom interaction are included:

**NONBONDED\_MIE** This section describes n-6 (Lennard-Jones) non-bonded interactions. The Lennard-Jones potential (12-6) is a subset of this potential. Non-bonded parameters are assigned by specifying atom type name followed by minimum energy, atom diameter, and repulsion exponent. In order to modify 1-4 interaction, a second minimum energy, atom diameter, and repulsion exponent need to be defined; otherwise, the same parameters would be considered for 1-4 interaction.

**NBFIX\_MIE** This section allows n-6 (Lennard-Jones) interaction between two pairs of atoms to be modified. This is done by specifying two atoms type names followed by minimum energy, atom diameter, and repulsion exponent. In order to modify 1-4 interaction, a second minimum energy, atom diameter, and repulsion exponent need to be defined; otherwise, the same parameter will be considered for 1-4 interaction.

**NOTE:** In EXOTIC force field, the definition of atom diameter( $\sigma$ ) is same for both NONBONDED\_MIE and NBFIX\_MIE.

Otherwise, the exotic file reuses the same geometry section headings - BONDS / ANGLES / DIHEDRALS / etc. The only difference in these sections versus in the CHARMM format force field file is that the energies are in Kelvin ('K'), the unit most commonly found for parameters in Monte Carlo chemical simulation literature. This precludes the need to convert to kcal/mol, the energy unit used in CHARMM.

The most frequently used section of the exotic files in the Mie potential section is NONBONDED\_MIE.

Here are the parameters that are used to simulate alkanes:

```

NONBONDED_MIE
!
!V(mie) = 4*eps*((sig_ij/r_ij)n-(sig_ij/r_ij)6)
!
!atom eps sig n eps,1-4 sig,1-4 n,1-4
CH4 161.00 3.740 14 0.0 0.0 0.0 ! Potoff, et al. '09
CH3 121.25 3.783 16 0.0 0.0 0.0 ! Potoff, et al. '09
CH2 61.00 3.990 16 0.0 0.0 0.0 ! Potoff, et al. '09

```

**NOTE:** Although the units (Angstroms) are the same, the exotic file uses  $\sigma$ , not the  $R_{min}$  used by CHARMM. The energy in the exotic file are expressed in Kelvin (K), as this is the standard convention in the literature.

## 8.6 Control File (\*.conf)

The control file is GOMC's proprietary input file. It contains key settings. The settings generally fall under three categories:

- Input/Simulation Setup
- System Settings for During Run
- Output Settings

**NOTE:** The control file is designed to recognize logic values, such as “yes/true/on” or “no/false/off”.

### 8.6.1 Input/Simulation Setup

In this section, input file names are listed. In addition, if you want to restart your simulation or use integer seed for running your simulation, you need to modify this section according to your purpose.

**Restart** Determines whether to restart and, if so, what step to restart from.

- Value 1: *< BOOLEAN >* - true if restart, false otherwise

**FirstStep** Determines what step to restart from. If Restart was set to true, step number needs to be specified; otherwise, the program will terminate.

- Value 1: *< ULONG >* - step to restart from

```

enable, step

Restart true
FirstStep 1000000
```

**PRNG** Dictates how to start the pseudo-random number generator (PRNG)

- Value 1: *< STRING >*
  - RANDOM: Randomizes Mersenne Twister PRNG with random bits based on the system time.

```

kind {RESTART, RANDOM, INTSEED}

PRNG RANDOM
```

- INTSEED: This option “seeds” the Mersenne Twister PRNG with a standard integer. When the same integer is used, the generated PRNG stream should be the same every time, which is helpful in tracking down bugs.
- RESTART: Used for restarting a previous simulation. This option in the Mersenne Twister’s state from a saved file.

```

kind {RESTART, RANDOM, INTSEED}

PRNG RESTART
```

**Random\_Seed** Defines the seed number. If “INTSEED” is chosen, seed number needs to be specified; otherwise, the program will terminate.

- Value 1: `< ULONG >` or `< UINT >`: If “INTSEED” command is used (See above example).

```
#####
kind {RESTART, RANDOM, INTSEED}
#####
PRNG INTSEED
Random_Seed 50
```

**ParaTypeCHARMM** Sets force field type to CHARMM style.

- Value 1: `< BOOLEAN >` - true if it is CHARMM force field, false if it is not.

```
#####
FORCE FIELD TYPE
#####
ParaTypeCHARMM true
```

**ParaTypeEXOTIC** Sets force field type to EXOTIC style.

- Value 1: `< BOOLEAN >` - true if it is EXOTIC force field, false if it is not.

```
#####
FORCE FIELD TYPE
#####
ParaTypeEXOTIC true
```

**ParaTypeMARTINI** Sets force field type to MARTINI style.

- Value 1: `< BOOLEAN >` - true if it is MARTINI force field, false if it is not.

```
#####
FORCE FIELD TYPE
#####
ParaTypeMARTINI true
```

**Parameters** Provides the name and location of the parameter file to use for the simulation.

- Value 1: `< STRING >` - Sets the name of the parameter file.

```
#####
FORCE FIELD TYPE
#####
ParaTypeCHARMM yes
Parameters ../../common/Par_TraPPE_Alkanes.inp
```

**Coordinates** Defines the PDB filenames (coordinates) for each box in the system.

- Value 1: `< INTEGER >` - Sets box number (first box is box ‘0’).
- Value 2: `< STRING >` - Sets PDB file name

**NOTE:** NVT and NPT ensembles requires only one PDB file and GEMC/GCMC requires two PDB files. If the number of PDB files is not compatible with the simulation type, the program will terminate.

Example of NVT or NPT ensemble

```
#####
INPUT PDB FILES - NVT or NPT ensemble
#####
Coordinates 0 STEP3_START_ISB.sys.pdb
```

Example of Gibbs or GC ensemble

```

INPUT PDB FILES - Gibbs or GC ensemble

Coordinates 0 STEP3_START_ISB_sys_BOX_0.pdb
Coordinates 1 STEP3_START_ISB_sys_BOX_1.pdb
```

**Structures** Defines the PSF filenames (structures) for each box in the system.

- Value 1: `< INTEGER >` - Sets box number (first box is box '0').
- Value 2: `< STRING >` - Sets PSF file name

**NOTE:** NVT and NPT ensembles requires only one PSF file and GEMC/GCMC requires two PSF files. If the number of PSF files is not compatible with the simulation type, the program will terminate.

Example of NVT or NPT ensemble

```

INPUT PSF FILES

Structure 0 STEP3_START_ISB_sys.psf
```

Example of Gibbs or GC ensemble

```

INPUT PSF FILES

Structure 0 STEP3_START_ISB_sys_BOX_0.pdb
Structure 1 STEP3_START_ISB_sys_BOX_1.pdb
```

## 8.6.2 System Settings for During Run Setup

This section contains all the variables not involved in the output of data during the simulation, or in the reading of input files at the start of the simulation. In other words, it contains settings related to the moves, the thermodynamic constants (based on choice of ensemble), and the length of the simulation.

Note that some tags, or entries for tags, are only used in certain ensembles (e.g. Gibbs ensemble). These cases are denoted with colored text.

**GEMC** (For Gibbs Ensemble runs only) Defines what type of Gibbs Ensemble simulation you want to run.

If neglected in Gibbs Ensemble, it simply defaults to constant volume (NVT) Gibbs Ensemble.

- Value 1: `< STRING >` - allows you to pick between isovolumetric ("NVT") and isobaric ("NPT") Gibbs ensemble simulations

- NVT: Run simulation with constant molecule number, volume, and temperature.

```

GEMC TYPE (DEFAULT IS NVT_GEMC

GEMC NVT
```

- NPT: Run simulation with constant molecule number, pressure, and temperature.

**Pressure** If "NPT" simulation is chosen, imposed pressure (in bar) needs to be specified; otherwise, the program will terminate.

- Value 1: < *DOUBLE* > - Constant pressure in bars.

```
#####
GEMC TYPE (DEFAULT IS NVT_GEMC
#####
GEMC NPT
Pressure 5.76
```

**Temperature** Sets the temperature at which the system will run.

- Value 1: < *DOUBLE* > - The distance to truncate the Lennard-Jones potential at.

**RcutLow** Sets a specific minimum possible in angstrom that reject any move that place any atom closer than specified distance.

- Value 1: < *DOUBLE* > - The minimum possible distance between any atoms.

**LRC** Defines whether or not long range corrections are used.

- Value 1: < *BOOLEAN* > - True to consider long range correction. In case of using “SHIFT” or “SWITCH” potential functions, LRC will be ignored.

**Exclude** Defines which pairs of bonded atoms should be excluded from non-bonded interactions.

- Value 1: < *STRING* > - Allows you to choose between “1-2”, “1-3”, and “1-4”.
  - 1-2** All interactions pairs of bonded atoms, except the ones that separated with one bond, will be considered and modified using 1-4 parameters defined in parameter file.
  - 1-3** All interaction pairs of bonded atoms, except the ones that separated with one or two bonds, will be considered and modified using 1-4 parameters defined in parameter file.
  - 1-4** All interaction pairs of bonded atoms, except the ones that separated with one, two or three bonds, will be considered using non-bonded parameters defined in parameter file.

**NOTE:** The default value is “1-3”.

**Potential** Defines the potential function type to calculate non-bonded interaction energy and force between atoms.

- Value 1: < *STRING* > - Allows you to pick between “VDW”, “SHIFT” and “SWITCH”.

**VDW** Nonbonded interaction energy and force calculated based on n-6 (Lennard-Johns) equation. This function will be discussed further in the Intermolecular energy and Virial calculation section.

```
#####
SIMULATION CONDITION
#####
Temperature 200.00
Potential VDW
LRC true
Rcut 10
Exclude 1-4
```

**SHIFT** This option forces the potential energy to be zero at Rcut distance. This function will be discussed further in the Intermolecular energy and Virial calculation section.

```
#####
SIMULATION CONDITION
#####
Temperature 200.00
Potential SHIFT
LRC false
Rcut 10
Exclude 1-4
```

**SWITCH** This option smoothly forces the potential energy to be zero at  $R_{cut}$  distance and starts modifying the potential at **Rswitch** distance. Depending on force field type, specific potential function will be applied. These functions will be discussed further in the Intermolecular energy and Virial calculation section.

**Rswitch** In the case of choosing “SWITCH” as potential function, a distance is set in which non-bonded interaction energy is truncated smoothly from to cutoff distance.

- Value 1: `< DOUBLE >` - Define switch distance in angstrom. If the “SWITCH” function is chosen, **Rswitch** needs to be defined; otherwise, the program will be terminated.

**NOTE:** In CHARMM force field, the 1-4 interaction needs to be considered. Choosing “Exclude 1-3” will modify 1-4 interaction based on 1-4 parameter in parameter file. If a kind force field is used, where 1-4 interaction needs to be ignored, such as TraPPE, either “exclude 1-4” needs to be chosen or 1-4 parameter needs to be assigned a value of zero in the parameter file.

**ElectroStatic** Considers coulomb interaction or not.

- Value 1: `< BOOLEAN >` - True if coulomb interaction needs to be considered and false if not.

**NOTE:** If MARTINI force field was used and charged molecule was used in simulation, **ElectroStatic** needs to be turn on. MARTINI force field uses short range coulomb interaction with constant dielectric 15.0.

**Dielectric** Defines dielectric constant for coulomb interaction in MARTINI force field.

- Value 1: `< DOUBLE >` - Sets dielectric value used in coulomb interaction.

**NOTE:** In MARTINI force field, **Dielectric** needs to be set to 15.0. If MARTINI force field was chosen and if **Dielectric** was not specified, a default value of 15.0 will be assigned.

**Ewald** Considers standard Ewald summation method for electrostatic calculation.

- Value 1: `< DOUBLE >` - “true” if Ewald summation calculation needs to be considered and “false” if not.

**NOTE:** By default, **ElectroStatic** will be set to true if Ewald summation method was used to calculate coulomb interaction.

**CachedFourier** Considers storing the reciprocal terms for Ewald summation calculation in order to improve the code performance. This option would increase the code performance with the cost of memory usage.

- Value 1: `< BOOLEAN >` - “true” to store reciprocal terms of Ewald summation calculation and “false” if not.

**NOTE:** By default, **CachedFourier** will be set to “true” if not value was set.

**Tolerance** Specifies the accuracy of the Ewald summation calculation. Ewald separation parameter and number of reciprocal vectors for the Ewald summation are determined based on the accuracy parameter.

- Value 1: `< DOUBLE >` - Sets the accuracy in Ewald summation calculation. A reasonable value for the accuracy is 0.00001.

**NOTE:** If “Ewald” was chosen and no value was set for **Tolerance**, the program will be terminated.

**PressureCalc** Considers to calculate the pressure or not. If it is set to true, the frequency of pressure calculation need to be set.

- Value 1: `< BOOLEAN >` - “True” enabling pressure calculation during the simulation, “false” disabling pressure calculation.
- Value 2: `< ULONG >` - The frequency of calculating the pressure.

**1-4scaling** Defines constant factor to modify 1-4 short range coulomb interaction.

- Value 1: `< DOUBLE >` - A fraction number between 0.0 and 1.0 that sets 1-4 scaling factor.

**NOTE:** CHARMM force field uses a value between 0.0 and 1.0. In EXOTIC force field, it needs to be set to 0.0 because 1-4 interaction will not be considered in this force field. In MARTINI force field, it needs to be set to 1.0 because 1-4 interaction will not be modified in this force field.

```

SIMULATION CONDITION

ElectroStatic true
Ewald true
Tolerance 0.00001
1-4scaling 0.0
```

**RunSteps** Sets the total number of steps to run (one move is performed for each step) (cycles = this value / number of molecules in the system)

- Value 1: `< ULONG >` - Total run steps

**EqSteps** Sets the number of steps necessary to equilibrate the system; averaging will begin at this step.

- Value 1: `< ULONG >` - Equilibration steps

**AdjSteps** Sets the number of steps per adjustment to the maximum constants associated with each move (e.g. maximum distance in *xyz* to displace, the maximum volume in A3 to swap, etc.)

- Value 1: `< ULONG >` - Number of steps per move adjustment

```

STEPS

RunSteps 25000000
EqSteps 5000000
AdjSteps 1000
```

**ChemPot** (**For Grand Canonical (GC) ensemble runs only**): Chemical potential at which simulation is run.

- Value 1: `< STRING >` - The rename to apply this chemical potential w.r.t.
- Value 2: `< DOUBLE >` - The chemical potential value in degrees Kelvin (should be negative).

**NOTE:** For binay systems, include multiple copies of the tag (one per residue kind).

```

Mol. Name Chem. Pot. (K)

ChemPot AR -968
```

**DisFreq** Fractional percentage at which displacement move will occur.

- Value 1: `< DOUBLE >` - % displace

**RotFreq** Fractional percentage at which rigid rotation move will occur.

- Value 1: `< DOUBLE >` - % rotate

**IntraSwapFreq** Fractional percentage at which particle will be removed from a box and inserted into the same box.

- Value 1: < *DOUBLE* > - % Intra molecule swap

**VolFreq** ( For isobaric-isothermal ensemble and Gibbs ensemble runs only ) Fractional percentage at which volume displacement move will occur.

- Value 1: < *DOUBLE* > - % of volumen swaps

**SwapFreq** ( For Gibbs and Grand Canonical (GC) ensemble runs only ) Fractional percentage at which particle swap move will occur.

- Value 1: < *DOUBLE* > - % of molecule swaps

```
#####
MOVE FREQUENCY
#####
DisFreq 0.59
RotFreq 0.10
VolFreq 0.01
SwapFreq 0.20
IntraSwapFreq 0.10
```

**NOTE:** All move percentages should add up to 1.0; otherwise, the program will terminate.

**useConstantArea** ( For Isobaric-Isothermal ensemble and Gibbs ensemble runs only ) Considers to change the volume of the simulation box by fixing the cross-sectional area (x-y plane).

- Value 1: < *BOOLEAN* > - If “true” volume will change only in z axis, If “false” volume will change with constant axis ratio.

**NOTE:** By default, **useConstantArea** will be set to “false” if no value was set. It means, the volume of the box will change in a way to maintain the constant axis ratio.

**BoxDim** Defines the axis lengths of simulation box. This tag may occur multiple times. It occurs once for NVT and NPT, but twice for Gibbs ensemble or GC ensemble.

- Value 1: < *INTEGER* > - Sets box number (first box is box ‘0’)
- Value 2: < *DOUBLE* > - x-axis length in Angstroms
- Value 3: < *DOUBLE* > - y-axis length in Angstroms
- Value 4: < *DOUBLE* > - z-axis length in Angstroms

**NOTE:** If the number of defined boxes were not compatible to simulation type, the program will be terminated.

Example for NVT and NPT ensemble:

```
#####
BOX DIMENSION #, X, Y, Z
#####
BoxDim 0 40.00 40.00 40.00
```

Example for Gibbs ensemble and GC ensemble:

```
#####
BOX DIMENSION #, X, Y, Z
#####
BoxDim 0 106.00 106.00 106.00
BoxDim 1 176.00 176.00 176.00
```

**CBMC\_First** Number of CBMC trials to choose the first seed position (Lennard-Jones trials for first seed growth)



- Value 1: `< INTEGER >` - Number of initial insertion sites to try

**CBMC\_Nth** Number of CBMC trials to choose the later seed positions (Lennard-Jones trials for first seed growth)

- Value 1: `< INTEGER >` - Number of LJ trials for growing later atom positions

**CBMC\_Ang** Number of CBMC bending angle trials to perform for geometry (per the coupled-decoupled CBMC scheme)

- Value 1: `< INTEGER >` - Number of trials per angle

**CBMC\_Dih** Number of CBMC dihedral angle trials to perform for geometry (per the coupled-decoupled CBMC scheme)

- Value 1: `< INTEGER >` - Number of trials per dihedral

```
#####
CBMC TRIALS
#####
CBMC_First 10
CBMC_Nth 4
CBMC_Ang 100
CBMC_Dih 30
```

### 8.6.3 Output Controls

This section contains all the values that control output in the control file. For example, certain variables control the naming of files dumped of the block-averaged thermodynamic variables of interest, the PDB files, etc.

**OutputName** Unique name for simulation used to name the block average, PDB, and PSF output files.

- Value 1: `< STRING >` - Unique phrase to identify this system.

```
#####
OUTPUT FILE NAME
#####
OutputName ISB_T_270_K
```

**CoordinatesFreq** Controls output of PDB file (coordinates). If PDB dumping was enabled, one file for NVT or NPT and two files for Gibbs ensemble or GC ensemble will be dumped.

- Value 1: `< BOOLEAN >` - “true” enables dumping these files; “false” disables dumping.
- Value 2: `< ULONG >` - Steps per dump PDB frame. It should be less than or equal to RunSteps. If this keyword could not be found in configuration file, its value will be assigned a default value to dump 10 frames.

**NOTE:** The PDB file contains an entry for every ATOM, in all boxes read. This allows VMD (which requires a constant number of atoms) to properly parse frames, with a bit of help. Atoms that are not currently in a specific box are given the coordinate (0.00, 0.00, 0.00). The occupancy value corresponds to the box a molecule is currently in (e.g. 0.00 for box 0; 1.00 for box 1).

**NOTE:** At the beginning of simulation, a merged PSF file contain “\_merged” phrase, in which all boxes will be dumped. It also contains the topology for every molecule in both boxes, corresponding to the merged PDB format. Loading PDB files into merged PSF file in VMD allows the user to visualize and analyze the results.

**RestartFreq** Controls the output of the last state of simulation at a specified step in PDB files (coordinates) that contain “\_restart” phrase. If PDB dumping was enabled, one file for NVT or NPT and two files for Gibbs ensemble or GC ensemble will be dumped.

- Value 1: `< BOOLEAN >` - “true” enables dumping these files; “false” disables dumping.
- Value 2: `< ULONG >` - Steps per dump last state of simulation to PDB files. It should be less than or equal to `RunSteps`. If this keyword could not be found in the configuration file, `RestartFreq` value will be assigned by default.

**NOTE:** The restart PDB file contains only `ATOM` that exist in each boxes at specified steps. This allows the user to use `psfgen` and `tcl` to build a new PSF file and reload it to `RESTART` the simulation.

**NOTE:** `CoordinatesFreq` must be a common multiple of `RestartFreq` or vice versa.

**ConsoleFreq** Controls the output to `STDIO` (“the console”) of messages such as acceptance statistics, and run timing info. In addition, instantaneously-selected thermodynamic properties will be output to this file.

- Value 1: `< BOOLEAN >` - “true” enables message printing; “false” disables dumping.
- Value 2: `< ULONG >` - Number of steps per print. If this keyword could not be found in the configuration file, the value will be assigned by default to dump 1000 output for `RunSteps` greater than 1000 steps and 100 output for `RunSteps` less than 1000 steps.

**BlockAverageFreq** Controls the block averages output of selected thermodynamic properties. Block averages are averages of thermodynamic values of interest for chunks of the simulation (for post-processing of averages or std. dev. in those values).

- Value 1: `< BOOLEAN >` - “true” enables printing block average; “false” disables it.
- Value 2: `< ULONG >` - Number of steps per block-average output file. If this keyword cannot be found in the configuration file, its value will be assigned a default to dump 100 output.

**HistogramFreq** Controls the histograms. Histograms are a binned listing of observation frequency for a specific thermodynamic variable. In this code, they also control the output of a file containing energy/particle samples; it only will be used in GC ensemble simulations for histogram reweighting purposes.

- Value 1: `< BOOLEAN >` - “true” enables printing histogram; “false” disables it.
- Value 2: `< ULONG >` - Number of steps per histogram output file. If this keyword cannot be found in the configuration file, a value will be assigned by default to dump 1000 output for `RunSteps` greater than 1000 steps and 100 output for `RunSteps` less than 1000 steps.

```
#####
STATISTICS Enable, Freq.
#####
CoordinatesFreq true 10000000
RestartFreq true 1000000
ConsoleFreq true 100000
BlockAverageFreq true 100000
HistogramFreq true 10000
```

The next section controls the output of the energy/particle sample file and the distribution file for particle counts, commonly referred to as the “histogram” output. This section is only required if Grand Canonical ensemble simulation was used.

**DistName** Sets short phrase to naming particle distribution file.

- Value 1: `< STRING >` - Short phrase which will be combined with `RunNumber` and `RunLetter` to use in the name of the binned histogram for particle distribution.

**HistName** Sets short phrase to naming energy sample file.

- Value 1: < *STRING* > - Short phrase, which will be combined with **RunNumber** and **RunLetter**, to use in the name of the energy/particle count sample file.

**RunNumber** Sets a number, which is a part of **DistName** and **HistName** file name.

- Value 1: < *UINT* > - Run number to be used in the above file names.

**RunLetter** Sets a letter, which is a part of **DistName** and **HistName** file name.

- Value 1: < *CHAR* > - Run letter to be used in above file names.

**SampleFreq** Controls histogram sampling frequency.

- Value 1: < *UINT* > - the number of steps per histogram sample.

```

OutHistSettings

DistName dis
HistName his
RunNumber 5
RunLetter a
SampleFreq 200
```

**OutEnergy\*\*\*, OutPressure\*\*\*, OutMolNumber\*\*, OutDensity\*\*, OutVolume\*\*\*, OutSurfaceTension\***  
Enables/Disables for specific kinds of file output for tracked thermodynamic quantities

(\*) = NVT ensemble, (\*) = NPT ensemble and Gibbs ensemble, (\*) = GC ensemble

- Value 1: < *BOOLEAN* > - “true” enables message output of block averages via this tracked parameter (and in some cases such as entry, components); “false” disables it.
- Value 2: < *BOOLEAN* > - “true” enables message output of a fluctuation into the console file via this tracked parameter (and in some cases, such as entry, components); “false” disables it.

```

ENABLE: BLK AVE., FLUC.

OutEnergy true true
OutPressure true true
OutMolNum true true
OutDensity true true
OutVolume true true
OutSurfaceTention false false
```

## 9 Sample Files

Here's a sample of how a typical **NVT ensemble** control file might be expected to look:

```
#=====
#= GOMC - NVT Control example
#=====

#####
##=====----- INPUT -----=====
#####

#####
ENABLE, STEP
#####
Restart false

#####
KIND {RESTART, RANDOM, INTSEED}
#####
PRNG RANDOM

#####
FORCE FIELD
#####
ParaTypeCHARMM true
Parameters ../../common/Par_MODEL_NAME.inp

#####
INPUT PDB FILES
#####
Coordinates 0 STEP3_START_XX_PHA_BOX_0.pdb

#####
INPUT PSF FILES
#####
Structure 0 STEP3_START_XX_PHA_BOX_0.psf

#####
=====----- SYSTEM -----=====
#####

#####
SIMULATION CONDITION
#####
Temperature 200.00
Potential VDW
LRC true
Rcut 10
Exclude 1-4
```

```

#####
ELECTROSTATIC
#####
ElectroStatic true
Ewald false
Tolerance 0.00001
1-4scaling 0.0

#####
STEPS
#####
RunSteps 25000000
EqSteps 5000000
AdjSteps 1000

#####
MOVE FREQUENCY
#####
DisFreq 0.80
RotFreq 0.10
IntraSwapFreq 0.10

#####
PRESSURE CALCULATION
#####
PressureCalc true 10000

#####
BOX DIMENSION #, X, Y, Z
#####
BoxDim 0 35.00 35.00 35.00

#####
CBMC TRIALS
#####
CBMC_First 10
CBMC_Nth 4
CBMC_Ang 100
CBMC_Dih 30

#####
=====-- OUTPUT -----
#####

#####
OUTPUT FILE NAME
#####
OutputName AR_200_00_K_2220_r5

```

```
#####
STATISTICS ENABLE, FREQ.
#####
CoordinatesFreq true 1000000
RestartFreq true 1000000
ConsoleFreq true 1000000
BlockAverageFreq true 1000000

#####
ENABLE: BLK AVF., FLUCK.
#####
OutEnergy true true
OutPressure true true
OutMolNum false false
OutDensity false false
```

Here's a sample of how a typical [Gibbs ensemble](#) control file might be expected to look:

```
=====
= GOMC - Gibbs ensemble Control example
=====

#####
ENABLE, STEP
#####
Restart false

#####
KIND RESTART, RANDOM, INTSEED
#####
PRNG INTSEED
Random_Seed 49

#####
FORCE FIELD
#####
ParaTypeEXOTIC true
Parameters Par_MODEL_NAME.inp

#####
INPUT PDB FILES
#####
Coordinates 0 STEP3_START_XX_PHA_BOX_0.pdb
Coordinates 1 STEP3_START_XX_PHA_BOX_1.pdb

#####
INPUT PSF FILES
#####
Structure 0 STEP3_START_XX_PHA_BOX_0.psf
Structure 1 STEP3_START_XX_PHA_BOX_1.psf

#####
===== SYSTEM =====
#####

#####
GEMC TYPE (DEFAULT IS NVT_GEMC)
#####
GEMC NPT
Pressure 2.50

#####
SIMULATION CONDITION
#####
Temperature 200.00
Potential SWITCH
LRC false
Rswitch 7
Rcut 10
RcutLow 1.0
Exclude 1-4
```

```

#####
ELECTROSTATIC
#####
Ewald false
ElectroStatic false

#####
STEPS
#####
RunSteps 25000000
EqSteps 5000000
AdjSteps 1000

#####
MOVE FREQUENCY
#####
DisFreq 0.69
RotFreq 0.10
VolFreq 0.01
SwapFreq 0.20
IntraSwapFreq 0.00

#####
PRESSURE CALCULATION
#####
PressureCalc true 10000

#####
BOX DIMENSION #, X, Y, Z
#####
BoxDim 0 35.00 35.00 35.00
BoxDim 1 45.00 45.00 45.00

#####
CBMC TRIALS
#####
CBMC_First 8
CBMC_Nth 4
CBMC_Ang 100
CBMC_Dih 30

#####
===== OUTPUT =====
#####

#####
OUTPUT FILE NAME
#####
OutputName AR_200_00_K_2220_r5

```



```

#####
STATISTICS ENABLE, FREQ.
#####
CoordinatesFreq true 1000000
RestartFreq true 1000000
ConsoleFreq true 1000000
BlockAverageFreq true 1000000

#####
ENABLE: BLK AVF., FLUCK.
#####
OutEnergy true true
OutPressure true true
OutMolNum true true
OutDensity true true

```

Here's a sample of how a typical **grand canonical** ensemble control file might be expected to look:

```
=====
= GOMC - Grand canonical ensemble Control example
=====
#####
ENABLE, STEP
#####
Restart false

#####
KIND RESTART, RANDOM, INTSEED
#####
PRNG RANDOM

#####
FORCE FIELD
#####
ParaTypeCHARMM false
ParaTypeEXOTIC true
Parameters Par_MODEL_NAME.inp

#####
INPUT PDB FILES
#####
Coordinates 0 STEP3_START_XX_PHA_BOX_0.pdb
Coordinates 1 STEP3_START_XX_PHA_ Reserv_BOX_1.pdb

#####
INPUT PSF FILES
#####
Structure 0 STEP3_START_XX_PHA_BOX_0.psf
Structure 1 STEP3_START_XX_PHA_ Reserv_BOX_1.psf

#####
===== SYSTEM =====
#####

#####
SIMULATION CONDITION
#####
Temperature 200.00
Potential VDW
LRC true
Rcut 10
Exclude 1-4

#####
ELECTROSTATIC
#####
Ewald true
ElectroStatic true
CachedFourier true
Tolerance 0.00001
1-4scaling 0.0
```

```

#####
STEPS
#####
RunSteps 25000000
EqSteps 5000000
AdjSteps 1000

#####
MOVE FREQUENCY
#####
DisFreq 0.20
RotFreq 0.20
SwapFreq 0.60

#####
PRESSURE CALCULATION
#####
PressureCalc false

#####
BOX DIMENSION #, X, Y, Z
#####
BoxDim 0 35.00 35.00 35.00
BoxDim 1 45.00 45.00 45.00

#####
CBMC TRIALS
#####
CBMC_First 8
CBMC_Nth 4
CBMC_Ang 100
CBMC_Dih 30

#####
Mol. Name Chem. Pot.
#####
ChemPot DME -2230

#####
===== OUTPUT =====
#####

#####
OUTPUT FILE NAME
#####
OutputName DME_200_00_K_2220

```

```

#####
STATISTICS ENABLE, FREQ.
#####
CoordinatesFreq true 1000000
RestartFreq true 1000000
ConsoleFreq true 1000000
BlockAverageFreq true 1000000
HistogramFreq true 100000

#####
OutHistSettings
#####
DistName dis
HistName his
RunNumber 5
RunLetter a
SampleFreq 200

#####
ENABLE: BLK AVF., FLUCK.
#####
OutEnergy true true
OutPressure false false
OutMolNum true true
OutDensity false false
OutSurfaceTension false false

```

## 10 GOMC's Output Files, Terminal Output

GOMC currently supports several kinds of output:

- STDIO (“console”) output
- File output
  - PDB
  - PSF
  - Block Averages

GOMC output units:

| Properties                | Units  | Properties      | Units          |
|---------------------------|--------|-----------------|----------------|
| Energy                    | $K$    | Volume          | $\text{\AA}^3$ |
| Pressure, Pressure Tensor | bar    | Density         | $kg/m^3$       |
| Heat of vaporization      | KJ/mol | Surface Tension | mN/m           |

### 10.1 Console Output

A variety of useful information relating to instantaneous statistical and thermodynamic data (move trials, acceptance rates, file I/O messages warnings, and other kinds of information) is printed to the **STDIO**, which, in Linux, will typically be displayed in the terminal. This output can be redirected into a log file in Linux using the “>” operator.

Statistical and thermodynamic information is provided in console output.

- Energy
  - Intermolecular (LJ)
  - Intramolecular bonded
  - Intramolecular nonbonded
  - Tail corrections
  - Electrostatic real
  - Electrostatic Reciprocal
  - Electrostatic self
  - Electrostatic correction
  - Total electrostatic energy (sum of real, reciprocal, self, and correction)
  - Total Energy (sum of the all energies)
- Pressure, Pressure Tensor ( $P_{xx}, P_{yy}, P_{zz}$ )
- Volume
- Total molecule number
- Total Density
- Surface Tension
- Mole fraction of each species

Detailed move, energy, and statistical or thermodynamic information for each simulation box will be printed in three different sections. Each section’s title will start with **MTITLE**, **ETITLE**, and **STITLE** for move, energy, and statistical information, respectively. The instantaneous values for each section will start with **MOVE\_#**, **ENER\_#**, and **STAT\_#** for move, energy, and statistical values, respectively. Where, **#** is the simulation box number. In addition, if pressure calculation is activated and enabled to print, pressure tensor will be printed in the console output file. This section starts with **PRES\_#** and print the diagonal value of pressure tensor  $P_{xx}$ ,  $P_{yy}$ , and  $P_{zz}$ , respectively. The second element after the title of each section is the step number.

In order to extract the desired information from the console file, “grep” and “awk” commands can be used with a proper title section. For example, in order to extract total energy of the system, the following command needs to be executed in terminal:

```
grep ‘‘ENER_0’’ output_console.log | awk ‘{print $3}’
```

Here, “output\_console.log” is the console output file and “\$3” represents the second element of the “ENERGY\_BOX\_0” section. The first section of this console output typically includes some info relating to the system, CPU, and RAM. In continue, console output includes information regarding the input file (configuration file) reading, force field reading, summary of the topology of the molecule, and minimum and maximum coordinate of molecules. This output is important; it may contain text relating to issues encountered if there was an error in the current run (e.g. a bad parameter, unknown keyword, missing parameters in the configuration file, etc.)

**NOTE**: Surface Tension is calculated using Virial method according to following equation,

$$\gamma = \frac{1}{2A_{xy}} \int_0^L \left( P_{zz} - \frac{P_{xx} + P_{yy}}{2} \right) dz \quad (1)$$

```

GOMC Serial Version 1.9
Started at: Sat Apr 22 21:44:50 2017
On hostname: potoff39.eng.wayne.edu

Total number of CPUs: 4
Total number of CPUs available: 4
Model name: Intel(R) Core(TM) i5-2500K CPU @ 3.30GHz

System name: Linux
Release: 2.6.32-642.4.2.el6.x86_64
Version: #1 SMP Tue Aug 23 19:58:13 UTC 2016
Kernel Architecture: x86_64
Total Ram: 7856.3MB
Used Ram: 5239.3MB
Working in the current directory /home3/soroush/Desktop/validation/GOMC_Examples\
/GCMC/isobutane/run2a_bridge

This code was compiled to support the grand canonical ensemble.

REMINDER: CHARMM force field has been selected!
Temperature of system has been set to 410.00000 K
Warning: Pressure calculation is turned off.
By default intra box swap frequency has been set to zero
Warning: Electrostatic energy would not be calculated!
Reading from CHARMM-Style Parameter File file: ../../../../common/Par_TraPPE_Alka\
nes_CHARMM.inp
Finished reading CHARMM-Style Parameter File file: ../../../../common/Par_TraPPE_\
Alkanes_CHARMM.inp
Reading from Box 1 PDB coordinate file file: ./STEP3_START_ISB_vap_BOX_0.pdb
Finished reading Box 1 PDB coordinate file file: ./STEP3_START_ISB_vap_BOX_0.pdb
Reading from Box 2 PDB coordinate file file: ./STEP3_START_ISB_reservoir_BOX_1.p\
db
Finished reading Box 2 PDB coordinate file file: ./STEP3_START_ISB_reservoir_BOX\
_1.pdb
Random number seed: 2018226010

Molecules in PSF:
Molecule Kind: ISB

Idx	name	type	charge	mass
0	C1	CH1	0.0000	13.0190
1	C2	CH3	0.0000	15.0350
2	C3	CH3	0.0000	15.0350
3	C4	CH3	0.0000	15.0350

Bonds:
[0 1] [0 2] [0 3]
Angles:
[1 0 3] [1 0 2] [2 0 3]
Dihedrals:

REMINDER! 1-3 and 1-4 Interaction is OFF
Minimum coordinates in box 0: x = 1.000, y = 20.816, z = 25.283
Maximum coordinates in box 0: x = 5.215, y = 28.682, z = 29.000
Minimum coordinates in box 1: x = 1.000, y = 1.000, z = 1.000
Maximum coordinates in box 1: x = 29.000, y = 29.000, z = 29.000

```

Next, the energy title and initial energy of the system's starting configuration will print:

```
#####
INITIAL SIMULATION ENERGY
ETITLE: STEP TOTAL INTRA(B) INTRA(NB) INTER(LJ)\
 LRC TOTAL_ELECT REAL RECIP SELF\
 CORR
ENER_0: 0 206.4495 364.4544 0.0000 -153.5288\
 -4.4761 0.0000 0.0000 0.0000 0.0000\
 -0.0000
ENER_1: 0 109688.7579 109688.7579 0.0000 0.0000\
 0.0000 0.0000 0.0000 0.0000 0.0000\
 -0.0000
```

After the simulation starts, move, energy, and statistical title, followed by their values for each simulation box, will print:

```
#####
STARTING SIMULATION
MTITLE: STEP DISTR DISACCEP DISACCEP% DISMAX\
 ROTATE ROTACCEP ROTACCEP% ROTMAX INTRASWAP\
 INTACCEP INTACCEP% TRANSFER TRANACCEP TRANACCEP%
ETITLE: STEP TOTAL INTRA(B) INTRA(NB) INTER(LJ)\
 LRC TOTAL_ELECT REAL RECIP SELF\
 CORR
STITLE: STEP TOTALMOL
Printed combined psf to file ISB_410_00_K_u_3135_r1a_merged.psf
MOVE_0: 10000 1924 886 46.0499 2.2351\
 1012 790 78.0632 15.0000 0\
 0 0.0000 3478 1870 53.7665
ENER_0: 10000 6190.3884 8704.4147 0.0000 -2294.6957\
 -219.3306 0.0000 0.0000 0.0000 0.0000\
 0.0000
STAT_0: 10000 14
MOVE_1: 10000 3586 1882 52.4819
ENER_1: 10000 363442.1856 363442.1856 0.0000 0.0000\
 0.0000 0.0000 0.0000 0.0000 0.0000\
 0.0000
STAT_1: 10000 588
Steps/sec. : 8109.0109
```

At the end of the run, timing information and other wrap up info will be printed.

**NOTE:** Printed energy and statistical values are instantaneous values.

**NOTE:** It's important to watch the acceptance rates and adjust the move percentages and CBMC trial amounts to get the desired rate of move acceptance.



## 10.2 PDB and PSF Files

The PDB and PSF output (merging of atom entries) has already been mentioned/explained in previous sections. To recap: The PDB file's `ATOM` entries' occupancy is used to represent the box the molecule is in for the current frame. All molecules are listed in order in which they were read (i.e. if box 0 has  $1..N_1$  molecules and box 1 has  $1..N_2$  molecules, then all of the molecules in box 0 are listed first and all the molecules in box 1, i.e.  $1..N_1, N_1 + 1..N_1 + N_2$ ). PDB frames are written as standard PDBs to consecutive file frames.

To visualize, open the PDB and PSF files output by VMD and use the command in the terminal:

```
pbj join connected
```

Use the TKConsole to get the current frame to obey the periodicity. Some peculiarities will still be observed, so please review the PDB file if anything looks odd (e.g. bonds will sometimes not show up in later frames). The GOMC team is in the process of improving VMD compatibility, but this may require changes to VMD to allow the files output to be read properly.

For Gibbs ensemble, the same PSF will be used to visualize either box, i.e.

```
vmd ISB_T_330.00_K_Run_0_MIE_BOX_0.pdb ISB_T_330.00_K_Run_0_MIE_merged.pdb
```

... for visualizing the first box and...

```
vmd ISB_T_330.00_K_Run_0_MIE_BOX_1.pdb ISB_T_330.00_K_Run_0_MIE_merged.pdb
```

... for visualizing the second box.

## 10.3 Block Output Files

GOMC tracks a number of thermodynamic variables of interest during the simulation and prints them all in one file for each box.

- Energy
  - Intermolecular (LJ)
  - Intramolecular bonded
  - Intramolecular nonbonded
  - Tail corrections
  - Electrostatic real
  - Electrostatic Reciprocal
  - Total Energy (sum of the all energies)
- Virial
- Pressure
- Surface Tension (using virial method)
- Volume
- Total molecule number
- Total Density
- Mole fraction of each species
- Heat of vaporization

At the beginning of each file, the title of each property followed by their average values is printed. Desired data can be extracted, as explained before, using the “awk” command. For example, in order to extract total density of the system, the following command need to be executed in terminal:

```
cat Blk_OUTPUTNAME_BOX_0.dat | awk '{print $13}'
```

Here, “Blk\_OUTPUTNAME\_BOX\_0.dat” is the block-average file for simulation box 0 and “\$13” represents the 13th column of the block file.

## 11 Putting it all together: Running a GOMC Simulation

It is strongly recommended that you download the test system provided at <http://gomc.eng.wayne.edu/downloads.html> or [https://github.com/GOMC-WSU/GOMC\\_Examples/tree/master](https://github.com/GOMC-WSU/GOMC_Examples/tree/master)

Run different simulation types in order to become more familiar with different parameter and configuration files (\*.conf).

To recap the previous examples, a simulation of isobutane will be completed for a single temperature point on the saturated vapor-liquid coexistence curve.

The general plan for running the simulation is:

1. Build GOMC (if not done already)
2. Copy GOMC executable to build directory
3. Create scripts, PDB, and topology file to build the system, plus in.dat file and parameter files to prepare for runtime
4. Build finished PDBs and PSFs using the simulation.
5. Run the simulation in the terminal.
6. Analyze the output.

Please, complete steps 1 and 2; then, traverse to the directory, which should now contain a single file “GOMC\_Serial.GEMC”. Next, six files need to be made:

- PDB file for isobutane
- Topology file describing isobutane residue
- Two \*.inp packmol scripts to pack two system boxes
- Two TCL scripts to input into PSFGen to generate the final configuration

### isobutane.pdb

```
REMARK 1 File created by GaussView 5.0.8
ATOM 1 C1 ISB 1 0.911 -0.313 0.000 C
ATOM 2 C2 ISB 1 1.424 -1.765 0.000 C
ATOM 3 C3 ISB 1 -0.629 -0.313 0.000 C
ATOM 4 C4 ISB 1 1.424 0.413 -1.257 C
END
```

### Top\_Branched\_Alkane.inp

```

* Custom top file -- branched alkanes
*
MASS 1 CH3 15.035 C !
MASS 3 CH1 13.019 C !

RESI ISB 0.00 ! isobutane { TraPPE
GROUP
ATOM C1 CH1 0.00 ! C3
ATOM C2 CH3 0.00 ! C2-C1
ATOM C3 CH3 0.00 ! C4
ATOM C4 CH3 0.00 !
BOND C1 C2 C1 C3 C1 C4
PATCHING FIRS NONE LAST NONE
END

```

#### pack\_box\_0.inp

```

tolerance 3.0
filetype pdb
output STEP2_ISB_packed_BOX_0.pdb

structure isobutane.pdb
number 1000
inside box 0. 0. 0. 68.00 68.00 68.00
end structure

```

#### pack\_box\_1.inp

```

tolerance 3.0
filetype pdb
output STEP2_ISB_packed_BOX_1.pdb

structure isobutane.pdb
number 1000
inside box 0. 0. 0. 68.00 68.00 68.00
end structure

```

#### build\_box\_0.inp

```

psfgen << ENDMOL
topology ./Top_Branched_Alkane.inp
segment ISB {
 pdb ./STEP2_ISB_packed_BOX_0.pdb
 first none
 last none
}
coordpdb ./STEP2_ISB_packed_BOX_0.pdb ISB
writepsf ./STEP3_START_ISB_sys_BOX_0.psf
writepdb ./STEP3_START_ISB_sys_BOX_0.pdb

```

#### build\_box\_1.inp

```

psfgen << ENDMOL
topology ./Top_Branched_Alkane.inp
segment ISB {
 pdb ./STEP2_ISB_packed_BOX_1.pdb
 first none
 last none
}
coordpdb ./STEP2_ISB_packed_BOX_1.pdb ISB
writepsf ./STEP3_START_ISB_sys_BOX_1.psf
writepdb ./STEP3_START_ISB_sys_BOX_1.pdb

```

These files can be created with a standard Linux or Windows text editor. Please, also copy a Packmol executable into the working directory.

Once those files are created, run in the terminal:

```

./packmol < pack_box_0.inp
./packmol < pack_box_1.inp

```

This will create the intermediate PDBs.

Then, run the PSFGen scripts to finish the system using the following commands:

```

vmd < ./build_box_0.inp
vmd < ./build_box_1.inp

```

This will create the intermediate PDBs.

To run the code a few additional things will be needed:

- A GOMC Gibbs ensemble executable
- A control file
- Parameter files.

Enter the control file (in.conf) in the text editor in order to modify it. Example files for different simulation types can be found in previous section.

Once these four files have been added to the output directory, the simulation is ready.

Assuming the code is named GOMC\_CPU\_GEMC, run in the terminal using:

```

./GOMC_CPU_GEMC in.conf > out_ISB_T_330.00_K_RUN_0.log &

```

For running GOMC in parallel, using openmp, run in the terminal using:

```

./GOMC_CPU_GEMC +p4 in.conf > out_ISB_T_330.00_K_RUN_0.log &

```

Here, 4 defines the number of processors that will be used to run the simulation in parallel.

Progress can be monitored in the terminal with the tail command:

```

tail -f out_ISB.log

```

**Congratulations!** You have examined a single-phase coexistence point on the saturated vapor-liquid curve using GOMC operating in the Gibbs ensemble.

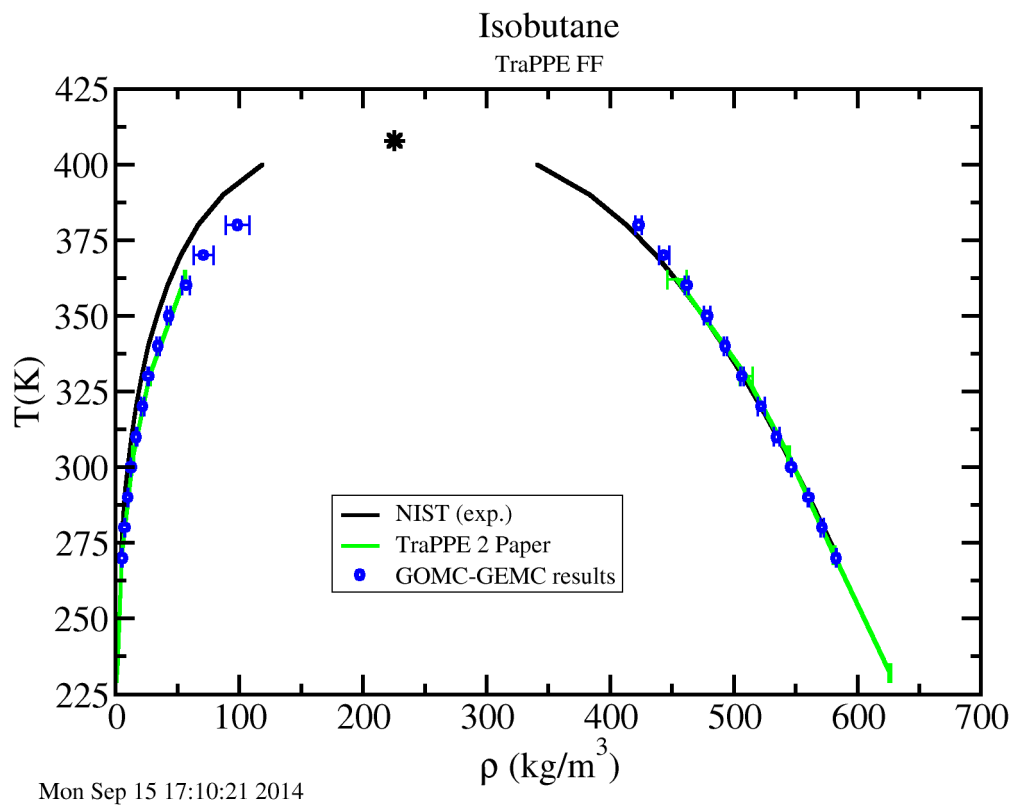


Figure 7: Repeating this process for multiple temperatures will allow you to obtain the following results.

## 12 Intermolecular Energy and Virial function (Van der Waals)

In this section, the virial and energy equation of Van der Waals interaction for different potential function are discussed in details.

### 12.1 VDW

This option calculates potential energy without any truncation.

- **Potential Calculation:** Interactions between atoms can be modeled with an n-6 potential, a Mie potential in which the attractive exponent is fixed. The Mie potential can be viewed as a generalized version of the 12-6 Lennard-Jones potential,

$$E_{ij} = C_{n_{ij}} \epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{n_{ij}} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \quad (2)$$

where  $r_{ij}$ ,  $\epsilon_{ij}$ , and  $\sigma_{ij}$  are, respectively, the separation, well depth, and collision diameter for the pair of interaction sites  $i$  and  $j$ . The constant  $C_n$  is a normalization factor such that the minimum of the potential remains at  $-\epsilon_{ij}$  for all  $n_{ij}$ . In the 12-6 potential,  $C_n$  reduces to the familiar value of 4.

$$C_{n_{ij}} = \left( \frac{n_{ij}}{n_{ij} - 6} \right) \left( \frac{n_{ij}}{6} \right)^{6/(n_{ij}-6)} \quad (3)$$

- **Virial Calculation:** Virial is basically the negative derivative of energy with respect to distance, multiplied by distance.

$$W_{ij} = -\frac{dE_{ij}}{dr} \times \frac{r_{ij}}{r_{ij}} \quad (4)$$

Using n-6 LJ potential defined above:

$$W_{ij} = 6C_{n_{ij}} \epsilon_{ij} \left[ \frac{n_{ij}}{6} \times \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{n_{ij}} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \times \frac{\vec{r}_{ij}}{r_{ij}^2} \quad (5)$$

**NOTE:** This option only evaluates the energy up to specified **Rcut** distance. Tail correction to energy and pressure can be specified to account for infinite cutoff distance.

### 12.2 SHIFT

This option forces the potential energy to be zero at **Rcut** distance.

- **Potential Calculation:** Interactions between atoms can be modeled with an n-6 potential,

$$E_{ij}(\text{shift}) = C_{n_{ij}} \epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{n_{ij}} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] - C_{n_{ij}} \epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{cut}} \right)^{n_{ij}} - \left( \frac{\sigma_{ij}}{r_{cut}} \right)^6 \right] \quad (6)$$

where  $r_{ij}$ ,  $\epsilon_{ij}$ , and  $\sigma_{ij}$  are, respectively, the separation, well depth, and collision diameter for the pair of interaction sites  $i$  and  $j$ . The constant  $C_n$  is a normalization factor according to Eq. 3, such that the minimum of the potential remains at  $-\epsilon_{ij}$  for all  $n_{ij}$ . In the 12-6 potential,  $C_n$  reduces to the familiar value of 4.

- **Virial Calculation:** Virial is basically the negative derivative of energy with respect to distance, multiplied by distance, Eq. 4.

Using **SHIFT** potential function defined above:

$$W_{ij}(\text{shift}) = 6C_{n_{ij}} \epsilon_{ij} \left[ \frac{n_{ij}}{6} \times \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{n_{ij}} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \times \frac{\vec{r}_{ij}}{r_{ij}^2} \quad (7)$$

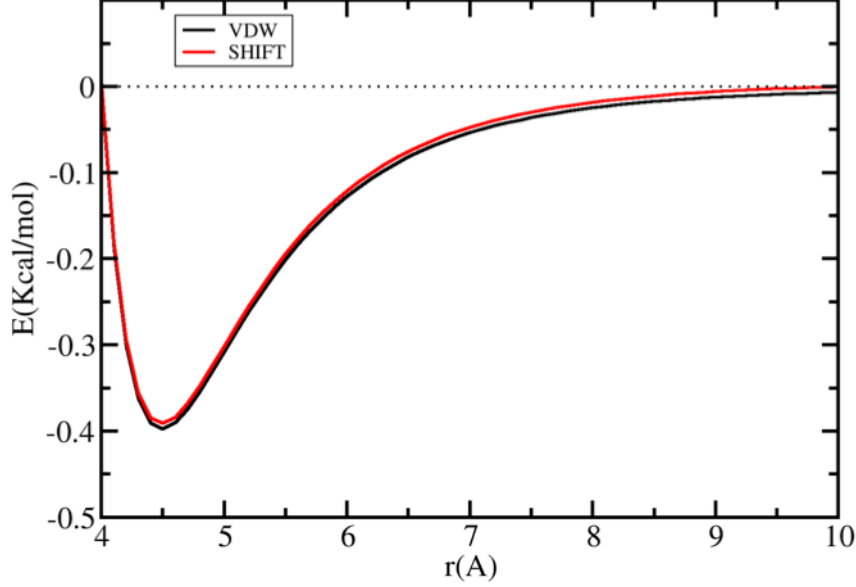


Figure 8: Graph of Van der Waals potential with and without the application of the **SHIFT** function. With the **SHIFT** function active, the potential by force was reduced to 0.0 at the **Rcut** distance. With the **SHIFT** function, there is a discontinuity where the potential is truncated.

### 12.3 SWITCH

This option in **CHARMM** or **EXOTIC** force field smoothly forces the potential energy to be zero at **Rcut** distance and starts modifying the potential at **Rswitch** distance.

- Potential Calculation: Interactions between atoms can be modeled with an n-6 potential,

$$E_{ij}(\text{switch}) = C_{n_{ij}} \epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{n_{ij}} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \times F_E \quad (8)$$

where  $r_{ij}$ ,  $\epsilon_{ij}$ , and  $\sigma_{ij}$  are, respectively, the separation, well depth, and collision diameter for the pair of interaction sites  $i$  and  $j$ . The constant  $C_n$  is a normalization factor according to Eq. 3, such that the minimum of the potential remains at  $-\epsilon_{ij}$  for all  $n_{ij}$ . In the 12-6 potential,  $C_n$  reduces to the familiar value of 4.

The factor  $F_E$  is defined as:

$$F_E = \begin{cases} 1 & r_{ij} \leq r_{\text{switch}} \\ \frac{(r_{\text{cut}}^2 - r_{ij}^2)^2 \times (r_{\text{cut}}^2 - 3r_{\text{switch}}^2 + 2r_{ij}^2)}{(r_{\text{cut}}^2 - r_{\text{switch}}^2)^3} & r_{\text{switch}} < r_{ij} < r_{\text{cut}} \\ 0 & r_{ij} \geq r_{\text{cut}} \end{cases}$$

- Virial Calculation: Virial is basically the negative derivative of energy with respect to distance, multiplied by distance, Eq. 4.

Using **SWITCH** potential function defined above:

$$W_{ij}(\text{switch}) = \left[ 6C_{n_{ij}} \epsilon_{ij} \left[ \frac{n_{ij}}{6} \times \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{n_{ij}} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \times \frac{F_E}{r_{ij}^2} - C_{n_{ij}} \epsilon_{ij} \left[ \left( \frac{\sigma_{ij}}{r_{ij}} \right)^{n_{ij}} - \left( \frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \times F_W \right] \times \vec{r}_{ij} \quad (9)$$

The factor  $F_W$  is defined as:

$$F_W = \begin{cases} 1 & r_{ij} \leq r_{switch} \\ \frac{12(r_{cut}^2 - r_{ij}^2) \times (r_{switch}^2 - r_{ij}^2)}{(r_{cut}^2 - r_{switch}^2)^3} & r_{switch} < r_{ij} < r_{cut} \\ 0 & r_{ij} \geq r_{cut} \end{cases}$$

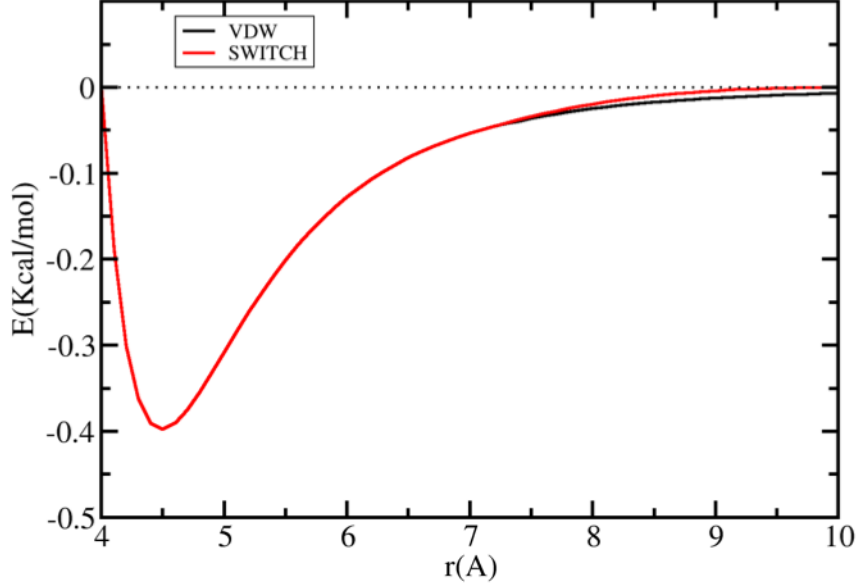


Figure 9: Graph of Van der Waals potential with and without the application of the SWITCH function. With the SWITCH function active, the potential is smoothly reduced to 0.0 at the Rcut distance.

## 12.4 SWITCH

This option in MARTINI force field smoothly forces the potential energy to be zero at Rcut distance and starts modifying the potential at Rswitch distance.

- Interactions between atoms can be modeled with an n-6 potential. In standard MARTINI,  $n$  is equal to 12,

$$E_{ij}(\text{switch}) = C_{n_{ij}} \epsilon_{ij} \left[ \sigma_{ij}^n \left( \frac{1}{r_{ij}^n} + \varphi_n(r_{ij}) \right) - \sigma_{ij}^6 \left( \frac{1}{r_{ij}^6} + \varphi_6(r_{ij}) \right) \right] \quad (10)$$

where  $r_{ij}$ ,  $\epsilon_{ij}$ , and  $\sigma_{ij}$  are, respectively, the separation, well depth, and collision diameter for the pair of interaction sites  $i$  and  $j$ . The constant  $C_n$  is a normalization factor according to Eq. 3, such that the minimum of the potential remains at  $-\epsilon_{ij}$  for all  $n_{ij}$ . In the 12-6 potential,  $C_n$  reduces to the familiar value of 4.

The factor  $\varphi_\alpha$  and constants are defined as:

$$\varphi_\alpha(r_{ij}) = \begin{cases} -C_\alpha & r_{ij} \leq r_{switch} \\ -\frac{A_\alpha}{3}(r_{ij} - r_{switch})^3 - \frac{B_\alpha}{4}(r_{ij} - r_{switch})^4 - C_\alpha & r_{switch} < r_{ij} < r_{cut} \\ 0 & r_{ij} \geq r_{cut} \end{cases}$$

$$A_\alpha = \alpha \frac{(\alpha + 1)r_{switch} - (\alpha + 4)r_{cut}}{r_{cut}^{(\alpha+2)}(r_{cut} - r_{switch})^2} \quad (11)$$



$$B_\alpha = \alpha \frac{(\alpha + 1)r_{switch} - (\alpha + 3)r_{cut}}{r_{cut}^{(\alpha+2)}(r_{cut} - r_{switch})^3} \quad (12)$$

$$C_\alpha = \frac{1}{r_{cut}^\alpha} - \frac{A_\alpha}{3}(r_{cut} - r_{switch})^3 - \frac{B_\alpha}{4}(r_{cut} - r_{switch})^4 \quad (13)$$

- Virial Calculation: Virial is basically the negative derivative of energy with respect to distance, multiplied by distance, Eq. 4.

Using the **SWITCH** potential function defined for **MARTINI** force field:

$$W_{ij}(\text{switch}) = C_{n_{ij}} \epsilon_{ij} \left[ \sigma_{ij}^n \left( \frac{n}{r_{ij}^{(n+1)}} + d\varphi_n(r_{ij}) \right) - \sigma_{ij}^6 \left( \frac{6}{r_{ij}^{(6+1)}} + d\varphi_6(r_{ij}) \right) \right] \times \frac{\vec{r}_{ij}}{r_{ij}} \quad (14)$$

The constants defined in Eq. 11-13 and the factor  $d\varphi_\alpha$  defined as:

$$d\varphi_\alpha(r_{ij}) = \begin{cases} 0 & r_{ij} \leq r_{switch} \\ A_\alpha(r_{ij} - r_{switch})^2 + B_\alpha(r_{ij} - r_{switch})^3 & r_{switch} < r_{ij} < r_{cut} \\ 0 & r_{ij} \geq r_{cut} \end{cases}$$

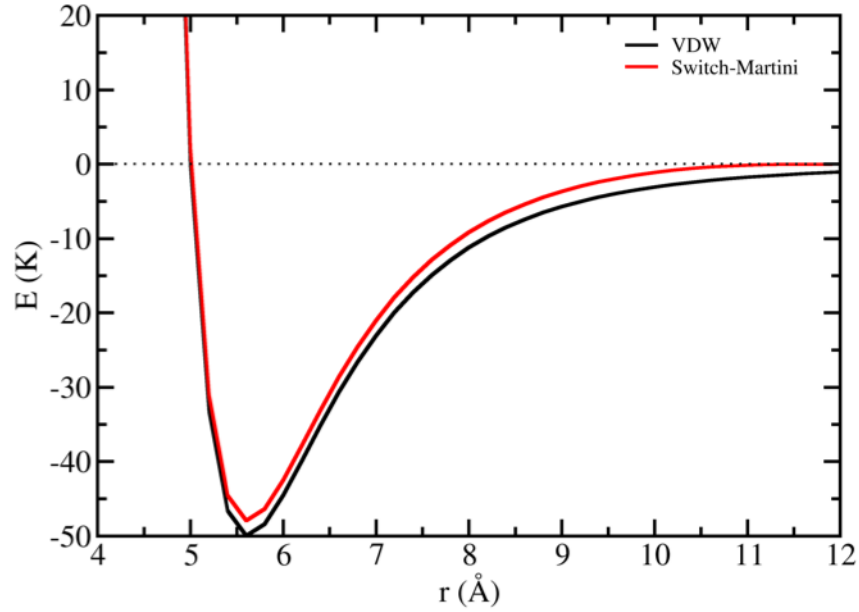


Figure 10: Graph of Van der Waals potential with and without the application of the **SWITCH** function in **MARTINI** force field. With the **SWITCH** function active, the potential is smoothly reduced to 0.0 at the  $R_{cut}$  distance.

## 13 Intermolecular Energy and Virial function (Electrostatic)

In this section, the virial and energy equation of electrostatic interaction for different potential function are discussed in details.

### 13.1 Ewald

This option calculate electrostatic energy using standard **Ewald Summation Method**.

**NOTE**: Once this option is activated, it would override the the electrostatic calculation using **VDW**, **SHDT**, and **SWITCH** functions.

- Potential Calculation: Coulomb interactions between atoms can be modeled as

$$E(\text{Ewald}) = E_{real} + E_{reciprocal} + E_{self} + E_{correction} \quad (15)$$

$E_{real}$ : Defines the short range electrostatic energy according to

$$E_{real} = \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N q_i q_j \frac{\text{erfc}(\alpha r_{ij})}{r_{ij}} \quad (16)$$

, where  $\alpha$  is **Ewald** separation parameter according to

$$\alpha = \frac{\sqrt{-\log(\text{Tolerance})}}{r_{cut}} \quad (17)$$

, where  $\text{Tolerance}$  is a parameter, controlling the desired accuracy.

$E_{reciprocal}$ : Defines the long range electrostatic energy according to,

$$E_{reciprocal} = \frac{1}{\epsilon_0 V} \frac{1}{2} \sum_{\vec{k} \neq 0} \frac{1}{k^2} \exp\left(\frac{-\vec{k}^2}{4\alpha^2}\right) \left[ |R_{sum}|^2 + |I_{sum}|^2 \right] \quad (18)$$

, where  $\vec{k}$  is reciprocal vector,  $R_{sum}$  and  $I_{sum}$  are,

$$R_{sum} = \sum_{i=1}^N q_i \cos(\vec{k} \cdot \vec{x}_i) \quad (19)$$

$$I_{sum} = \sum_{i=1}^N q_i \sin(\vec{k} \cdot \vec{x}_i) \quad (20)$$

$E_{self}$ : Defines the self energy according to,

$$E_{self} = -\frac{\alpha}{4\pi\epsilon_0\sqrt{\pi}} \sum_{i=1}^N q_i^2 \quad (21)$$

$E_{correction}$ : Defines intra-molecule nonbonded enegy,

$$E_{correction} = -\frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{j=1}^N \sum_{l=1}^{N_j} \sum_{m=1}^{N_j} q_{j_l} q_{j_m} \frac{\text{erf}(\alpha r_{j_l j_m})}{r_{j_l j_m}} \quad (22)$$

- **Virial Calculation:** Virial is basically the negative derivative of energy with respect to distance, multiplied by distance, Eq. 4. Coulomb force between atoms can be modeled as,

$$W(\text{Ewald}) = W_{real} + W_{reciprocal} \quad (23)$$

$W_{real}$ : Defines the short range electrostatic force according to,

$$W_{real} = \frac{1}{4\pi\epsilon_0} \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N q_i q_j \left[ \frac{\text{erfc}(\alpha r_{ij})}{r_{ij}} + \frac{2\alpha}{\sqrt{\pi}} \exp(-\alpha^2 r_{ij}^2) \right] \times \frac{\vec{r}_{ij}}{r_{ij}^2} \quad (24)$$

$W_{reciprocal}$ : Defines the long range electrostatic force according to,

$$W_{reciprocal} = \frac{1}{\epsilon_0 V} \frac{1}{2} \sum_{\vec{k} \neq 0} \left[ \frac{1}{\vec{k}^2} \exp\left(\frac{-\vec{k}^2}{4\alpha^2}\right) \left( |R_{sum}|^2 + |I_{sum}|^2 \right) \left( 1 - \frac{\vec{k}^2}{2\alpha^2} \right) \right] + \sum_{i=1}^N \frac{1}{\epsilon_0 V} \sum_{\vec{k} \neq 0} \left[ \frac{q_i}{\vec{k}^2} \exp\left(\frac{-\vec{k}^2}{4\alpha^2}\right) \left[ I_{sum} \times \cos(\vec{k} \cdot \vec{x}_i) - R_{sum} \times \sin(\vec{k} \cdot \vec{x}_i) \right] \right] \times (\vec{k} \cdot \vec{r}_{ic}) \quad (25)$$

, where  $\vec{r}_{ic}$  is the vector between atom and the center of the mass of the molecule.

## 13.2 SHIFT

This option forces the electrostatic energy to be zero at **Rcut** distance.

- **Potential Calculation:** Coulomb interactions between atoms can be modeled as

$$E(\text{SHIFT}) = \frac{q_i q_j}{4\pi\epsilon_0} \left( \frac{1}{r_{ij}} - \frac{1}{r_{cut}} \right) \quad (26)$$

- **Virial Calculation:** Virial is basically the negative derivative of energy with respect to distance, multiplied by distance, Eq. 4. Coulomb force between atoms can be modeled as,

$$E(\text{SHIFT}) = \frac{q_i q_j}{4\pi\epsilon_0} \left( \frac{1}{r_{ij}} \times \frac{\vec{r}_{ij}}{r_{ij}^2} \right) \quad (27)$$