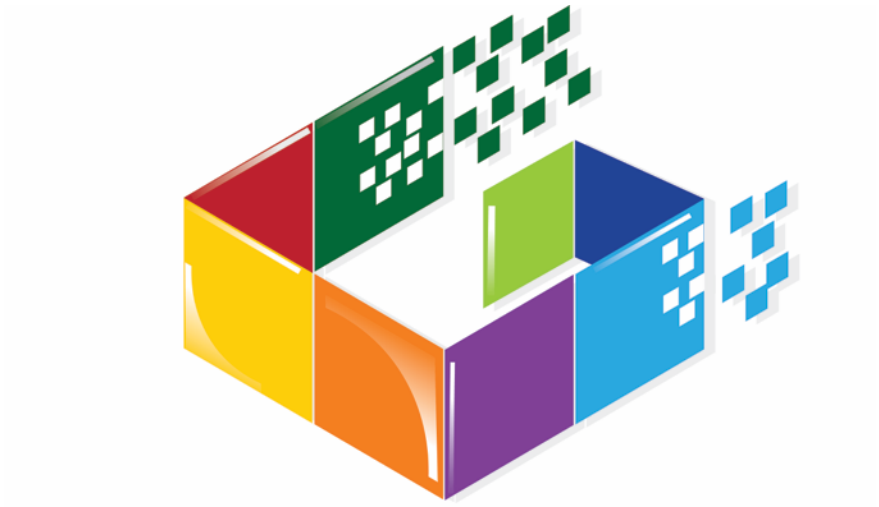


GOMC

User Manual
Version 2.30

Distributed by the Potoff and Schwiebert Groups

May 8, 2018

Contents

1 Tutorial Overview

This document will instruct a new user how to download, compile, prepare the input files, 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, compiling a GOMC executable, and preparing input files such as PDB, PSF, Parameter, and Configuration file. Executable is then used to calculate the saturated vapor and liquid equilibria (VLE) using Gibbs Ensemble Monte Carlo on systems of pure isobutane (R600a), a branched alkane that whose application as a refrigerant/propellant is increasing. The Transferable Potentials for Phase Equilibria (TraPPE) united atom (UA) force field is used to describe the molecular geometry constraints and the intermolecular interactions.

`http://en.wikipedia.org/wiki/Isobutane`

2 Introduction

GPU Optimized Monte Carlo (GOMC) is open-source software for simulating many-body molecular systems using the Metropolis Monte Carlo algorithm. GOMC is written in object oriented C++, which was chosen since it offers a good balance between code development time, interoperability with existing software elements, and code performance. The software may be compiled as a single-threaded application, a multi-threaded application using OpenMP, or to use many-core heterogeneous CPU-GPU architectures using OpenMP and CUDA. GOMC officially supports Windows 7 or newer and most modern distribution of GNU/Linux. This software has the ability to compile on recent versions of macOS; however, such a platform is not officially supported.

GOMC employs widely-used simulation file types (PDB, PSF, CHARMM-style parameter file) and supports polar and non-polar linear and branched molecules. GOMC can be used to study vapor-liquid and liquid-liquid equilibria, adsorption in porous materials, surfactant self-assembly, and condensed phase structure for complex molecules.

GOMC currently is capable of simulating systems in the following ensembles:

- Canonical (NVT)
- Isobaric-isothermal (NPT)
- Grand canonical (μVT)
- Constant volume Gibbs (NVT-Gibbs)
- Constant pressure Gibbs (NPT-Gibbs)

GOMC supports the following Monte Carlo moves:

- Rigid-body displacement
- Rigid-body rotation
- Regrowth using coupled-decoupled configurational-bias
- Intra-box swap using coupled-decoupled configurational-bias

- Inter-box swap using coupled-decoupled configurational-bias
- Volume exchange (both isotropic and anisotropic)

GOMC supports various all-atom, united-atom, and coarse grained force fields:

- OPLS
- CHARMM
- TraPPE
- Mie
- Martini

3 Software Requirements

3.1 C++11 Compliant Compiler

- Linux/macOS
  - icpc (Intel C++ Compiler)

    In Linux, the Intel compiler will generally produce the fastest CPU executables (when running on Intel Core processors). Type the following command in a terminal:

    ```
    $ icpc --version
    ```

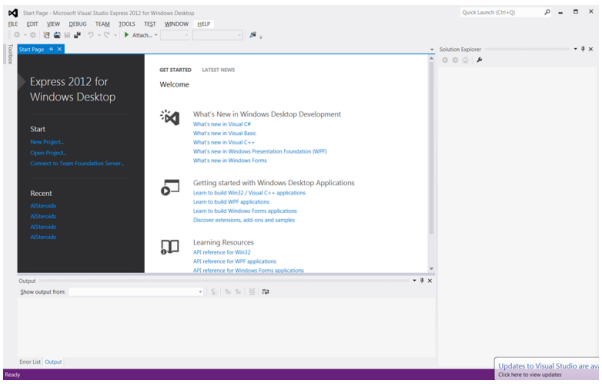
    If gives a version number 16.0.3 (2016 Initial version) or later, you're all set. Otherwise, we recommend upgrading.

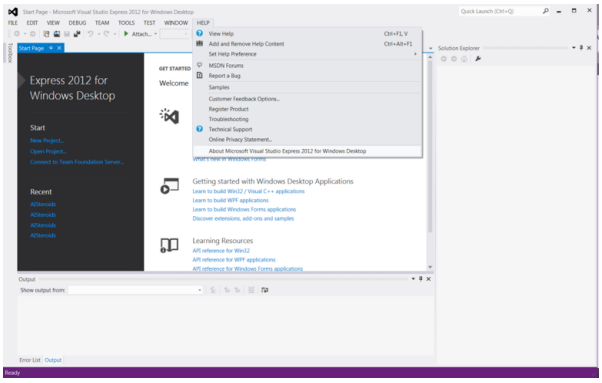
  - g++ (GNU GCC)
    Type the following command in a terminal.

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

    If gives a version number 4.4 or later, you're all set. Otherwise, we recommend upgrading.

- Windows
  - Visual Studio Microsoft's Visual Studio 2010 or later is recommended.
    To check the version:
    Help (top tab) → *About Microsoft Visual Studio*





3.2 CMake

To check if cmake is installed:

```
$ which cmake
```

To check the version number:

```
$ cmake --version
```

The minimum required version is 2.8. However, we recommend to use version 3.2 or later.

3.3 CUDA Toolkit

CUDA is required to compile the GPU executable in both Windows and Linux. However, is not required to compile the CPU code. To download and install CUDA visit NVIDIA's webpage:

```
https://developer.nvidia.com/cuda-downloads
https://developer.nvidia.com/cuda
```

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.

To check if nvcc is installed:

```
$ which nvcc
```

To check the version number:

```
$ nvcc --version
```

The GPU builds of the code requires NVIDIA's CUDA 8.0 or newer:

4 Recommended Software Tools

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

4.1 Packmol

Packmol is a free molecule packing tool (written in Fortran), created by José Mario Martínez, a professor of mathematics at the State University of Campinas, Brazil. Packmol allows a specified number of molecules to be packed at defined separating distances within a certain region of space. More information regarding downloading and installing Packmol is available on their homepage:

`http://www.ime.unicamp.br/~martinez/packmol`

WARNING: 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. It is highly suggested to used the optimized structure of the molecule as the input file to packmol.

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

4.2 VMD

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

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

Although GOMC uses the same fundamental file types ? PDB (coordinates) and PSF (topology) as VMD, it uses some special tricks to obey certain rules of those file formats.
One useful purpose of VMD is visualization and analyze your systems.

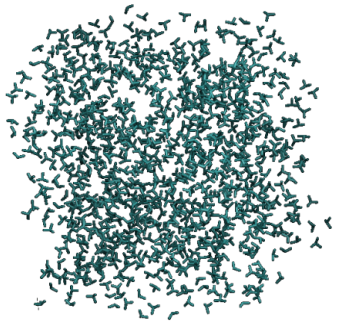


Figure 1: A system of united atom isobutane molecules

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

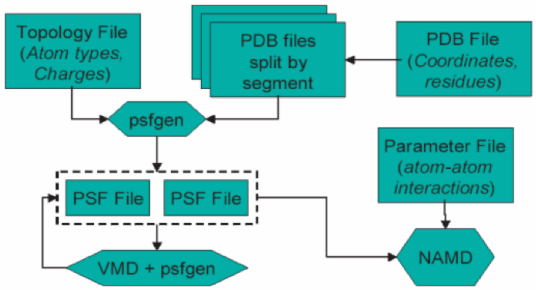


Figure 2: An overview of the PSFGen file generation process and its relationship to VMD/NAMD

To read more about PSFGen, reference:

Plugin homepage @ UIUC
`http://www.ks.uiuc.edu/Research/vmd/plugins/psfgen`

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

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

5 How to get the software

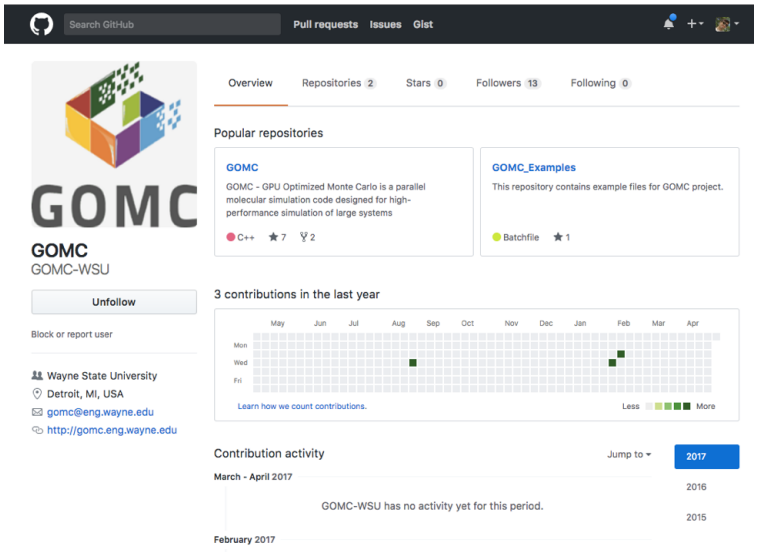
The CPU and GPU code are merged together under GOMC project. Currently, version control is handled through the GitHub repository. The latest GOMC release, Example files, and User Manual can be downloaded from GOMC website or GitHub repository.

5.1 GitHub

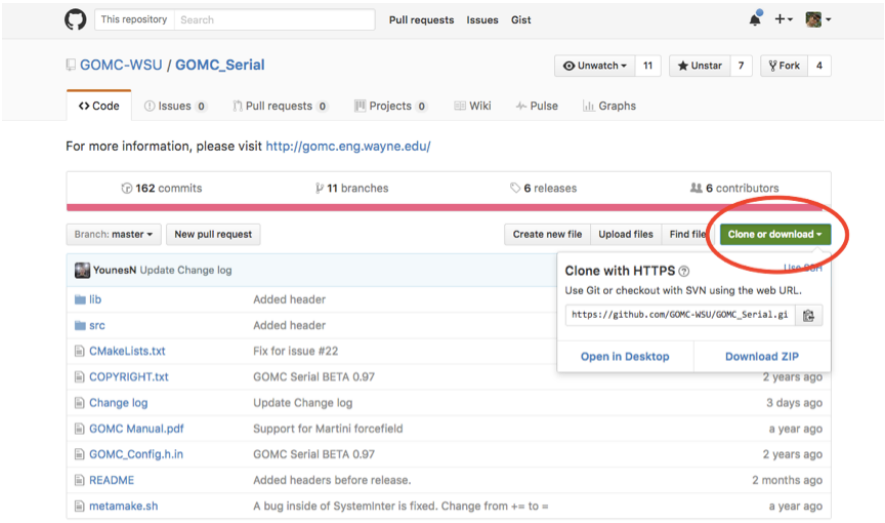
The posted builds in Master branch are "frozen" versions of the code that have been validated for a number of systems and ensembles. Other branches are created as a means of implementing new features. The latest

updated code builds, manual, example files, and other resources can be obtained via the following GitHub repository:

`https://github.com/GOMC-WSU`



GOMC and Examples repository can be found under the main page. Under GOMC repository, the code and manual can be found. Each repository can be downloaded by clicking on the Clone or download tab.

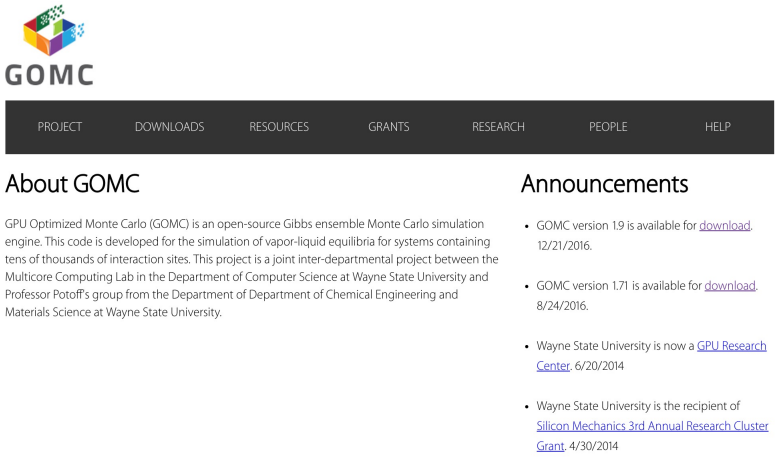


5.2 Website

To access the GOMC website, please click on the following link:

`http://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.



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

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

6 Compiling GOMC

GOMC generates four executable files for CPU code; `GOMC_CPU_GEMC` (Gibbs ensemble), `GOMC_CPU_NVT` (NVT ensemble), `GOMC_CPU_NPT` (isobaric-isothermal ensemble), and `GOMC_CPU_GCMC` (Grand canonical ensemble). In case of installing CUDA Toolkit, GOMC will generate additional four executable files for GPU code; `GOMC_GPU_GEMC`, `GOMC_GPU_NVT`, `GOMC_GPU_NPT`, and `GOMC_GPU_GCMC`.
This section guid users to compile GOMC in Linux or Windows.

6.1 Linux

First, navigate your command line to the GOMC base directory. To compile GOMC on Linux, give permission to "metamake.sh" by running the following command and execute it.

```
$ chmod u+x metamake.sh
$ ./metamake.sh
```

This script will create a bin directory and run cmake file to compile the code as well. All executable files will be generated in the "bin" directory.

6.2 Windows

To compile GOMC on in Windows, follow these steps:

1. Open the Windows-compatible CMake GUI.
2. Set the Source Folder to the GOMC root folder.
3. Set the build Folder to your Build Folder.

4. Click configure, select your compiler/environment
5. Wait for CMake to finish the configuration.
6. Click configure again and click generate.
7. Open the CMake-generated project/solution etc. to the desired IDE (e.g Visual Studio).
8. Using the solution in the IDE of choice build GOMC per the IDE's standard release compilation/executable generation methods.

NOTE: You can also use CMake from the Windows command line if its directory is added to the PATH environment variable.

6.3 Configuring CMake

subsubsectionConfigure CMAKE GOMC use CMAKE to generate multi-platform intermediate files to compile the project. In this section, you can find all the information needed to configure CMAKE.
We recommend using a different directory for the cmake output than the home directory of the project as cmake tend to generate lots of files.
CMake has a ridiculously expansive set of options, so this document will only reproduce the most obviously relevant ones. When possible, options should be passed into CMake via command line options rather than the CMakeCached.txt file:

CMAKE_BUILD_TYPE To get the best performance you should build the project in release mode. In cmake GUI you can set the value of "CMAKE_BUILD_TYPE" to "Release" and in cmake command line you can add the following to the cmake:

```
-DCMAKE_BUILD_TYPE=Release
```

To compile the GOMC in debug mode, in cmake GUI, change the value of "CMAKE_BUILD_TYPE" to "Debug" and in cmake command line you can add the following to the cmake:

```
-DCMAKE_BUILD_TYPE=Debug
```

Other options are "< None | ReleaseWithDebInfo | MinSizeRel >".

CMAKE_CXX_COMPILER This option will set the compiler. It is recommended to use the Intel Compiler and linking tools, if possible (icc/icpc/etc.). They significantly outperform the default GNU and Visual Studio compiler tools and are available for free for academic use with registration.

CMAKE_CXX_FLAGS_RELEASE:STRING 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 from "-O3 -DNDEBUG" to "-O3 -qopenmp -DNDEBUG". Recompile the GOMC by typing the command:

```
$ make
```

ENSEMBLE_NVT You can turn the compilation of CPU version of NVT ensemble on or off using this option.
`-DENSEMBLE_NVT=<On | Off >`

ENSEMBLE_NPT You can turn the compilation of CPU version of NPT ensemble on or off using this option.
`-DENSEMBLE_NPT=<On | Off >`

ENSEMBLE_GCMC You can turn the compilation of CPU version of GCMC ensemble on or off using this option.
`-DENSEMBLE_GCMC=<On | Off >`

ENSEMBLE_GEMC You can turn the compilation of CPU version of GEMC ensemble on or off using this option.
`-DENSEMBLE_GEMC=<On | Off >`

ENSEMBLE_GPU_NVT You can turn the compilation of GPU version of NVT ensemble on or off using this option.
`-DENSEMBLE_GPU_NVT=<On | Off >`

ENSEMBLE_GPU_NPT You can turn the compilation of GPU version of NPT ensemble on or off using this option.
`-DENSEMBLE_GPU_NPT=<On | Off >`

ENSEMBLE_GPU_GCMC You can turn the compilation of GPU version of GCMC ensemble on or off using this option.
`-DENSEMBLE_GPU_GCMC=<On | Off >`

ENSEMBLE_GPU_GEMC You can turn the compilation of GPU version of GEMC ensemble on or off using this option.
`-DENSEMBLE_GPU_GEMC=<On | Off >`

7 Input File Formats

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

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

7.1 PDB File

GOMC requires only one PDB file for NVT and NPT ensembles. However, GOMC requires two PDB files for GEMC and GCMC ensembles.

7.1.1 What is PDB file

The term PDB can refer to the Protein Data Bank (`http://www.rcsb.org/pdb/`), to a data file provided there, or to any file following the PDB format. Files in the PDB include various information such as the name of the compound, the ATOM and HETATM records containing the coordinates of the molecules, and etc. PDB widely used by NAMD, GROMACS, CHARMM, ACEMD, and Amber. GOMC ignore everything in a PDB file except for the `REMARK`, `CRYST1`, `ATOM`, and `END` records. An overview of the PDB standard can be found here:

`http://www.wwpdb.org/documentation/file-format-content/format33/sect2.html#HEADER`
`http://www.wwpdb.org/documentation/file-format-content/format33/sect8.html#CRYST1`
`http://www.wwpdb.org/documentation/file-format-content/format33/sect9.html#ATOM`

PDB contains foure major parts; `REMARK`, `CRYST1`, `ATOM`, and `END`. Here is the definition of each field and how GOMC is using them to get the information it requires.

- `REMARK`: This header records present experimental details, annotations, comments, and information not included in other records (`http://www.wwpdb.org/documentation/file-format-content/format33/sect2.html#HEADER`). However, GOMC uses this header to print simulation informations.

  Max Displacement ($\mathring{A}$)

  Max Rotation (Degree)

  Max volume exchange ($\mathring{A}^3$)

  Monte Carlo Steps (MC)

- `CRYST1`: This header records the unit cell dimension parameters (`http://www.wwpdb.org/documentation/file-format-content/format33/sect8.html#CRYST1`).

  Lattice constant: a, b, c ($\mathring{A}$)

  Lattice angles: α, β, γ (Degree)

- `ATOM`: The ATOM records present the atomic coordinates for standard amino acids and nucleotides. They also present the occupancy and temperature factor for each atom (`http://www.wwpdb.org/documentation/file-format-content/format33/sect9.html#ATOM`).

  ATOM: Record name.

  serial: Atom serial number.

name: Atom name.

resName: Residue name.

chainID: Chain identifier.

resSeq: Residue sequence number.

x: Coordinates for X ($\mathring{A}$).

y: Coordinates for Y ($\mathring{A}$).

z: Coordinates for Z ($\mathring{A}$).

occupancy: GOMC uses to define which atoms belong to which box.

beta: Beta orTemperature factor. GOMC uses this value to define the mobility of the atoms.

element: Element symbol.

- `END`: A frame in the PDB file is terminated with the keyword.

Here are the PDB output of GOMC for the first molecule of isobutane:

```
REMARK    GOMC  122.790  3.14159  3439.817  1000000
CRYST1  35.245   35.245   35.245     90.00    90.00   90.00
ATOM         1       C1       ISB         1    0.911  -0.313   0.000  0.00  0.00   C
ATOM         2       C2       ISB         1    1.424  -1.765   0.000  0.00  0.00   C
ATOM         3       C3       ISB         1   -0.629  -0.313   0.000  0.00  0.00   C
ATOM         4       C4       ISB         1    1.424   0.413  -1.257  0.00  0.00   C
END
```

The fields seen here in order from left to right are the record type, atom ID, atom name, residue name, residue ID, x, y, and z coordinates, occupancy, temperature factor (called beta), and segment name.

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.

Important: NOTE on PDB Format Conventions:

- 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)
- The beta value in GOMC code is used to define the mobility of the molecule.

  Beta = 0.00: molecule can move and transfer within and between boxes.

  Beta = 1.00: molecule is fixed in its position.

  Beta = 2.00: molecule can move within the box but cannot be transferred between boxes.

7.1.2 Generating PDB file

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

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

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

2. Next, packings are calculated to place the simulation in a region of vapor-liquid coexistence. There are a couple of ways to do this in Gibbs ensemble:

   - Pack both boxes to a single middle density, which is an average of the liquid and vapor densities.
   - Same as previous method, 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 cube 0.1 0.1 0.1 70.20
end structure
```

   Copy the above text into"`pack_isobutane.inp`" file, save it and run the script by typing the following line into the terminal:

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

7.2 PSF File

GOMC requires only one PSF file for NVT and NPT ensembles. However, GOMC requires two PSF files for GEMC and GCMC ensembles.

7.2.1 What is PSF file

Protein structure file (PSF), contains all of the molecule-specific information needed to apply a particular force field to a molecular system. The CHARMM force field is divided into a topology file, which is needed to generate the PSF file, and a parameter file, which supplies specific numerical values for the generic CHARMM potential function. The topology file defines the atom types used in the force field; the atom names, types, bonds, and partial charges of each residue type; and any patches necessary to link or otherwise mutate these basic residues. The parameter file provides a mapping between bonded and nonbonded interactions involving the various combinations of atom types found in the topology file and specific spring constants and similar parameters for all of the bond, angle, dihedral, improper, and van der Waals terms in the CHARMM potential function. PSF file widely used by by NAMD, CHARMM, and X-PLOR.

The PSF file contains six main sections: remarks, atoms, bonds, angles, dihedrals, and impropers (dihedral force terms used to maintain planarity). Each section starts with a specific header described bellow:

- `NTITLE`: remarks on the file.
  The following is taken from a PSF file for isobutane:

```
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 }
```

- `NATOM`: Defines the atom names, types, and partial charges of each residue type.

  `atom ID`

  `segment name`

  `residue ID`

  `residue name`

  `atom name`

  `atom type`

  `atom charge`

  `atom mass`

  The following is taken from a PSF file for isobutane:

```
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
```

  The fields in the atom section, from left to right are atom ID, segment name, residue ID, residue name, atom name, atom type, charge, mass, and an unused 0.

- `NBOND`: The covalent bond section lists four pairs of atoms per line.
  The following is taken from a PSF file for isobutane:

```
3000  !BOND:  bonds
   1  2       1  3  1  4  5  6
   5  7       5  8
```

- `NTHETA`: The angle section lists three triples of atoms per line.
  The following is taken from a PSF file for isobutane:

```
3000  !NTHETA:  angles
   2  1         4  2  1  3  3  1  4
   6  5         8  6  5  7  7  5  8
```

- `NPHI`: The dihedral sections list two quadruples of atoms per line.
- `NIMPHI`: The improper sections list two quadruples of atoms per line. GOMC currently does not support improper. For the molecules without dihedral or improper, PDF file look like the following:

```
0  !NPHI: dihedrals

0  !NIMPHI: impropers
```

- (other sections such as cross terms)

Important: NOTE on PSF Format Conventions:

- 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 .
- Improper entries are read and stored, but are not currently used. Support will eventually be added for this.

7.2.2 Generating PSF file

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

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

coordpdb ./STEP2_ISB_packed_BOX_0.pdb ISB

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

Typically, one script is run per box to generate a finalized PDB/PSF for that box. The script requires one additional file, the NAMD-style topology file. While GOMC does not directly read or interact with this file, it's typically used to generate the PSF and, hence, is considered one of the integral file types. It will be briefly discussed in the following section.

7.3 Topology File

A CHARMM forcefield topology file contains all of the information needed to convert a list of residue names into a complete PSF structure 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 topology file for isobutane:

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

AUTOGENERATE ANGLES DIHEDRALS

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

END
```

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

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

- Topology Tutorial: `http://www.ks.uiuc.edu/Training/Tutorials/science/topology/topology-tutorial.pdf`
- NAMD Tutorial: Examining the Topology File (`http://www.ks.uiuc.edu/Training/Tutorials/science/topology/topology-html/node4.html`)
- Developing Topology and Parameter Files: `http://www.ks.uiuc.edu/Training/Tutorials/science/forcefield-tutorial/forcefield-html/node6.html`
- NAMD Tutorial: Topology Files (`http://www.ks.uiuc.edu/Training/Tutorials/namd/namd-tutorial-win-html/node25.html`)

7.4 Parameter File(s):

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

- "`CHARMM`" (Chemistry at Harvard Molecular Mechanics) compatible parameter file
- "`EXOTIC`" parameter file

If the parameter file type is not specified or if the chosen file is missing, an error will result.
Both force field file options are whitespace separated files with sections preceded by a tag. When a known tag (representing a molecular interaction in the model) is encountered, reading of that section of the force field begins. Comments (anything after a * or !) and whitespace are ignored. Reading concludes when the end of the file is reached or another section tag is encountered.

CHARMM format parameter file
`CHARMM` contains a widely used model for describing energies in Monte Carlo and molecular dynamics simulations. It is intended to be compatible with other codes that use such a format, such as `NAMD`. For a general overview of the `CHARMM` force field, see:
`http://www.charmmtutorial.org/index.php/The_Energy_Function`

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

$$U_{\texttt{bond}} = \sum_{\texttt{bonds}} K_b(b - b_0)^2 \qquad U_{\texttt{dihedral}} = \sum_{\texttt{dihedrals}} K_\phi[1 + \cos(n\phi - \delta)]$$

$$U_{\texttt{angle}} = \sum_{\texttt{angles}} K_\theta(\theta - \theta_0)^2 \qquad U_{\texttt{LJ}} = \sum_{\texttt{nonbonded}} \epsilon_{ij} \left[\left(\frac{R_{min_{ij}}}{r_{ij}} \right)^{12} - 2 \left(\frac{R_{min_{ij}}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{\epsilon r_{ij}}$$

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 K_b.

  `NOTE:` GOMC does not sample bond stretch.

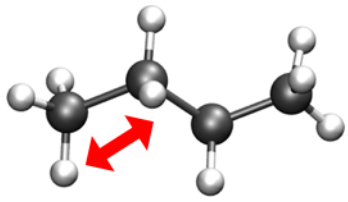


Figure 3: Oscillations about the equilibrium bond length

- `ANGLES`
  - Describe the conformational lbehavior of an angle (ϑ) between three atoms, one of which is shared branch point to the other two. To fix any angle and ignore the related angle energy, put a very large value i.e. "999999999999" for K_θ.

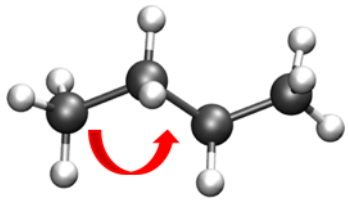


Figure 4: Oscillations of 3 atoms about an equilibrium bond angle

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

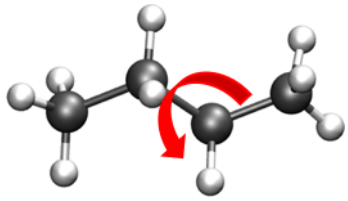


Figure 5: Torsional rotation of 4 atoms about a central bond

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

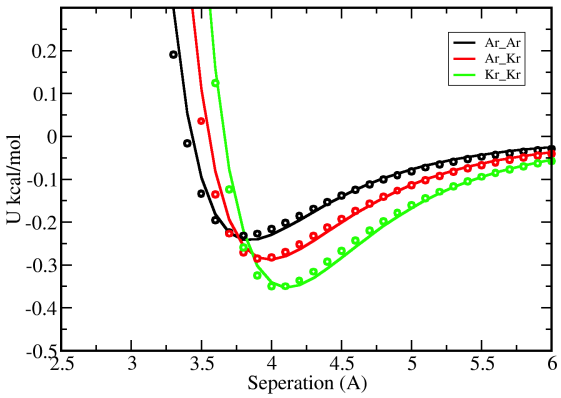


Figure 6: Non-bonded energy terms (electrostatics and Lenard-Jones)

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

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

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

7.4.1 BONDS

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

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

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

7.4.2 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. In order to fix the angle, it requires to set a large value for K_θ. By assigning a large value like 9999999999, specified angle will be fixed and energy of that angle will considered to be zero.

Here is an example of what is necessary for isobutane:

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

Some CHARMM `ANGLES` section entries include Urey-Bradley potentials (K_{ub}, b_{ub}), in addition to the standard quadratic angle potential. The constants related to this potential function are currently read, but the logic has not been added to calculate this potential function. Support for this potential function will be added in later versions of the code.

7.4.3 DIHEDRALS

The final major bonded interactions section of the `CHARMM` compliant parameter file are the `DIHEDRALS`. Each dihedral is composed of a dihedral series of 1 or more terms. Often, there are 4 to 6 terms in a dihedral. Angles for the dihedrals' deltas are given in degrees.
Since isobutane has no dihedral, here are the parameters pertaining to 2,3-dimethylbutane:

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

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

to literature.

7.4.4 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.

7.4.5 NONBONDED

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

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

NOTE: The R_{min} is different from 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.

7.4.6 NBFIX

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
```

7.5 Exotic Parameter file

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

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

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

NOTE: Although the units (Angstroms) are the same, the exotic file uses 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.

7.6 Control File (*.conf)

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

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

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

7.6.1 Input/Simulation Setup

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

Restart Determines whether to restart the simulation from previous simulation or not.

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

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

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

```
##################################
# kind {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.

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

Random_Seed Defines the seed number. If "INTSEED" is chosen, seed number needs to be specified; otherwise, the program will terminate.

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

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

ParaTypeCHARMM Sets force field type to `CHARMM` style.

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

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

ParaTypeEXOTIC Sets force field type to `EXOTIC` style.

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

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

ParaTypeMARTINI Sets force field type to MARTINI style.

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

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

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

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

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

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

- Value 1: $< INTEGER >$ - Sets box number (first box is box '0').

- Value 2: $< STRING >$ - Sets PDB file name

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

Example of NVT or NPT ensemble

```
##################################
# INPUT PDB FILES - NVT or NPT ensemble
##################################
Coordinates 0 STEP3_START_ISB_sys.pdb
```

Example of Gibbs or GC ensemble

```
##################################
# INPUT PDB FILES - Gibbs or GC ensemble
##################################
Coordinates 0 STEP3_START_ISB_sys_BOX_0.pdb
Coordinates 1 STEP3_START_ISB_sys_BOX_1.pdb
```

NOTE: In case of `Restart true`, the restart PDB output file from GOMC (OutputName_BOX_0_restart.pdb) can be used for each boxe.

Example of Gibbs ensemble when `Restart` mode is active

```
################################
# INPUT PDB FILES
################################
Coordinates 0 ISB_T_270_k_BOX_0_restart.pdb
Coordinates 1 ISB_T_270_k_BOX_1_restart.pdb
```

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

- Value 1: $< INTEGER >$ - Sets box number (first box is box '0').

- Value 2: $< STRING >$ - Sets PSF file name

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

  Example of NVT or NPT ensemble

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

  Example of Gibbs or GC ensemble

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

  NOTE: In case of `Restart true`, the PSF output file from GOMC (OutputName_merged.psf) can be used for both boxes.

  Example of Gibbs ensemble when Restart mode is active

```
################################
# INPUT PSF FILES
################################
Structure 0 ISB_T_270_k_merged.psf
Structure 1 ISB_T_270_k_merged.psf
```

7.6.2 System Settings for During Run Setup

This section contains all the variables not involved in the output of data during the simulation, or in the reading of input files at the start of the simulation. In other words, it contains settings related to the moves, the thermodynamic constants (based on choice of ensemble), and the length of the simulation.
Note that some tags, or entries for tags, are only used in certain ensembles (e.g. Gibbs ensemble). These cases are denoted with colored text.

GEMC (For Gibbs Ensemble runs only) Defines what type of Gibbs Ensemble simulation you want to run.
If neglected in Gibbs Ensemble, it simply defaults to constant volume (NVT) Gibbs Ensemble.

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

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

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

```
################################
# GEMC TYPE (DEFAULT IS NVT_GEMC
################################
GEMC NVT
```

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

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

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

Temperature Sets the temperature at which the system will run.

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

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

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

LRC Defines whether or not long range corrections are used.

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

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

- Value 1: $< STRING >$ - Allows you to choose between "1-2", "1-3", and "1-4".

  1-2 All interactions pairs of bonded atoms, except the ones that separated with one bond, will be considered and modified using 1-4 parameters defined in parameter file.

  1-3 All interaction pairs of bonded atoms, except the ones that separated with one or two bonds, will be considered and modified using 1-4 parameters defined in parameter file.

  1-4 All interaction pairs of bonded atoms, except the ones that separated with one, two or three bonds, will be considered using non-bonded parameters defined in parameter file.

  NOTE: The default value is "1-4".

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

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

- Value 1: $< STRING >$ - Allows you to pick between "VDW", "SHIFT" and "SWITCH".

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

```
################################
# SIMULATION CONDITION
################################
Temperature 270.00
Potential VDW
LRC true
Rcut 10
Exclude 1-4
```

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

```
################################
# SIMULATION CONDITION
################################
Temperature 270.00
Potential SHIFT
LRC false
Rcut 10
Exclude 1-4
```

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

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

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

ElectroStatic Considers coulomb interaction or not. This function will be discussed further in the Intermolecular energy and Virial calculation section.

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

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

Ewald Considers standard Ewald summation method for electrostatic calculation. This function will be discussed further in the Intermolecular energy and Virial calculation section.

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

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

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

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

`NOTE:` By default, `CachedFourier` will be set to "true" if not value was set.

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

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

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

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

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

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

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

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

1-4scaling Defines constant factor to modify intra-molecule coulomb interaction.

- Value 1: $< DOUBLE >$ - A fraction number between 0.0 and 1.0.

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

```
################################
# SIMULATION CONDITION
################################
ElectroStatic true
Ewald true
Tolerance 0.00001
1-4scaling 0.0
```

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

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

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

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

AdjSteps Sets the number of steps per adjustment to the maximum constants associated with each move (e.g. maximum distance in xyz to displace, the maximum volume in $\AA^3$ to swap, etc.)

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

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

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

- Value 1: $< STRING >$ - The resname to apply this chemical potential.
- 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).
NOTE: If there is a molecule kind that cannot be transfer between boxes (in PDB file the beta value is set to 1.00 or 2.00), an arbitrary value (e.g. 0.00) can be assigned to the resname.

```
################################
# Mol.  Name Chem.  Pot.  (K)
################################
ChemPot AR -968
```

Fugacity (For Grand Canonical (GC) ensemble runs only): Fugacity at which simulation is run.

- Value 1: $< STRING >$ - The resname to apply this fugacity.
- Value 2: $< DOUBLE >$ - The fugacity value in bar.

NOTE: For binary systems, include multiple copies of the tag (one per residue kind).
NOTE: If there is a molecule kind that cannot be transfer between boxes (in PDB file the beta value is set to 1.00 or 2.00) an arbitrary value e.g. 0.00 can be assigned to the resname.

```
################################
# Mol.  Name Fugacity (bar)
################################
Fugacity AR 0.1
Fugacity Si 0.0
Fugacity O 0.0
```

DisFreq Fractional percentage at which displacement move will occur.

- Value 1: $< DOUBLE >$ - % Displacement

RotFreq Fractional percentage at which rigid rotation move will occur.

- Value 1: $< DOUBLE >$ - % Rotatation

IntraSwapFreq Fractional percentage at which particle will be removed from a box and inserted into the same box using configurational bias algorithm.

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

RegrowthFreq Fractional percentage at which part of the molecule will be deleted and then regrown using configurational bias algorithm.

- Value 1: $< DOUBLE >$ - % Molecular growth

VolFreq (For isobaric-isothermal ensemble and Gibbs ensemble runs only) Fractional percentage at which particle will be removed from one box and inserted into the other box using configurational bias algorithm.

- Value 1: $< DOUBLE >$ - % Volume swaps

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

- Value 1: $< DOUBLE >$ - % Molecule swaps

```
#################################
# MOVE FREQEUNCY
#################################
DisFreq 0.49
RotFreq 0.10
VolFreq 0.01
SwapFreq 0.20
IntraSwapFreq 0.10
RegrowthFreq 0.10
```

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

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

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

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

FixVolBox0 (For adsorption simulation in 'NPT Gibbs ensemble runs only) Changing the volume of fluid phase (Box 1) to maintain the constant imposed pressure and temperature, while keeping the volume of adsorbed phase (Box 0) fix.

- Value 1: $< BOOLEAN >$ - If "true" volume of adsorbed phase will remain constant, If "false" volume of adsorbed phase will change.

CellBasisVector Defines the shape and size of the simulation periodic cell. `CellBasisVector1`, `CellBasisVector2`, `CellBasisVector3` represent the cell basis vector a, b, c, respectively. This tag may occur multiple times. It occurs once for `NVT` and `NPT`, but twice for Gibbs ensemble or GC ensemble.

- Value 1: $< INTEGER >$ - Sets box number (first box is box '0')
- Value 2: $< DOUBLE >$ - x value of cell basis vector in Angstroms
- Value 3: $< DOUBLE >$ - y value of cell basis vector in Angstroms
- Value 4: $< DOUBLE >$ - z value of cell basis vector in Angstroms

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

Example for `NVT` and `NPT` ensemble. In this example, each vector is perpendicular to the other two ($\alpha = 90, \beta = 90, \gamma = 90$), as indicated by a single x, y, or z value being specified by each and making a rectangular 3-D box:

```
#################################
# BOX DIMENSION #, X, Y, Z
#################################
CellBasisVector1 0 40.00 00.00 00.00
CellBasisVector2 0 00.00 40.00 00.00
CellBasisVector3 0 00.00 00.00 80.00
```

Example for `Gibbs ensemble` and `GC ensemble` ensemble. In this example, In the first box, only vector a and c are perpendicular to each other ($\alpha = 90, \beta = 90, \gamma = 120$), and making a non-orthogonal simulation cell with the cell length a, b, c of 36.91, 39.91, and 76.98 Angstroms, respectively. In the second box, each vector is perpendicular to the other two ($\alpha = 90, \beta = 90, \gamma = 90$), as indicated by a single x, y, or z value being specified by each and making a cubic box:

```
################################
# BOX DIMENSION #, X, Y, Z
################################
CellBasisVector1 0 36.91 00.00 00.00
CellBasisVector2 0 -18.45 31.96 00.00
CellBasisVector3 0 00.00 00.00 76.98

CellBasisVector1 1 60.00 00.00 00.00
CellBasisVector2 1 00.00 60.00 00.00
CellBasisVector3 1 00.00 00.00 60.00
```

Warning: In case of `Restart true`, box dimension does not need to be specified. If it is specified, program will read it but it will be ignored and replaced by the printed cell dimensions and angles in the restart PDB output file from GOMC (OutputName_BOX_0_restart.pdb and OutputName_BOX_1_restart.pdb).

CBMC_First Number of CBMC trials to choose the first atom 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 atom positions (Lennard-Jones trials for first seed growth)

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

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

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

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

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

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

7.6.3 Output Controls

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

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

- Value 1: $< STRING >$ - Unique phhrase to identify this system.

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

CoordinatesFreq Controls output of PDB file (coordinates). If PDB dumping was enabled, one file for NVT or NPT and two files for Gibbs ensemble or GC ensemble will be dumped into OutputName_BOX_n.pdb, where `n` defines the box number.

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

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

`NOTE:` At the beginning of simulation, a merged PSF file will be dumped into OutputName_merged.pdb, 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. In addition, this file can be used to load into GOMC once restart simulation was active.

RestartFreq Controls the output of the last state of simulation at a specified step in PDB files (coordinates) OutputName_BOX_n_restart.pdb, where `n` defines the box number. Header part of this file contains important information and will be needed to restart the simulation:

- Simulation cell dimensions and angles.
- Maximum amount of displacement ($\mathring{A}$), rotation (θ), and volume ($\mathring{A}^3$) that used in `Displacement`, `Rotation`, and `Volume` move.

If PDB dumping was enabled, one file for NVT or NPT and two files for Gibbs ensemble or GC ensemble will be dumped.

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

`NOTE:` The restart PDB file contains only `ATOM` that exist in each boxes at specified steps. This allows the user to load this file into GOMC once restart simulation was active.
`NOTE:` `CoordinatesFreq` must be a common multiple of `RestartFreq` or vice versa.

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

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

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

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

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

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

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

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

DistName Sets short phrase to naming particle distribution file.

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

HistName Sets short phrase to naming energy sample file.

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

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

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

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

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

SampleFreq Controls histogram sampling frequency.

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

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

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

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

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

```
#################################
# ENABLE: BLK AVE., FLUC.
#################################
OutEnergy true true
OutPressure true true
OutMolNum true true
OutDensity true true
OutVolume true true
OutSurfaceTention false false
```

8 GOMC's Output Files, Terminal Output

GOMC currently supports several kinds of output:

- STDIO ("console") output
- File output
  - PDB
  - PSF
  - Block Averages

GOMC output units:

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

8.1 Console Output

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

```
$ GOMC_CPU_NVT in.conf > out_isobutane.log &
```

Statistical and thermodynamic information is provided in console output.

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

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

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

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

Here, "output_console.log" is the console output file and "$3" represents the second element of the "ENERGY_BOX_0" section.

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

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

The first section of this console output typically includes some information relating the system, CPU, GPU, and RAM. In continue, console output includes information regarding the input file (configuration file), force field reading, summary of the structure of the molecule, bonded parameter, and minimum and maximum coordinate of molecules. This output is important; it may contain text relating to issues encountered if there was an error in the current run (e.g. a bad parameter, unknown keyword, missing parameters in the configuration file, etc.)

```
Info: GOMC Version 2.20
Info: Start Time: Mon Nov 27 20:21:07 2017
Info: Host Name: ####
CPU information:
Info: Total number of CPUs: 4
Info: Total number of CPUs available: 4
Info: Model name: Intel(R) Core(TM) i5-2500K CPU @ 3.30GHz
Info: System name: Linux
Info: Release: 3.10.0-514.26.1.el7.x86_64
Info: Version: #1 SMP Wed Jun 28 15:10:01 CDT 2017
Info: Kernel Architecture: x86_64
Info: Total Ram: 7806.1MB
Info: Used Ram: 6970.0MB
Info: Working in the current directory: ~/Desktop/validation/GOMC_Examples/GCMC/isobutane/run2a_bridge
Info: GOMC COMPILED TO RUN GRAND CANONICAL ENSEMBLE.
Info: Number of threads                  1

Reading Input File:                      in.conf
Info: Random seed                        Active
Info: PARAMETER file: CHARMM format!
Info: Input Temperature                  410.0000 K
Info: Non-truncated potential            Active
Info: Long Range Correction              Active
Info: Cutoff                             10.0000 A
Info: Exclude                            ONE-FOUR
Warning: Modified 1-4 VDW parameters will be ignored!
Info: Pressure calculation               Inactive
Info: Total number of steps              1000000
Info: Number of equilibration steps      500000
Info: Move adjustment frequency          1000
Info: Displacement move frequency        0.2000
Info: Rotation move frequency            0.1000
Info: Molecule swap move frequency       0.7000
Info: Box  0:  Periodic Cell Basis 1     30.000   0.000   0.000
Info: Box  0:  Periodic Cell Basis 2      0.000  30.000   0.000
Info: Box  0:  Periodic Cell Basis 3      0.000   0.000  30.000
Info: Box  1:  Periodic Cell Basis 1     30.000   0.000   0.000
Info: Box  1:  Periodic Cell Basis 2      0.000  30.000   0.000
Info: Box  1:  Periodic Cell Basis 3      0.000   0.000  30.000
Info: Chemical potential                 ISB    -3135.0000 K
Info: Output name                        ISB_410_00_K_u_3135_r1a
Info: Coordinate frequency               1000000
Info: Restart frequency                  1000000
Info: Console output frequency           10000
Info: Average output frequency           100000
Info: Histogram output frequency         100000
Info: Histogram sample frequency         200
Default: Intra-Swap move frequency       0.0000
Default: Short Range Cutoff              1.0000
Warning: 1-4 Electrostatic scaling set, but will be ignored.
Finished Reading Input File:             in.conf
```

```
Reading from CHARMM-Style parameter file:       ../../../common/Par_TraPPE_Alkanes_CHARMM.inp
Reading BONDS parameters.
Reading ANGLES parameters.
Reading DIHEDRALS parameters.
Reading NONBONDED parameters.
Finished reading CHARMM-Style parameter file:   ../../../common/Par_TraPPE_Alkanes_CHARMM.inp
Reading from box 0 PDB coordinate file:         STEP3_START_ISB_vap_BOX_0.pdb
Finished reading box 0 PDB coordinate file:     STEP3_START_ISB_vap_BOX_0.pdb
Reading from box 1 PDB coordinate file:         STEP3_START_ISB_reservoir_BOX_1.pdb
Finished reading box 1 PDB coordinate file:     STEP3_START_ISB_reservoir_BOX_1.pdb
Random number seed: 1086667780

Molecules in PSF:
Molecule Kind: ISB
Idx     name    type    charge  mass
0       C1      CH1     0.0000  13.0190
1       C2      CH3     0.0000  15.0350
2       C3      CH3     0.0000  15.0350
3       C4      CH3     0.0000  15.0350

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

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

Dihedrals:

Bonds parameter:
Atom Types                    Kb(K)                b0(A)
CH1  CH3                        FIX              1.5400

Angles parameter:
Atom Types                Ktheta(K)       theta0(degree)
CH3  CH1  CH3          31250.002516             112.0000

Dihedrals parameter:
Atom Types                  Kchi(K)    n   delta(degree)

Minimum coordinates in box 0: x =    1.000, y =   20.816, z =   25.283
Maximum coordinates in box 0: x =    5.215, y =   28.682, z =   29.000
Wrapping molecules inside the simulation box 0:
Minimum coordinates in box 1: x =    1.000, y =    1.000, z =    1.000
Maximum coordinates in box 1: x =   29.000, y =   29.000, z =   29.000
Wrapping molecules inside the simulation box 1:
```

Next, the energy and statistic title, initial energy and statistic of the system's starting configuration will print:
NOTE: If total energy of simulation is greater that $1.0e^{14}$, `System Total Energy Calculation` will be performed at `EqSteps` to preserve energy value.

```
################################################################################
########################## INITIAL SIMULATION ENERGY ###########################

ETITLE:      STEP           TOTAL        INTRA(B)       INTRA(NB)       INTER(LJ)\
               LRC     TOTAL_ELECT            REAL           RECIP            SELF\
              CORR

ENER_0:         0        180.2229        181.3420          0.0000          0.0000\
          -1.1190          0.0000          0.0000          0.0000          0.0000\
          -0.0000

ENER_1:         0     109688.7579     109688.7579          0.0000          0.0000\
           0.0000          0.0000          0.0000          0.0000          0.0000\
          -0.0000

STITLE:      STEP        TOTALMOL

STAT_0:         0               1

STAT_1:         0             600
```

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

```
################################################################################
############################## STARTING SIMULATION #############################

MTITLE:      STEP          DISTRY       DISACCEPT      DISACCEPT%          DISMAX\
           ROTATE       ROTACCEPT      ROTACCEPT%          ROTMAX       INTRASWAP\
        INTACCEPT      INTACCEPT%        TRANSFER      TRANACCEPT     TRANACCEPT%

ETITLE:      STEP           TOTAL        INTRA(B)       INTRA(NB)       INTER(LJ)\
               LRC     TOTAL_ELECT            REAL           RECIP            SELF\
              CORR

STITLE:      STEP        TOTALMOL

Printed combined psf to file ISB_410_00_K_u_3135_r1a_merged.psf
MOVE_0:     10000            2001             936         46.7766          2.2711\
             1004             814         81.0757         15.0000               0\
                0          0.0000            3539            1895         53.5462

ENER_0:     10000       3140.6213      32612.5048          0.0000     -26561.2770\
       -2910.6065          0.0000          0.0000          0.0000          0.0000\
            0.0000

STAT_0:     10000              51

MOVE_1:     10000            3456            1945         56.2789

ENER_1:     10000     345561.7122     345561.7122          0.0000          0.0000\
            0.0000          0.0000          0.0000          0.0000          0.0000\
            0.0000

STAT_1:     10000             550

Steps/sec. : 8972.0132
```

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: In order to keep the format of console file consistent, if absolute value of calculated properties of simulation is greater that $1.0e^{11}$, the value of 999999999 will be printed instead.
NOTE: Since mol fraction value is very small compare to other properties, 8 digit precision was used instead of 4 digit to print out the value.
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.

8.2 Block Output Files

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

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

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

```
cat Blk_OutputName_BOX_0.dat | awk '{print $13}'
```

Here, "Blk_OutputName_BOX_0.dat" is the block-average file for simulation box 0 and "$13" represents the 13th column of the block file.

NOTE: In order to keep the format of console file consistent, if absolute value of calculated properties of simulation is greater that $1.0e^{11}$, the value of 999999999 will be printed instead.
NOTE: Since mol fraction value is very small compare to other properties, 8 digit precision was used instead of 4 digit to print out the value.

8.3 Visualizing Simulation

If `CoordinatesFreq` is enabled in configuration file, GOMC will output the molecule coordinates every specified stpes. 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..N1 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 output PDB and PSF files by GOMC using VMD, type this command in the terminal:

For all simulation except Gibbs ensemble that has one simulation box:

```
$ vmd ISB_T_270_k_merged.psf ISB_T_270_k_BOX_0.pdb
```

For Gibbs ensemble, visualizing the first box:

```
$ vmd ISB_T_270_k_merged.psf ISB_T_270_k_BOX_0.pdb
```

For Gibbs ensemble, visualizing the second box:

```
$ vmd ISB_T_270_k_merged.psf ISB_T_270_k_BOX_1.pdb
```

`NOTE:` Restart coordinate file (OutputName_BOX_0_restart.pdb) cannot be visualize using merged psf file, because atom number does not match. However, you can still open it in vmd using following command and vmd will automatically find the bonds of the molecule based on the coordinates.

```
$ vmd ISB_T_270_k_BOX_0_restart.pdb
```

9 Putting it all together: Running a GOMC Simulation

It is strongly recommended that you download the test system provided at
`http://gomc.eng.wayne.edu/downloads.html` or
`https://github.com/GOMC-WSU/GOMC_Examples/tree/master`

Run different simulation types in order to become more familiar with different parameter and configuration files (*.conf).
To recap the previous examples, a simulation of isobutane will be completed for a single temperature point on the saturated vapor-liquid coexistence curve.
The general plan for running the simulation is:

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

Please, complete steps 1 and 2; then, traverse to the directory, which should now contain a single file "GOMC_CPU_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 2 CH1 13.019 C !

AUTOGENERATE ANGLES DIHEDRALS

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

pack_box_0.inp

```
tolerance 3.0
filetype pdb
output STEP2_ISB_packed_BOX_0.pdb

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

pack_box_1.inp

```
tolerance 3.0
filetype pdb
output STEP2_ISB_packed_BOX_1.pdb

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

build_box_0.inp

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

build_box_1.inp

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

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

Once those files are created, run in the terminal:

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

This will create the intermediate PDBs.

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

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

This will create the intermediate PDBs.
To run the code a few additional things will be needed:

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

Enter the control file (in.conf) in the text editor in order to modify it. Example files for different simulation types can be found in previous section.
Once these four files have been added to the output directory, the simulation is ready.

Assuming the code is named `GOMC_CPU_GEMC`, run in the terminal using:

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

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

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

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

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

```
tail −f out_ISB.log
```

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

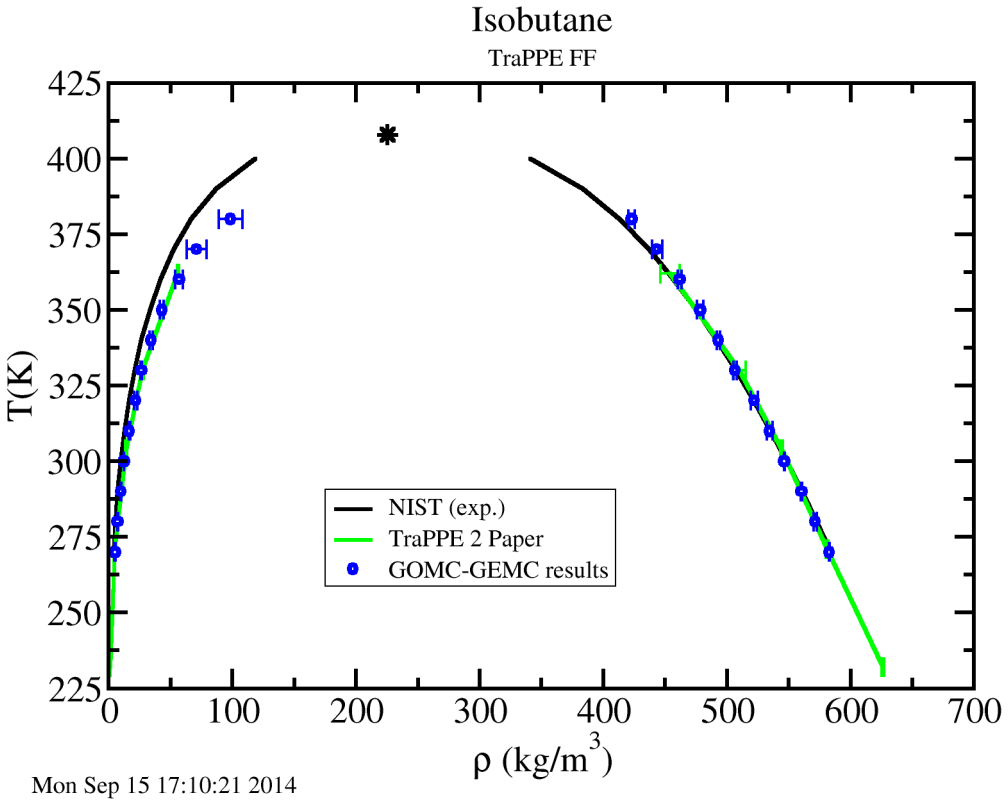


Figure 7: Repeating this process for multiple temperatures will allow you to obtain the following results.

10 Intermolecular Energy and Virial function (Van der Waals)

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

10.1 VDW

This option calculates potential energy without any truncation.

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

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

  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 $-\epsilon_{ij}$ for all n_{ij}. In the 12-6 potential, C_n reduces to the familiar value of 4.

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

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

$$W_{ij} = -\frac{dE_{ij}}{dr} \times \frac{\rightharpoonup r_{ij}}{r_{ij}} \tag{4}$$

  Using n−6 LJ potential defined above:

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

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

10.2 SHIFT

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

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

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

  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 according to Eq. 3, such that the minimum of the potential remains at $-\epsilon_{ij}$ for all n_{ij}. In the 12-6 potential, C_n reduces to the familiar value of 4.

- Virial Calculation: Virial is basically the negative derivative of energy with respect to distance, multiplied by distance, Eq. 4.
  Using `SHIFT` potential function defined above:

$$W_{ij}(\texttt{shift}) = 6 C_{n_{ij}} \epsilon_{ij} \left[\frac{n_{ij}}{6} \times \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{n_{ij}} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^{6} \right] \times \frac{\overrightarrow{r_{ij}}}{{r_{ij}}^2} \tag{7}$$

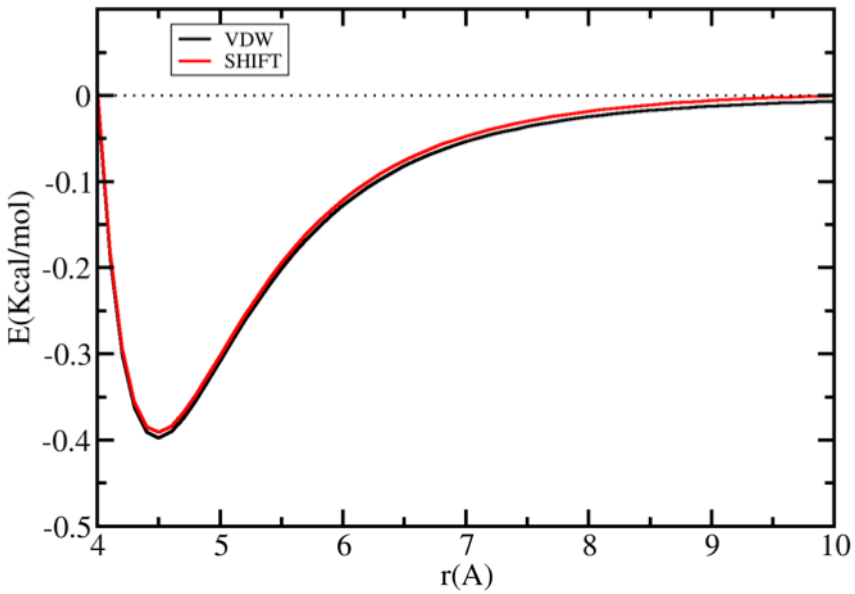


Figure 8: Graph of Van der Waals potential with and without the application of the `SHIFT` function. With the `SHIFT` function active, the potential by force was reduced to 0.0 at the `Rcut` distance. With the `SHIFT` function, there is a discontinuity where the potential is truncated.

10.3 SWITCH

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

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

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

  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 according to Eq. 3, such that the minimum of the potential remains at $-\epsilon_{ij}$ for all n_{ij}. In the 12-6 potential, C_n reduces to the familiar value of 4.

  The factor F_E is defined as:

$$F_E = \begin{cases} 1 & r_{ij} \le r_{switch} \\ \frac{\left({r_{cut}}^2 - {r_{ij}}^2\right)^2 \times \left({r_{cut}}^2 - 3{r_{switch}}^2 + 2{r_{ij}}^2\right)}{\left({r_{cut}}^2 - {r_{switch}}^2\right)^3} & r_{switch} < r_{ij} < r_{cut} \\ 0 & r_{ij} \ge r_{cut} \end{cases} \tag{9}$$

- Virial Calculation: Virial is basically the negative derivative of energy with respect to distance, multiplied by distance, Eq. 4.
  Using `SWITCH` potential function defined above:

$$W_{ij}(\texttt{switch}) = \left[6C_{n_{ij}}\epsilon_{ij}\left[\frac{n_{ij}}{6} \times \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{n_{ij}} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \times \frac{F_E}{{r_{ij}}^2} - C_{n_{ij}}\epsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{n_{ij}} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \times F_W\right] \times \overrightarrow{r_{ij}} \tag{10}$$

The factor F_W is defined as:

$$F_W = \begin{cases} 1 & r_{ij} \leq r_{switch} \\ \frac{12\left({r_{cut}}^2 - {r_{ij}}^2\right) \times \left({r_{switch}}^2 - {r_{ij}}^2\right)}{\left({r_{cut}}^2 - {r_{switch}}^2\right)^3} & r_{switch} < r_{ij} < r_{cut} \\ 0 & r_{ij} \geq r_{cut} \end{cases} \tag{11}$$

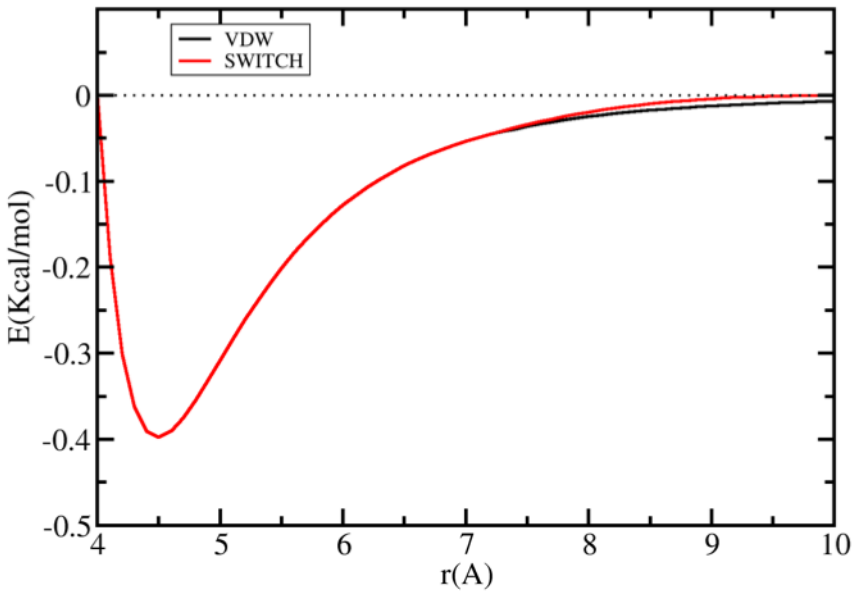


Figure 9: Graph of Van der Waals potential with and without the application of the `SWITCH` function. With the `SWITCH` function active, the potential is smoothly reduced to 0.0 at the `Rcut` distance.

10.4 SWITCH (MARTINI)

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

- Potential Calculation: Interactions between atoms can be modeled with an n−6 potential. In standard `MARTINI`, n is equal to 12,

$$E_{ij}(\texttt{switch}) = C_{n_{ij}} \epsilon_{ij} \left[{\sigma_{ij}}^n \left(\frac{1}{{r_{ij}}^n} + \varphi_n(r_{ij}) \right) - {\sigma_{ij}}^6 \left(\frac{1}{{r_{ij}}^6} + \varphi_6(r_{ij}) \right) \right] \tag{12}$$

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 according to Eq. 3, such that the minimum of the potential remains at $-\epsilon_{ij}$ for all n_{ij}. In the 12-6 potential, C_n reduces to the familiar value of 4.

The factor φ_α and constants are defined as:

$$\varphi_\alpha(r_{ij}) = \begin{cases} -C_\alpha & r_{ij} \leq r_{switch} \\ -\frac{A_\alpha}{3}(r_{ij} - r_{switch})^3 - \frac{B_\alpha}{4}(r_{ij} - r_{switch})^4 - C_\alpha & r_{switch} < r_{ij} < r_{cut} \\ 0 & r_{ij} \geq r_{cut} \end{cases} \tag{13}$$

$$A_\alpha = \alpha \frac{(\alpha+1)r_{switch} - (\alpha+4)r_{cut}}{{r_{cut}}^{(\alpha+2)}(r_{cut} - r_{switch})^2} \tag{14}$$

$$B_\alpha = \alpha \frac{(\alpha+1)r_{switch} - (\alpha+3)r_{cut}}{{r_{cut}}^{(\alpha+2)}(r_{cut} - r_{switch})^3} \tag{15}$$

$$C_\alpha = \frac{1}{{r_{cut}}^\alpha} - \frac{A_\alpha}{3}(r_{cut} - r_{switch})^3 - \frac{B_\alpha}{4}(r_{cut} - r_{switch})^4 \tag{16}$$

- Virial Calculation: Virial is basically the negative derivative of energy with respect to distance, multiplied by distance, Eq. 4.
  Using the `SWITCH` potential function defined for `MARTINI` force field:

$$W_{ij}(\texttt{switch}) = C_{n_{ij}}\epsilon_{ij}\left[{\sigma_{ij}}^n\left(\frac{n}{{r_{ij}}^{(n+1)}} + d\varphi_n(r_{ij})\right) - {\sigma_{ij}}^6\left(\frac{6}{{r_{ij}}^{(6+1)}} + d\varphi_6(r_{ij})\right)\right] \times \frac{\overrightarrow{r_{ij}}}{r_{ij}} \tag{17}$$

The constants defined in Eq. 14-16 and the factor $d\varphi_\alpha$ defined as:

$$d\varphi_\alpha(r_{ij}) = \begin{cases} 0 & r_{ij} \leq r_{switch} \\ A_\alpha(r_{ij} - r_{switch})^2 + B_\alpha(r_{ij} - r_{switch})^3 & r_{switch} < r_{ij} < r_{cut} \\ 0 & r_{ij} \geq r_{cut} \end{cases} \tag{18}$$

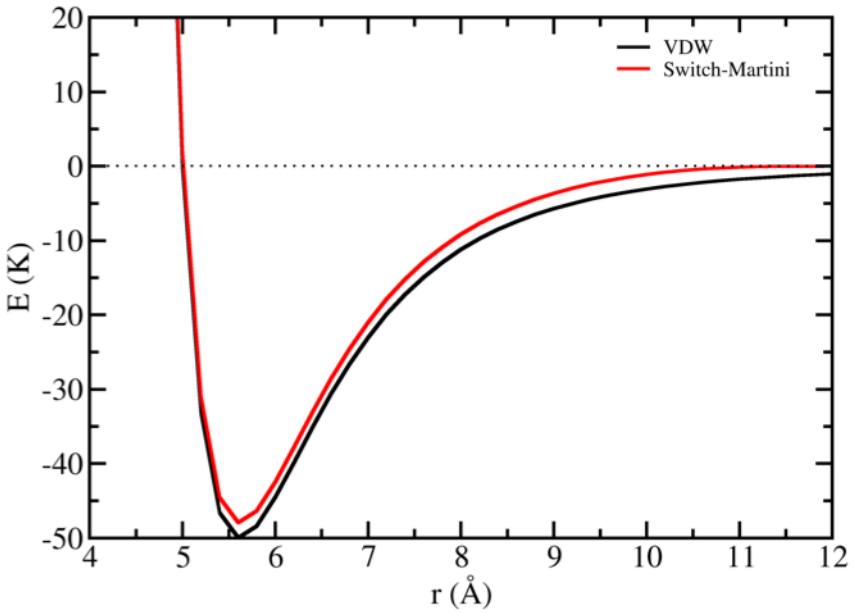


Figure 10: Graph of Van der Waals potential with and without the application of the `SWITCH` function in `MARTINI` force field. With the `SWITCH` function active, the potential is smoothly reduced to 0.0 at the `Rcut` distance.

11 Intermolecular Energy and Virial function (Electrostatic)

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

11.1 Ewald

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

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

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

$$E(\texttt{Ewald}) = E_{real} + E_{reciprocal} + E_{self} + E_{correction} \tag{19}$$

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

$$E_{real} = \frac{1}{4\pi\epsilon_0}\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} q_i q_j \frac{\mathrm{erfc}(\alpha r_{ij})}{r_{ij}} \tag{20}$$

, where α is `Ewald` separation parameter according to

$$\alpha = \frac{\sqrt{-\log(Tolerance)}}{r_{cut}} \tag{21}$$

, where $Tolerance$ is a parameter, controlling the desired accuracy.

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

$$E_{reciprocal} = \frac{1}{\epsilon_0 V}\frac{1}{2}\sum_{\vec{k}\neq 0}\frac{1}{\vec{k}^2}\exp\left(\frac{-\vec{k}^2}{4\alpha^2}\right)\left[\left|R_{sum}\right|^2 + \left|I_{sum}\right|^2\right] \tag{22}$$

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

$$R_{sum} = \sum_{i=1}^{N} q_i \cos\left(\vec{k}.\vec{x_i}\right) \tag{23}$$

$$I_{sum} = \sum_{i=1}^{N} q_i \sin\left(\vec{k}.\vec{x_i}\right) \tag{24}$$

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

$$E_{self} = -\frac{\alpha}{4\pi\epsilon_0\sqrt{\pi}}\sum_{i=1}^{N} {q_i}^2 \tag{25}$$

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

$$E_{correction} = -\frac{1}{4\pi\epsilon_0}\frac{1}{2}\sum_{j=1}^{N}\sum_{l=1}^{N_j}\sum_{m=1}^{N_j} q_{j_l} q_{j_m}\frac{\mathrm{erf}(\alpha r_{j_l j_m})}{r_{j_l j_m}} \tag{26}$$

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

$$W(\texttt{Ewald}) = W_{real} + W_{reciprocal} \tag{27}$$

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

$$W_{real} = \frac{1}{4\pi\epsilon_0}\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} q_i q_j \left[\frac{\text{erfc}(\alpha r_{ij})}{r_{ij}} + \frac{2\alpha}{\sqrt{\pi}}\exp(-\alpha^2 {r_{ij}}^2)\right] \times \frac{\overrightarrow{r_{ij}}}{{r_{ij}}^2} \tag{28}$$

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

$$\begin{aligned} W_{reciprocal} = \frac{1}{\epsilon_0 V}\frac{1}{2}\sum_{\overrightarrow{k}\neq 0}\left[\frac{1}{\overrightarrow{k}^2}\exp\left(\frac{-\overrightarrow{k}^2}{4\alpha^2}\right)\left(\left|R_{sum}\right|^2 + \left|I_{sum}\right|^2\right)\left(1-\frac{\overrightarrow{k}^2}{2\alpha^2}\right)\right] + \\ \sum_{i=1}^{N}\frac{1}{\epsilon_0 V}\sum_{\overrightarrow{k}\neq 0}\left[\frac{q_i}{\overrightarrow{k}^2}\exp\left(\frac{-\overrightarrow{k}^2}{4\alpha^2}\right)\left[I_{sum}\times\cos(\overrightarrow{k}.\overrightarrow{x_i}) - R_{sum}\times\sin(\overrightarrow{k}.\overrightarrow{x_i})\right]\right] \times \left(\overrightarrow{k}.\overrightarrow{r_{ic}}\right) \end{aligned} \tag{29}$$

, where $\overrightarrow{r_{ic}}$ is the vector between atom and the center of the mass of the molecule.

11.2 SHIFT

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

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

$$E(\texttt{SHIFT}) = \frac{q_i q_j}{4\pi\epsilon_0}\left(\frac{1}{r_{ij}} - \frac{1}{r_{cut}}\right) \tag{30}$$

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

$$W(\texttt{SHIFT}) = \frac{q_i q_j}{4\pi\epsilon_0}\left(\frac{1}{r_{ij}} \times \frac{\overrightarrow{r_{ij}}}{{r_{ij}}^2}\right) \tag{31}$$

11.3 SWITCH

This option in `CHARMM` or `EXOTIC` force field forces the electrostatic energy to be zero at `Rcut` distance.

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

$$E(\texttt{SWITCH}) = \frac{q_i q_j}{4\pi\epsilon_0}\left(\left(\frac{r_{ij}}{r_{cut}}\right)^2 - 1.0\right)^2 \frac{1}{r_{ij}} \tag{32}$$

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

$$W(\texttt{SWITCH}) = \frac{q_i q_j}{4\pi\epsilon_0}\left[\left(\left(\frac{r_{ij}}{r_{cut}}\right)^2 - 1.0\right)^2 \frac{1}{{r_{ij}}^2} - \left(\frac{4}{{r_{cut}}^2}\right)\left(\left(\frac{r_{ij}}{r_{cut}}\right)^2 - 1.0\right)\right] \times \frac{\overrightarrow{r_{ij}}}{r_{ij}} \tag{33}$$

11.4 SWITCH (MARTINI)

This option in `MARTINI` force field smoothly forces the potential energy to be zero at `Rcut` distance and starts modifying the potential at `"Rswitch = 0.0"` distance.

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

$$E(\texttt{SWITCH}) = \frac{q_i q_j}{4\pi\epsilon_0\epsilon_1}\left(\frac{1}{r_{ij}} + \varphi_1(r_{ij})\right) \tag{34}$$

  , where ϵ_1 is the dielectric constant, which in `MARTINI` force field is equal to 15.0 and $\varphi_\alpha(r_{ij})$ is defined in Eq. 13-16.

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

$$W(\texttt{SWITCH}) = \frac{q_i q_j}{4\pi\epsilon_0\epsilon_1}\left(\frac{1}{{r_{ij}}^2} + d\varphi_1(r_{ij})\right) \times \frac{\overrightarrow{r_{ij}}}{r_{ij}} \tag{35}$$

  , where $d\varphi_1(r_{ij})$ is defined in Eq. 18.

12 Get Help or Technical Support

For get any help or technical support, please send message to `GOMC gitter`:

`https://gitter.im/GOMC_WSU/Lobby`

or send email to:

- Jeffrey Potoff: `jpotoff@wayne.edu`
- Loren Schwiebert: `loren@wayne.edu`