USER'S MANUAL

version 1.90

Development Version

Distributed by the Potoff and Schwiebert Groups

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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-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.

Introduction (What is GOMC?)

Monte Carlo (MC) simulation is a type of simulation driven by stochastic processes. The "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, 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. Pressure calculation for a charged system and support for cyclic molecules is being developed.

How to get the software

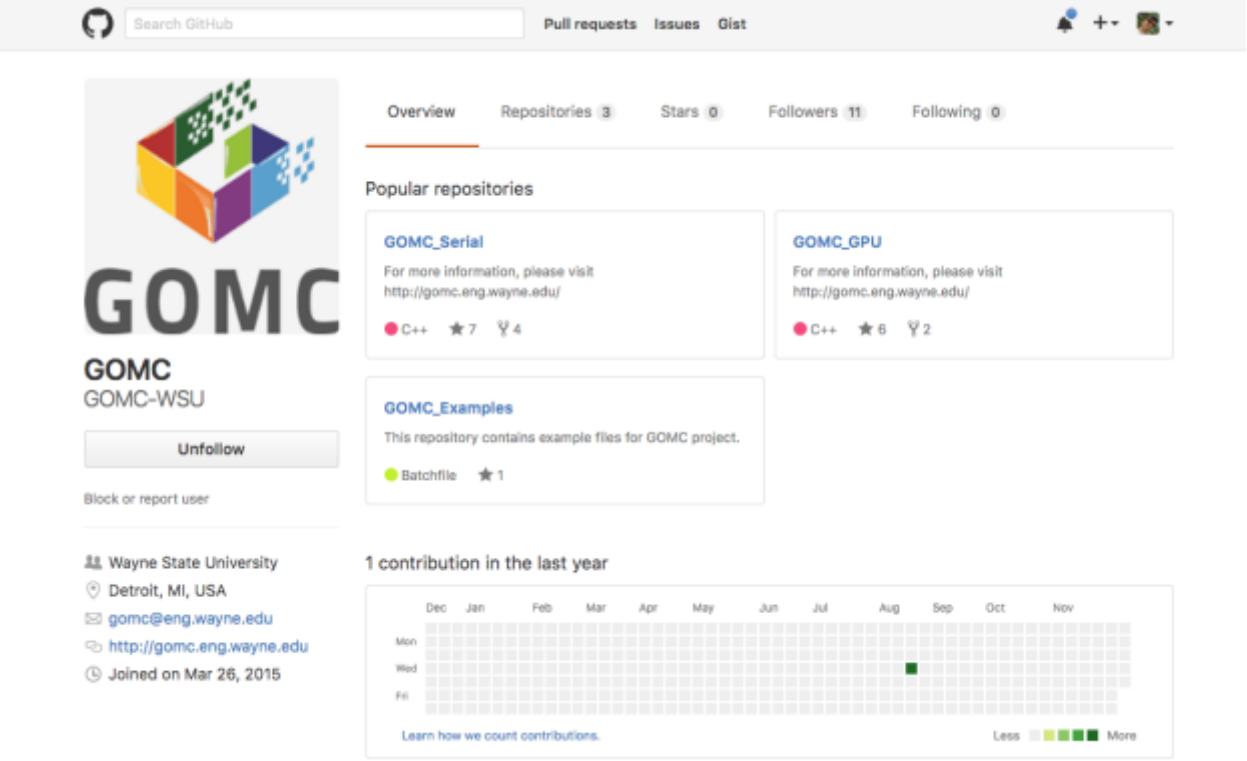
The latest public code builds, the project logo, manual, and other resources can be obtained via the following website:

gomc.eng.wayne.edu

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.

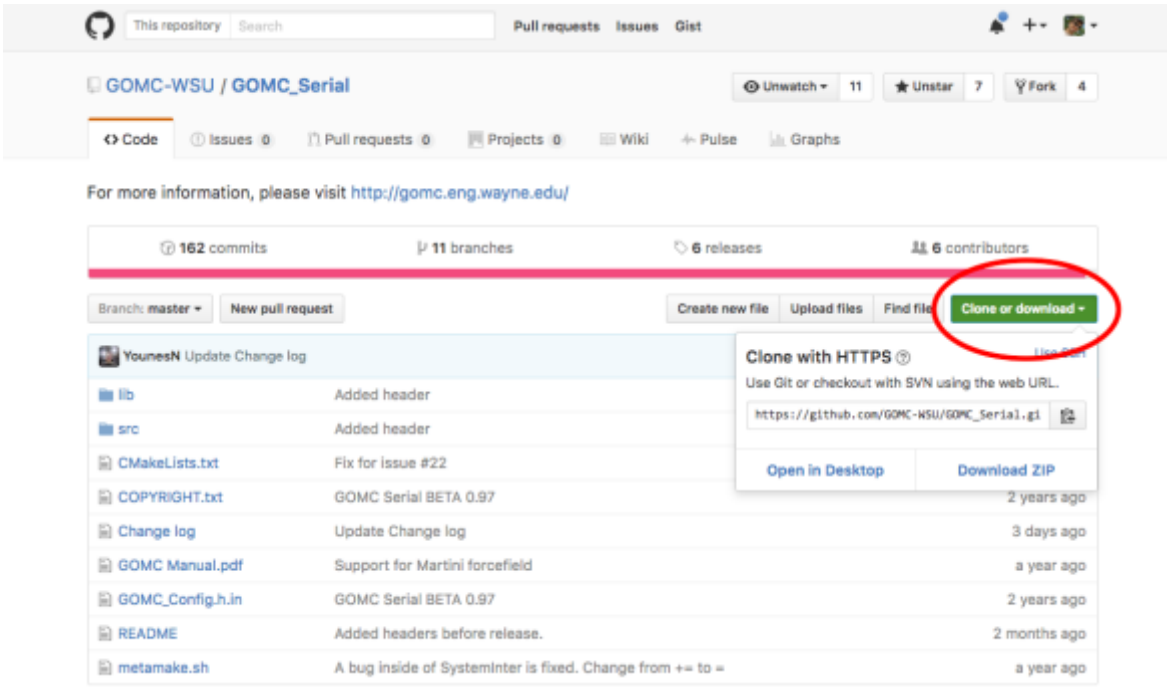
Currently version control is handled through the GitHub repository. The posted builds in Master branch are “frozen” versions of the code that have been validated for a number of systems and ensembles. Other branches are created as a means of implementing new features. The latest updated code builds,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

https://github.com/GOMC-WSU



The CPU, GPU, and Examples repositories 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/



Platform and Software Requirements

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.

Required Software Prequisites

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

1. C++03 Compliant Compiler
    a. Linux/OS X
        i. icc (Intel c++ compiler)
        Type 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).

        ii. g++ (GNU GCC)
        Type 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.

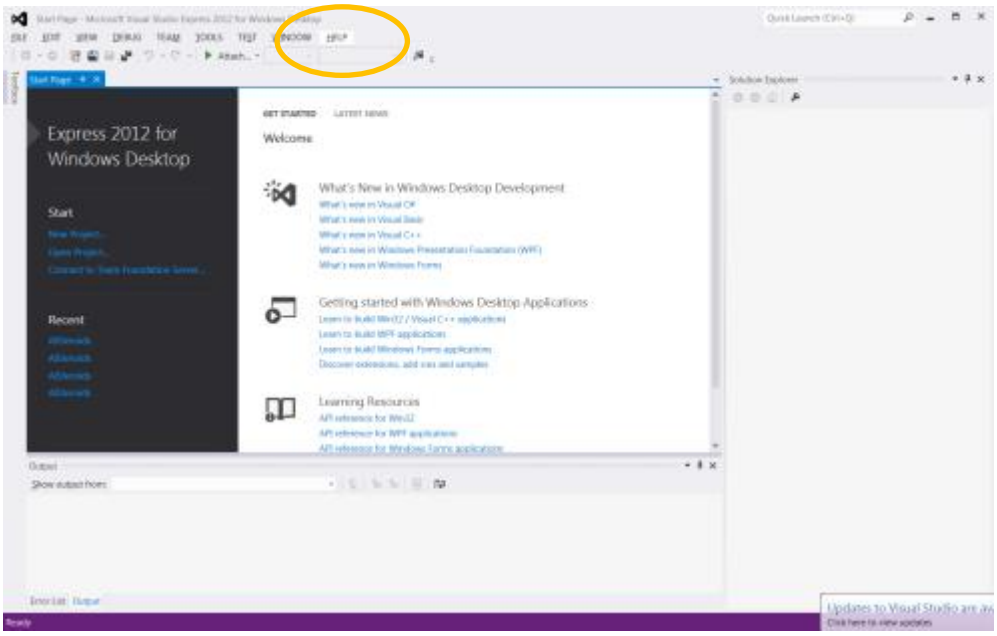
b. Windows

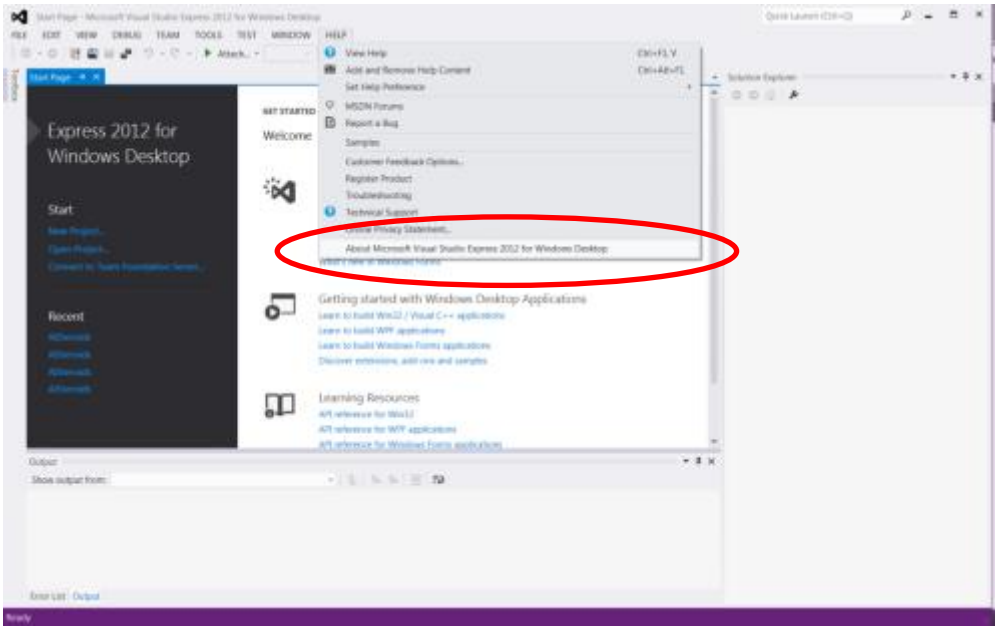
i. Visual Studio

Microsoft's Visual Studio 2010 or later is recommended.

To check the version:

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





2. cmake (if compiling on Linux)

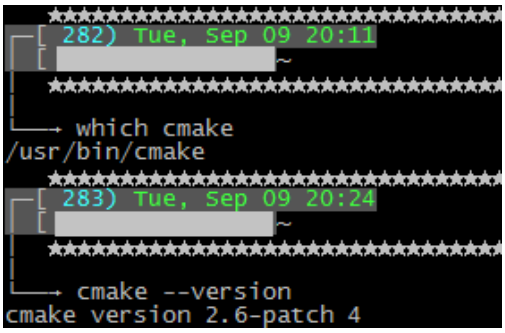
   To check if cmake is installed

   ```
   which cmake
   ```

   To check version number:

   ```
   cmake --version
   ```

   Here's an example from one of our systems:



3. nvcc/CUDA libs

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

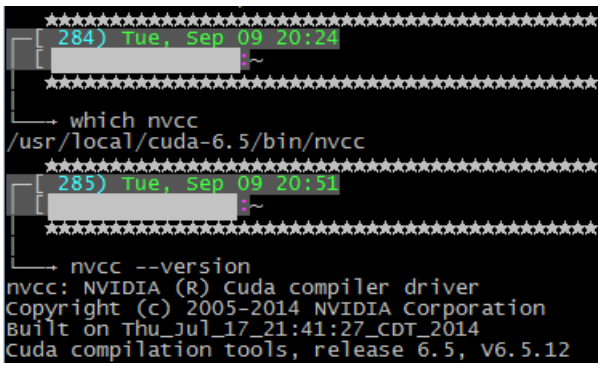
   To check if nvcc is installed

   ```
   which nvcc
   ```

   To check version number:

   ```
   nvcc --version
   ```

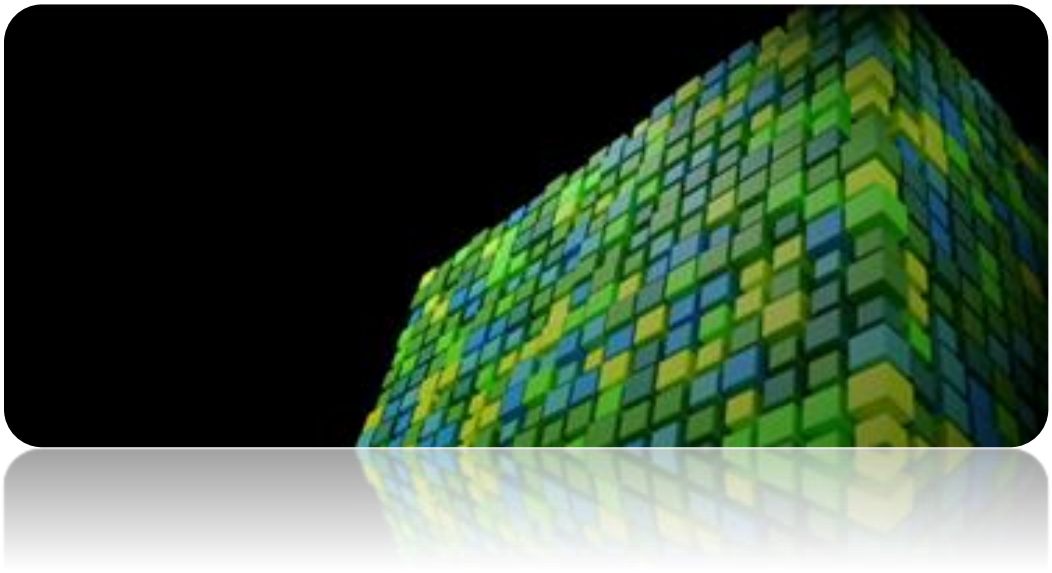
   Here's an example from one of our systems:



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.

Highly Recommended Software Tools

NOTE:

These listed programs are used in this manual and are generally to be considered **necessary.**

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 out here:

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

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

One useful purpose of VMD is visualization of your systems.

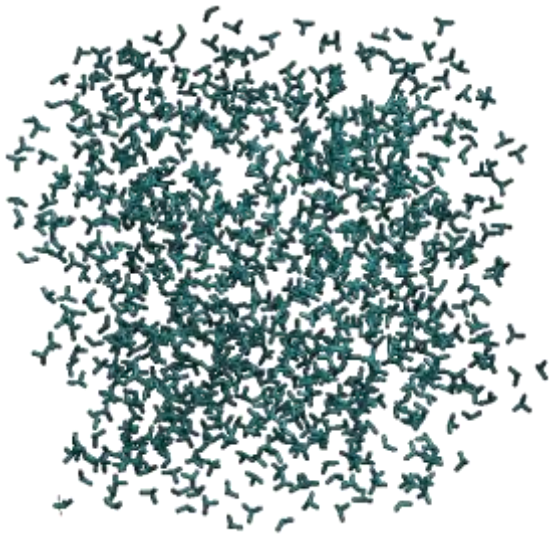


Figure 1 : A system of united atom isobutane molecules is seen above

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.

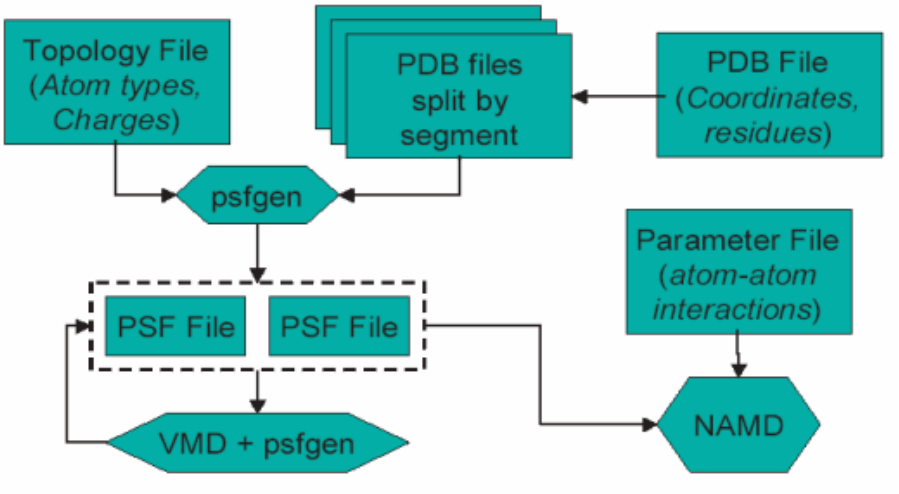


Figure 2 : An overview of the PSFGen file generation process and its relationship to VMD/NAMD

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

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 to 2 Angstroms smaller than the simulation box size. This prevents hard overlaps over the periodic boundary.

Other Useful Software Tools

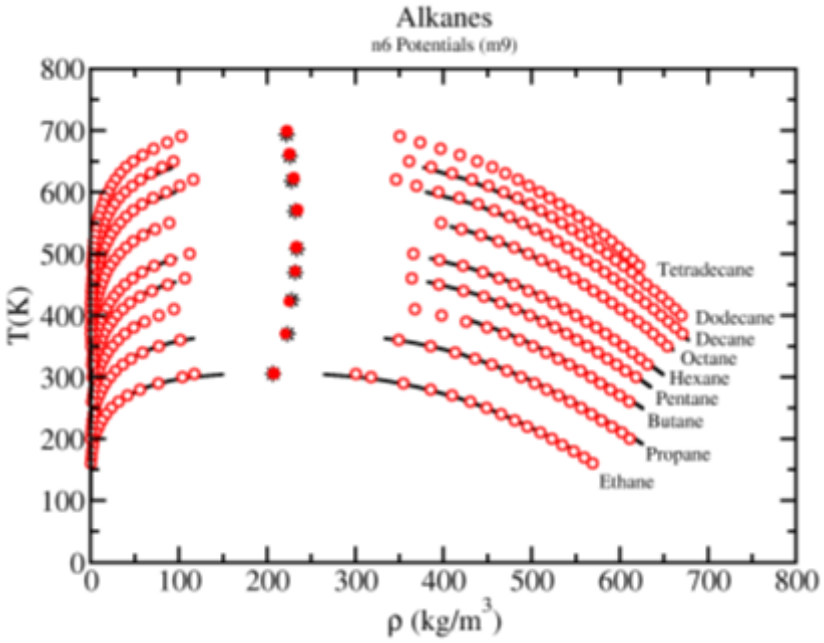
Grace

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/

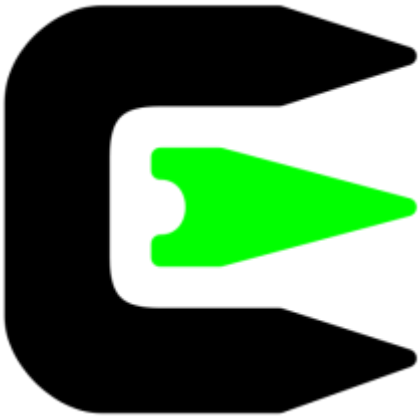
When compiled, Grace's executable in Linux is typically named "xmgrace". This tool allows the production of high quality, precise line and dot graphs, ideal for visualizing much of the thermodynamic data from the GOMC engine. Below is an example of the results of simulations of saturated VLE densities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



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.

Compiling GOMC

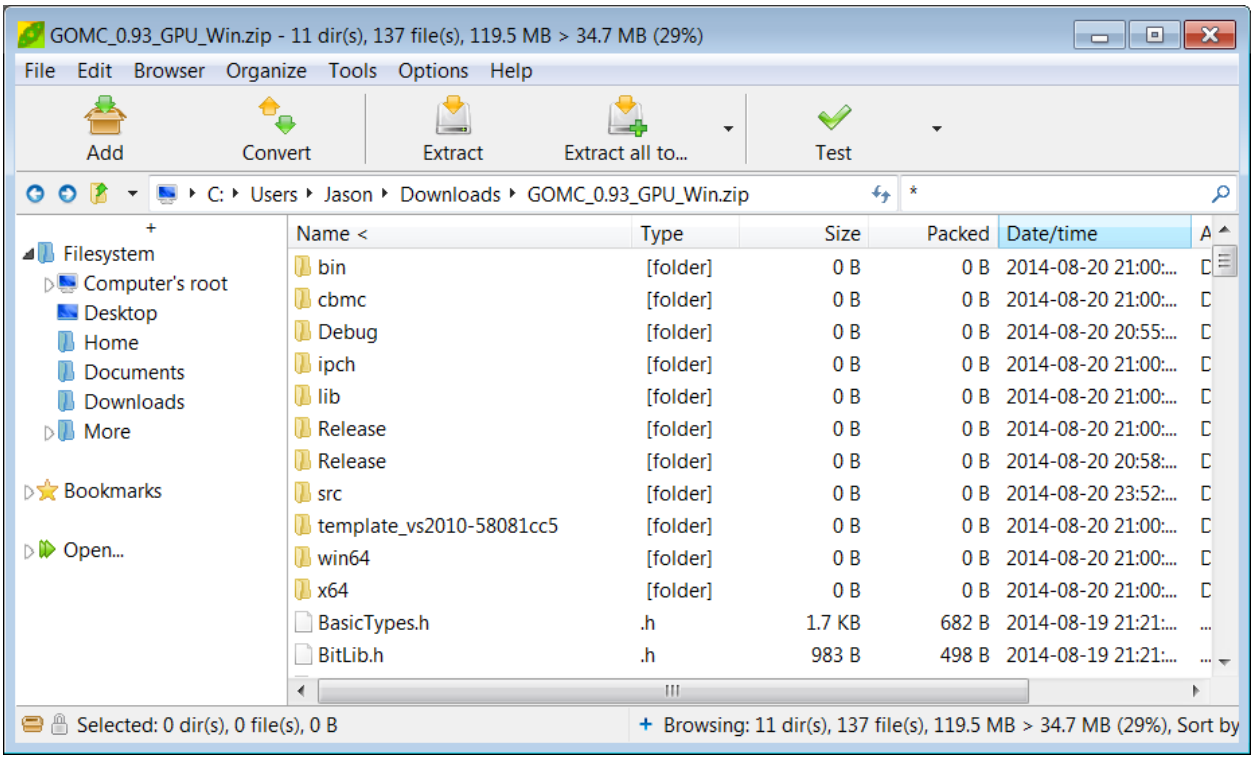
Extracting the Code

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:

```
tar –xzvf  <file name>.tar.gz
```

Compiling the Code

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, just go to the directory of the project, and then type:

```
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.

```
# CUDA code generation flags
GENCODE_SM10    := -gencode arch=compute_10,code=sm_10
GENCODE_SM20    := -gencode arch=compute_20,code=sm_21
GENCODE_SM30    := -gencode arch=compute_30,code=sm_30
GENCODE_SM35    := -gencode arch=compute_35,code=sm_35
GENCODE_FLAGS   :=  $(GENCODE_SM30)
```

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).

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

```
make all
```

which will use the Makefile to compile a GPU-compatible executable called "GOMC.out". To run this 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:

```
./metamake.sh
```

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

```
cd bin
```

and type:

```
make
```

Three executables – GOMC_Serial_GEMC (Gibbs ensemble), GOMC_Serial_NVT (NVT 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".

```
########################
# EXTERNAL cache entries
########################

//Path to a program.
CMAKE_AR:FILEPATH=/usr/bin/ar

//Choose the type of build, options are: None Debug Release RelWithDebInfo
// MinSizeRel.
CMAKE_BUILD_TYPE:STRING=Release

//Enable/Disable color output during build.
CMAKE_COLOR_MAKEFILE:BOOL=ON

//CXX compiler.
CMAKE_CXX_COMPILER:FILEPATH=/usr/bin/c++
```

To

```
########################
# EXTERNAL cache entries
########################

//Path to a program.
CMAKE_AR:FILEPATH=/usr/bin/ar

//Choose the type of build, options are: None Debug Release RelWithDebInfo
// MinSizeRel.
CMAKE_BUILD_TYPE:STRING=Debug

//Enable/Disable color output during build.
CMAKE_COLOR_MAKEFILE:BOOL=ON

//CXX compiler.
CMAKE_CXX_COMPILER:FILEPATH=/usr/bin/c++
```

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.

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
```

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 or files
- PSF file or files
- Parameter file

PDB

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.

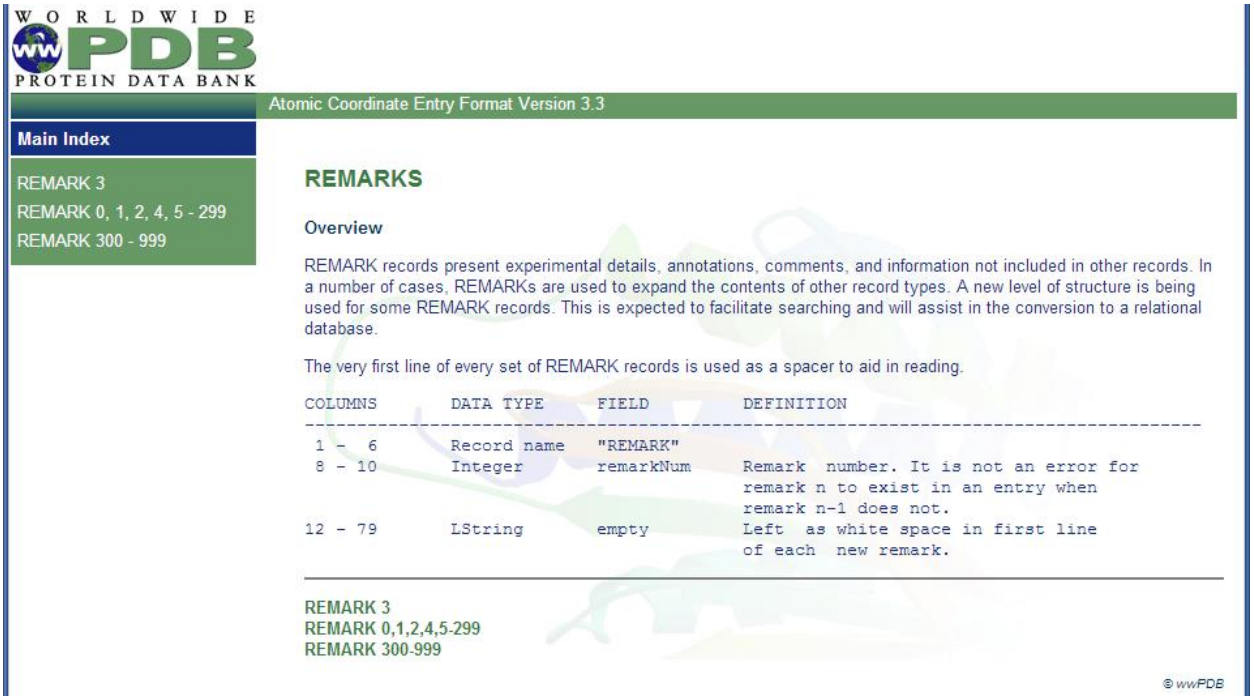
GOMC recognizes the following keywords in PDB files:

- 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.

Here is an example

```
REMARK    1_________2_________3_________4_________5_________6_________7_________8
REMARK  8901234567890123456789012345678901234567890123456789012345678901234567890
CRYST1   71.490   71.490   71.490  90.00  90.00  90.00 P 1           1
ATOM      1 C1   ISB A   1      24.378  36.667  45.645  0.00  0.00      ISB  C
```

This file indicates a box size of 71.49 Angstroms per side. The '90.00' entries, indicate the cell is cubic.

NOTE:

Non-cubic cells are not yet 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 alphanumerical 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 in these 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,

```
REMARK    1_________2_________3_________4_________5_________6_________7_________8
REMARK  8901234567890123456789012345678901234567890123456789012345678901234567890
CRYST1   71.490   71.490   71.490  90.00  90.00  90.00 P 1         1
ATOM      1 C1   ISB A   1      24.378  36.667  45.645  0.00  0.00      ISB  C
```

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 support, 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.

Pending Improvement

Note: Currently, a box is limited to hold up to 9,999 residues, or 99,999 atom entries, sticking to decimal integer numbering. Like NAMD/X-PLOR, an upcoming code modification will add support for using hexadecimal in the molecule numbering of 9,999 residues (see: NAMD), and using the alphanumeric overflow defined in the X-PLOR spec.

The modification will allow for a maximum of:
9,999 (standard uint) + 999 x 26 (overflow, alphanumeric) → 35,973 molecules (residue #s)
99,999 (standard uint) + 9,999 x 26 (overflow, alphanumeric) → 359,973 ATOM entries

Pass either of these and an "overflow" solution is hit, where it will print stars to the respective field. This file should still be readable, but is considered unsafe in terms of portability, as it will work for GOMC and NAMD, but may fail for other codes.

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

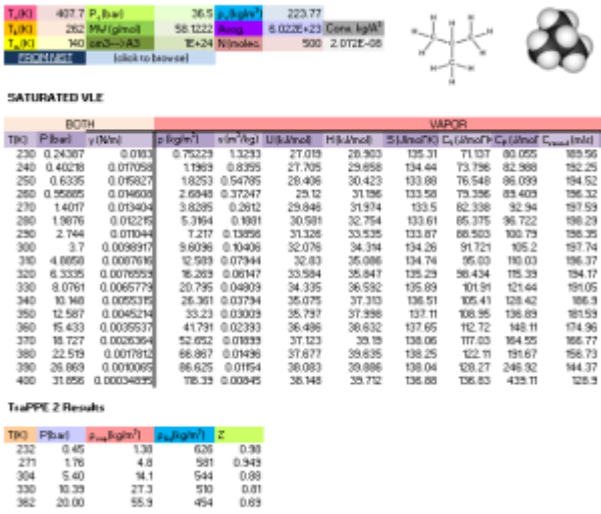
With that overview of the format in mind, the following steps describe how a PDB file is typically built.

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. 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 A). This technique can be handy in the constant pressure Gibbs ensemble.
- Pack one box to the predicted liquid density and the other to the vapor density.



A good reference for getting the information needed to estimate packing is the NIST Web Book database of pure compounds:

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

3. After packing is determined, a basic pack can be performed with a Packmol script. Here is one example:

```
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:

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

PSF File

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_Alkanes.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 consider 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 !NBOND: bonds
       1       2       1       3       1       4       5       6
       5       7       5       8
       .
       .
       .
3997    3998    3997    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
       .
       .
       .
```

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   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
```

Note the keyword **END** must be used to terminate this file and keywords related to the autogeneration 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/force field-tutorial/force field-html/node6.html
"NAMD Tutorial: 25. Topology Files"
http://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-win-html/node25.html

courtesy of UIUC.

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 be 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

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

$$U_{bond} = \sum_{bonds} K_b (b - b^0)^2$$

$$U_{angle} = \sum_{angles} K_\theta (\theta - \theta^0)^2$$

$$U_{dihedral} = \sum_{dihedrals} K_\varphi (1 + \cos(n\varphi - \delta))$$

$$U_{LJ} = \sum_{nonb,pairs} \varepsilon_{ij} \left[\left(\frac{r_{ij}^{min}}{r_{ij}} \right)^{12} - 2 \left(\frac{r_{ij}^{min}}{r_{ij}} \right)^{6} \right]$$

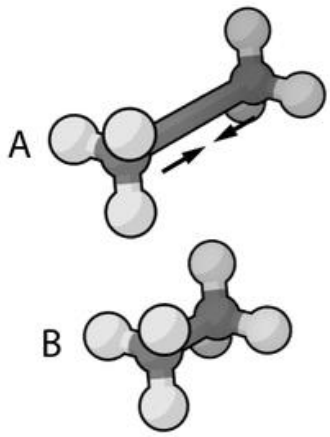
$$U_{elec} = \sum_{nonb,pairs} \frac{q_i q_j}{\epsilon r_{ij}}$$

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 Kb.

  Note:

  GOMC does not sample bond stretch.



[Image Courtesy of Wikimedia Commons]

- **ANGLES**
  - Describes the conformational behavior of an angle (ϑ) between three atoms, one of which is shared branch point to the other two.

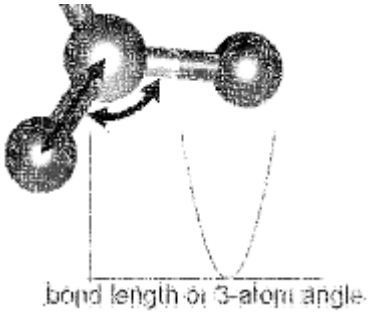


Image Courtesy of Wikimedia Commons

- **DIHEDRALS** Describes crankshaft-like rotation behavior about a central bond in a series of three consecutive bonds (rotation is given as φ)

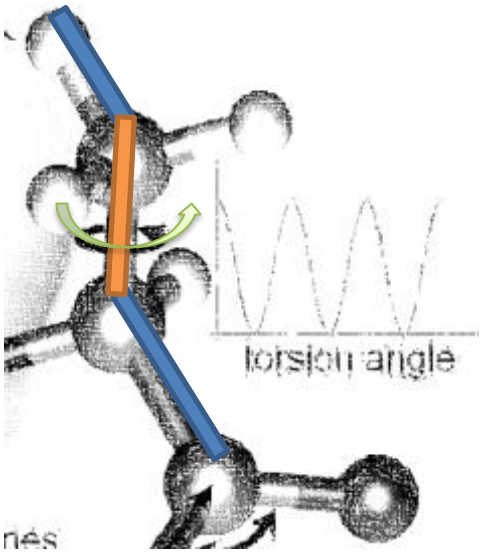


Image Courtesy of Wikimedia Commons

- **NONBONDED** This tag name only should only be used if CHARMM force field is 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, same parameter will be considered for 1-4 interaction.

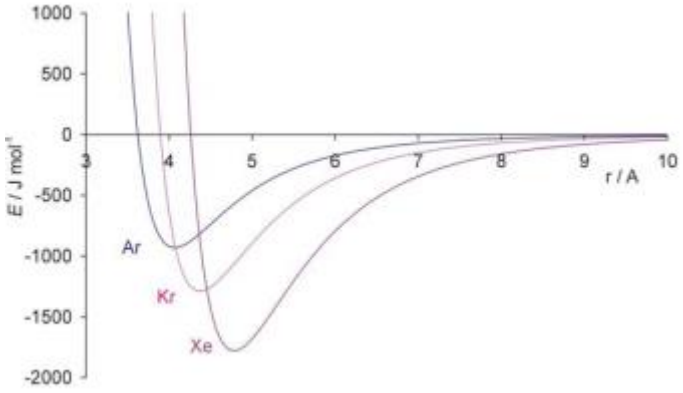


Image Courtesy of the Univ. of Bristol

- **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**, **IMPROPERS**, **NONBONDED**, **NBFIX**. Other sections such as **CMAP** are not currently read or supported.

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.

ANGLES (bond bending), where θ and θ_0 are commonly measured in degrees and K_θ 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.

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 the literature.

IMPROPERS – 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 iscritical. Here's an example with our isobutane potential models:

```
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 σ. σ 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 σ to R_{min}, simply multiply σ 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
```

"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(σ) is same for both **NONBONDED_MIE** and **NBFIX_FIE**.

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
```

Here is an example if there is need to modify CH3 CH2 interaction:

```
NBFIX_MIE
!
!V(mie) = 4*eps*((sig_ij/r_ij)^n-(sig_ij/r_ij)^6)
!
!atom   atom   eps       sig     n    eps,1-4    sig,1-4     n,1-4
CH2     CH3   81.10     2.540    16     31.10    1.540        16!
```

NOTE:

Although the units (Angstroms) are the same, the exotic file uses σ, *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.

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.

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.

  (WARNING: Restarts are not currently supported)

  - 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 be terminated.

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

    Example:

```
##################################
# 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.

      Example:

```
#####################################
# 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 loads in the Mersenne Twister's state from a saved file.

  (WARNING: Restarts are not currently supported)

  Example:

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

- Random_Seed: Define seed number. If "INTSEED" is chosen, seed number needs to be specified; otherwise, the program will be terminated.

  - Value 1: ULONG or UINT: If "INTSEED" command is used (see above example).

  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.

  Example:

```
####################################
# 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.

    Example:
    ```
    ####################################
    # FORCE FIELD TYPE
    ####################################
    ParaTypeEXOTIC        true
    ```

- **ParaTypeMARTINI:** Sets force field to MARTINI.
    - Value 1: <BOOLEAN> – true if it is MARTINI force field, false if it is not.

    Example:
    ```
    ####################################
    # 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 parameter file

    Example:
    ```
    ####################################
    # 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 ensemble 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 be terminated.

Example (NVT ensemble):

```
#####################################
# INPUT PDB FILES
#####################################
Coordinates 0 STEP3_START_ISB_sys.pdb
```

Example (Gibbs ensemble or GC ensemble):

```
#####################################
# INPUT PDB FILES
#####################################
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 ensemble requires only one PSF file and GEMC/GCMC require two PSF files. If the number of PSF files is not compatible with the simulation type, the program will be terminated.

Example (NVT ensemble):

```
#####################################
# INPUT PSF FILES
#####################################
Structure  0   STEP3_START_ISB_sys.psf
```

Example (Gibbs ensemble or GC ensemble):

```
#####################################
# INPUT PSF FILES
#####################################
Structure   0   STEP3_START_ISB_sys_BOX_0.psf
Structure   1   STEP3_START_ISB_sys_BOX_1.psf
```

System Settings for During Run Setup

This section contains all the variables not involved in the output of data during the simulation, or in with 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 mole number, volume and temperature.

    Example:
    ```
    ###################################
    # GEMC TYPE (DEFULT IS NVT_GEMC)
    ###################################
    GEMC            NVT
    ```

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

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

  - Value 1: <DOUBLE> – Constant pressure in bars

  Example:
  ```
  ###################################
  # GEMC TYPE (DEFULT IS NVT_GEMC)
  ###################################
  GEMC            NPT
  Pressure        5.76
  ```

- Temperature: Sets the temperature at which the system will run.

  - Value 1: <DOUBLE> – constant temperature of simulation in degrees Kelvin

- Rcut: Sets a specific radius that non-bonded interaction energy and force will be considered and calculated using defined potential function.

  - Value 1: <DOUBLE> – maximum distance for the Lennard-Jones potential

- 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 interaction 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 nonbonded parameters defined in parameter file.

    Note:
    If no value was detected, by default “1-3” will be considered.

- Potential: Defines the potential function type to calculate nonbonded interaction energy and force between atoms.
  - Value 1: <STRING> – Allows you to pick between “VDW”, “SHIFT” and “SWITCH”
    - VDW: Non-bonded 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.

      Example:

```
##############################
# 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.

Example:

```
##############################
# 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 Rcut 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. If the "SWITCH" function is chosen, Rswitch needs to be defined; otherwise, the program will be terminated.

    Example:

```
##############################
# SIMULATION CONDITION
##############################
Temperature     200.00
Potential   SWITCH
Rswitch     7
Rcut        10
LRC         false
Exclude     1-3
```

Note/Warning:

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.

Warning:

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.

Warning:

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 Ewald summation method for electrostatic calculation.
    - Value 1: <BOOLEAN> – True if Ewald summation calculation needs to be considered and false if not.

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

- `Tolerance`: Specifies the accuracy of the Ewald summation calculation. Ewald separation parameter and number of reciprocal vectors for the Ewald summation is determined based on the accuracy parameter.
    - Value 1: < DOUBLE > – Sets the accuracy in Ewald summation calculation. A reasonable value for the accuracy is 0.0001.

Warning:
If “Ewald” was chosen and no value was set for `Tolerance`, program will be terminated.

- `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.

Warning:

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.

Example:

```
################################
# ELECTROSTATIC
################################
ElectroStatic          true
Ewald                  true
Tolerance              0.0001
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 A^3 to swap, etc.)

    - Value 1: <ULONG> – number of steps per move adjustment

    Example:

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

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

    - Value 1: <STRING> – The resname to apply this chemical potential w.r.t.

    - Value 2: <DOUBLE>– The chemical potential value in degrees Kelvin (should be negative).

    Note:
    For binary systems include multiple copies of the tag (one per residue kind).

    Example:

```
##################################################
#                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:** Fractional percentage at which volume displacement move will occur

    - Value 1: <DOUBLE> – (For Gibbs Ensemble runs only) % of volume swaps

- **SwapFreq:** Fractional percentage at which particle swap move will occur

    - Value 1: <DOUBLE> – (For Gibbs and GC Ensemble runs only) % of molecule swaps

    Example:

```
################################
# 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 be terminated.

- **BoxDim**: Defines the axis lengths of simulation box. This tag may occur multiple times. It occurs once for NVT, 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 (NVT ensemble):

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

Example (Gibbs ensemble or GC ensemble):

```
###################################
# BOX DIMENSION #, X, Y, Z
###################################
BoxDim  0   106.60 106.60 106.60
BoxDim  1   176.60 176.60 176.60
```

- **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.

    Example:

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

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

    Example:

```
########################################
# OUTPUT FILE NAME
########################################
OutputName  ISB_T_270.00_K
```

- **CoordinatesFreq**: Controls output of PDB file (coordinates) and PRNG state. If PDB dumping was enabled one file for NVT 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/Warning:
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 contains an entry for every ATOM, 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 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, RunSteps value will be assigned by default.

Note/Warning:
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.

Warning:
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 in order 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" enable 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.

      Example:

```
#####################################
# 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 GC 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.

    Example:

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

- `OutEnergy`***,`OutPressure`***,`OutMolNumber`**,`OutDensity`**, `OutVolume`*: Enables/disables for specific kinds of file output for tracked thermodynamic quantities

  (*) = NVT ensemble (*) = Gibbs ensemble (*) = GC ensemble

  - Value 1: <BOOLEAN> – "true" enable message output of block averages via this tracked parameter (and in some cases such as entry, components); "false" disables it.

  - Value 2: <BOOLEAN> – "true" enable message output of a fluctuation into the console file via tracked parameter (and in some cases such as entry, components); "false" disables it.

Example:

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

Sample Files

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

```
#=====================================================
#=       GOMC 1.90 - 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             0.0001
1-4scaling            0.0
```

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

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


#################################
# 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 1.90 - Gibbs ensemble Control example              =
#=================================================================


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

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

####################################
# 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_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 (DEFULT IS NVT_GEMC)
##################################
GEMC       NPT
Pressure   2.50
```

```
##############################
# SIMULATION CONDITION
##############################
Temperature     200.00
Potential       SWITCH
LRC             false
Rswitch         7
Rcut            10
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      0.0



################################
# 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 1.90 - Grand canonical ensemble Control example       =
#===========================================================

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

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

#####################################
# 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       SHIFT
LRC             false
Rcut            10
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      0.0


##################################
# 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    AR             -2230


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

#########################
# OUTPUT FILE NAME
#########################
OutputName  AR_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
```

GOMC's Output Files, Terminal Output

GOMC currently supports several kinds of output:

- ❖ STDIO ("console") Output
- ❖ File Output
    - o PDB
    - o PSF
    - o Block Averages

GOMC output units:

Properties	Units	Properties	Units
Energy	K	Volume	$Å^3$
Pressure	bar	Density	Kg/m^3
Heat of vaporization	KJ/mol		

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 formatted 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 non-bonded
    - Tail corrections
    - Electrostatic real
    - Electrostatic Reciprocal
    - Electrostatic self
    - Electrostatic correction
    - Total electrostatic energy (sum of real, recip, self, and correction)
    - Total Energy (sum of the all energies)
- Pressure (bar)
- Volume
- Total molecule number
- Total Density
- Mole fraction of each species

Detail 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_BOX_#, ETITLE_BOX_#, and STITLE_BOX_# for move, energy, and statistical information, respectively. Where, # is the simulation box number. The instantaneous values for each section will start with MOVE_BOX_#, ENERGY_BOX_#, and STAT_BOX_# for move, energy, and statistical values, respectively. Where, # is the simulation box 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 commands need to be executed in terminal:

```
grep "ENERGY_BOX_0"   output_console.log | awk '{print $2}'
```

Here, "output_console.log" is the console output file and "$2" 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, and summary of the topology of the molecule. 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.)

```
GOMC Serial Version 1.9
Started at: Fri Dec  9 11:32:06 2016
On hostname:

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: 5537.9MB
Working in the current directory /home3/soroush/Desktop/validation/GOMC_Serial-d\
evelopment_1.90/GOMC_Examples-master/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 410.0 K
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: 3715890227

Molecules in PSF:

Molecule Kind: ISB
Idx     name    type    charge  mass
0       C1      CH1     0.0     13.0
1       C2      CH3     0.0     15.0
2       C3      CH3     0.0     15.0
3       C4      CH3     0.0     15.0

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
```

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

```
########################## INITIAL SIMULATION ENERGY ##########################
ETITLE_BOX_0    TOTAL           INTRA(B)        INTRA(N)        INTER(LJ)       \
LRC             TOTAL_ELECT     REAL            RECIP           SELF            \
CORR

ENERGY_BOX_0    13948327.3067   45654.5668      0.0000          13930559.9077   \
-27887.1678     0.0000          0.0000          0.0000          0.0000          \
-0.0000

ETITLE_BOX_1    TOTAL           INTRA(B)        INTRA(N)        INTER(LJ)       \
LRC             TOTAL_ELECT     REAL            RECIP           SELF            \
CORR

ENERGY_BOX_1    -50964.1052     45617.9658      0.0000          -73954.5137     \
-22627.5572     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_BOX_0    DISTRY          DISACCEPT       DISACCEPT%      DISMAX          \
ROTATE          ROTACCEPT       ROTACCEPT%      ROTMAX          INTRASWAP       \
INTACCEPT       INTACCEPT%      TRANSFER        TRANACCEPT      TRANACCEPT%     \
VOLUME          VOLACCEPT       VOLACCEPT%      VOLMAX          STEP

ETITLE_BOX_0    TOTAL           INTRA(B)        INTRA(N)        INTER(LJ)       \
LRC             TOTAL_ELECT     REAL            RECIP           SELF            \
CORR
STITLE_BOX_0    VOLUME          PRESSURE        TOTALMOL        MOLFRAC_ISB     \
MOLFRAC_NEO     TOT_DENSITY

MTITLE_BOX_1    DISTRY          DISACCEPT       DISACCEPT%      DISMAX          \
ROTATE          ROTACCEPT       ROTACCEPT%      ROTMAX          INTRASWAP       \
INTACCEPT       INTACCEPT%      TRANSFER        TRANACCEPT      TRANACCEPT%     \
VOLUME          VOLACCEPT       VOLACCEPT%      VOLMAX          STEP

ETITLE_BOX_1    TOTAL           INTRA(B)        INTRA(N)        INTER(LJ)       \
LRC             TOTAL_ELECT     REAL            RECIP           SELF            \
CORR
STITLE_BOX_1    VOLUME          PRESSURE        TOTALMOL        MOLFRAC_ISB     \
MOLFRAC_NEO     TOT_DENSITY
```

```
Printed combined psf to file isobutane_neopentane_NVT_360_00_K.psf
MOVE_BOX_0      34495           16823           48.7694         0.7357          \
4957            3255            65.6647         3.1416          0               \
0               0.0000          10113           2730            26.9950         \
972             532             54.7325         4918.0028       100000

ENERGY_BOX_0    -370026.7079    574198.7059     0.0000          -855334.0152    \
-88891.3986     0.0000          0.0000          0.0000          0.0000          \
0.0000

STAT_BOX_0      290054.9351     3.2014          832             0.4916          \
0.5084          310.8204

MOVE_BOX_1      34237           17117           49.9956         9.8999          \
5050            4101            81.2079         3.1416          0               \
0               0.0000          10176           3062            30.0904         \
0               0               0.0000          500.0000        100000

ENERGY_BOX_1    101802.2911     128352.3062     0.0000          -24274.1917     \
-2275.8234      0.0000          0.0000          0.0000          0.0000          \
0.0000

STAT_BOX_1      452930.0289     15.2367         168             0.5417          \
0.4583          39.7598
```

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.

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 output by VMD and use the command in the terminal:

```
pbc 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 outputted 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.

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 non-bonded
    - Tail corrections
    - Electrostatic real
    - Electrostatic Reciprocal
    - Total Energy (sum of the all energies)
- Virial
- Pressure
- 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, which is total density.

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.aspx and run different simulation types in order to become more familiar with different parameter and configuration files (in.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 GEMC GCMC 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:

```
./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
```

Note, you probably will have to first make your scripts executable using:

```
chmod a+x build_box_*.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_Serial_GEMC, run using:

```
./GOMC_Serial_GEMC in.conf > out_ISB_T_330.00_K_RUN_0.log &
```

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

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

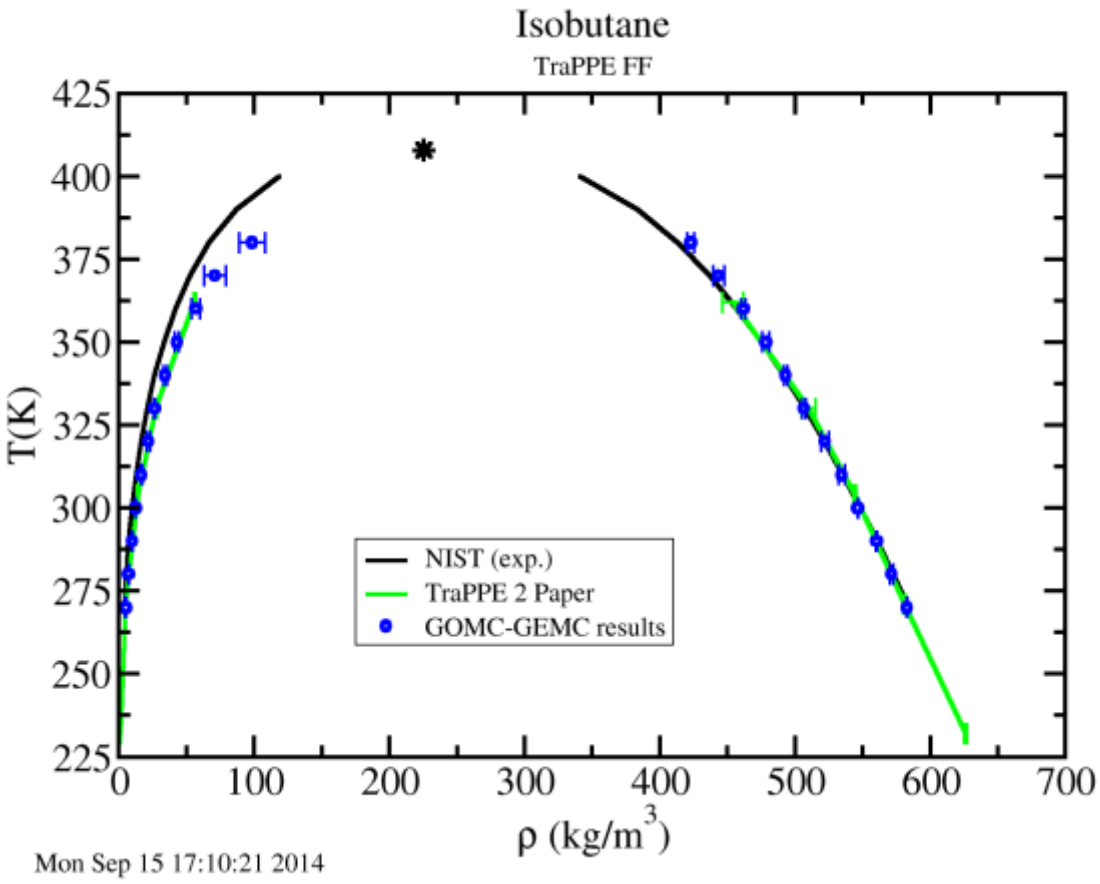
Here, 4 defines the number of processors that will be used to run the simulation in parallel.

Progress can be monitored with the tail command:

```
tail –f out_ISB*log
```

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

This process can be repeated multiple times to produce new results (saving the old results for later comparisons) to produce averages. It is recommended that at least three simulations be run per point; although, for larger/longer simulations, it is sometimes appropriate to run only one simulation.



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

Intermolecular Energy and Virial function:

- 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,

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

      where r_{ij}, ε_{ij}, and σ_{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 such that the minimum of the potential remains at $-\varepsilon_{ij}$ for all n_{ij}. In the 12-6 potential, C_n reduces to the familiar value of 4.

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

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

$$W_{ij} = -\frac{dE_{ij}}{dr} \times \frac{\overrightarrow{r_{IJ}}}{r_{ij}}$$

  Using n-6 LJ potential defined above:

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

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.

- 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,

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

where r_{ij}, ε_{ij}, and σ_{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 $-\varepsilon_{ij}$ for all n_{ij}. In the 12-6 potential, C_n reduces to the familiar value of 4.

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

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

$$W_{ij} = -\frac{dE_{ij}}{dr} \times \frac{\overrightarrow{r_{ij}}}{r_{ij}}$$

Using SHIFT potential function defined above:

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

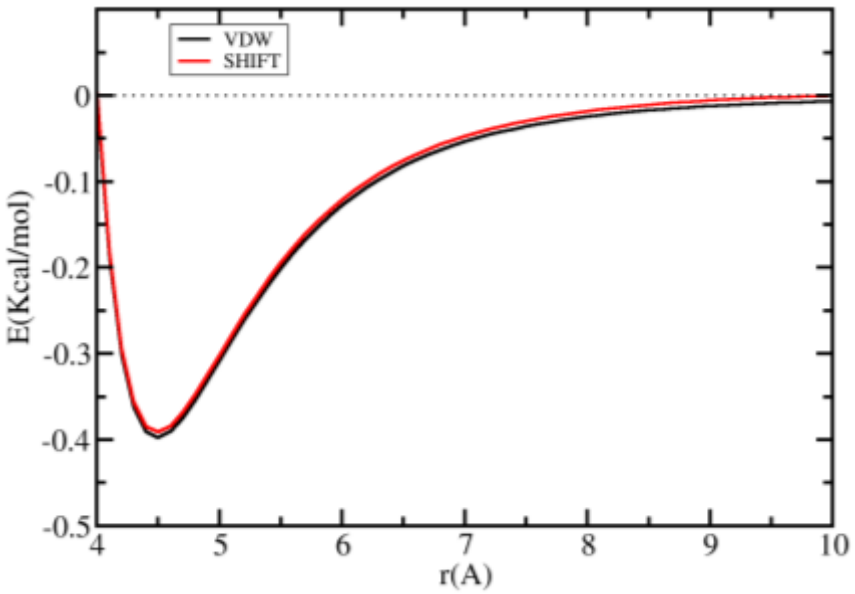


Figure 3: Graph of van der Waals potential with and without the application of the SHIFT function. With the SHIFT function active, the potential by forced reduced to 0.0 at the Rcut distance. Without the SHIFT function, there is a discontinuity where the potential is truncated.

- **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,

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

      where r_{ij}, ε_{ij}, and σ_{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 used such that the minimum of the potential remains at $-\varepsilon_{ij}$ for all n_{ij}. In the 12-6 potential, C_n reduces to the familiar value of 4.

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

      The factor F_E is defined as:

$$F_E = \begin{cases} 1 & r_{ij} \le r_{\text{switch}} \\ \dfrac{\left({r_{\text{cut}}}^2 - {r_{ij}}^2\right)^2 \times \left({r_{\text{cut}}}^2 - 3\times{r_{\text{switch}}}^2 + 2\times{r_{ij}}^2\right)}{({r_{\text{cut}}}^2 - {r_{switch}}^2)^3} & r_{\text{switch}} < r_{ij} < r_{\text{cut}} \\ 0 & r_{ij} \ge r_{\text{cut}} \end{cases}$$

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

$$W_{ij} = -\frac{dE_{ij}}{dr}\times\frac{\overrightarrow{r_{IJ}}}{r_{ij}}$$

      Using the SWITCH potential function defined above:

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

      The factor F_W is defined as:

$$F_W = \begin{cases} 1 & r_{ij} \le r_{\text{switch}} \\ \dfrac{12\left({r_{\text{cut}}}^2 - {r_{ij}}^2\right)\times\left({r_{\text{switch}}}^2 - {r_{ij}}^2\right)}{({r_{\text{cut}}}^2 - {r_{switch}}^2)^3} & r_{\text{switch}} < r_{ij} < r_{\text{cut}} \\ 0 & r_{ij} \ge r_{\text{cut}} \end{cases}$$

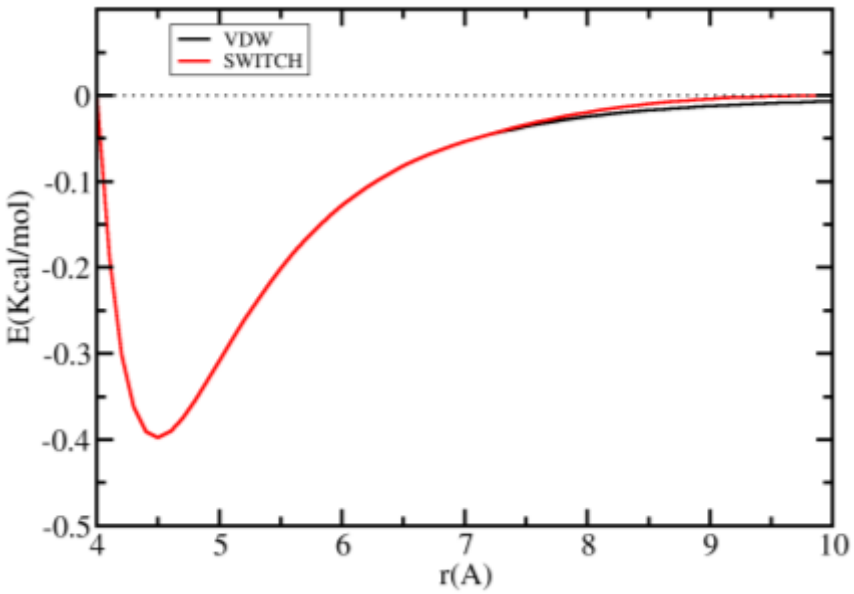


Figure 4: Graph of van der Waals potential with and without the application of the SWITCH function. With the SWITCH function active, the potential is smoothly reduced to 0 at the Rcut distance.

- **SWITCH**: This option in MARTINI force field smoothly forces the potential energy to be zero at Rcut distance and start modifying the potential at Rswitch distance.

    - Potential calculation: Interactions between atoms. Rswitch is set to 0.0 for coulomb interaction.

$$E_{ij}(\text{switch}) = 4\,\varepsilon_{ij}\left[{\sigma_{ij}}^{12}\left(\frac{1}{{r_{ij}}^{n}} + \varphi_{12}(r_{ij})\right) - {\sigma_{ij}}^{6}\left(\frac{1}{{r_{ij}}^{6}} + \varphi_{6}(r_{ij})\right)\right] + \frac{q_i q_j}{4\pi\varepsilon_0\varepsilon_1}\left(\frac{1}{r_{ij}} + \varphi_1(r_{ij})\right)$$

The factor φ_α is defined as:

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

$$\begin{cases} A_\alpha = \alpha \frac{(\alpha+1)r_{\text{switch}} - (\alpha+4)r_{cut}}{r_{cut}^{(\alpha+2)}(r_{cut} - r_{\text{switch}})^2} \\ B_\alpha = \alpha \frac{(\alpha+1)r_{\text{switch}} - (\alpha+3)r_{cut}}{r_{cut}^{(\alpha+2)}(r_{cut} - r_{\text{switch}})^3} \\ C_\alpha = \frac{1}{r_{cut}^\alpha} - \frac{A}{3}(r_{cut} - r_{\text{switch}})^3 + \frac{B}{4}(r_{cut} - r_{\text{switch}})^4 \end{cases}$$

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

$$W_{ij} = -\frac{dE_{ij}}{dr} \times \frac{\overrightarrow{r_{ij}}}{r_{ij}}$$

Using SWITCH potential function defined above:

$$\mathrm{W_{ij}(switch)} = 4\,\varepsilon_{ij}\left[{\sigma_{ij}}^{12}\left(\frac{12}{{r_{ij}}^{(12+2)}} + \frac{{\varphi'}_{12}(r_{ij})}{r_{ij}}\right) - {\sigma_{ij}}^{6}\left(\frac{6}{{r_{ij}}^{(6+2)}} + \frac{{\varphi'}_{6}(r_{ij})}{r_{ij}}\right)\right]$$

The factor ${\varphi'}_\alpha$ is defined as:

$${\varphi'}_\alpha(r_{ij}) = \begin{cases} 0 & r_{ij} < r_{switch} \\ A_\alpha(r_{ij} - r_{switch})^2 + B_\alpha(r_{ij} - r_{switch})^3 & r_{switch} < r_{ij} < r_{cut} \\ 0 & r_{ij} > r_{cut} \end{cases}$$

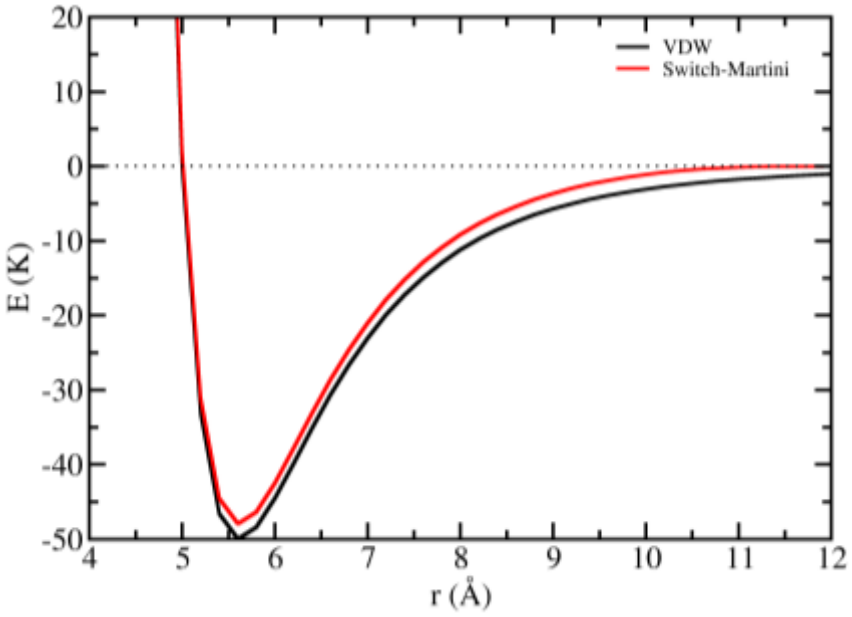


Figure 5: Graph of van der Waals potential with and without the application of the SWITCH function in MARTINI force field. With the SWITCH function active, the potential is smoothly reduced to 0.0 at the Rcut distance.

How to Get Help/Technical Support

Please, send an email to ***gomc@eng.wayne.edu***