GIBS: Grand Canonical Monte Carlo Simulation Program for Computing Ion Distributions around Biomolecules in Hard Sphere Solvents

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# Synopsis

GIBS is a Grand canonical Monte Carlo (GCMC) simulation program for computing the thermodynamic properties of ionic solutions and their distributions around biomolecules. GIBS implements algorithms that automate the excess chemical potential calculations for a given target salt concentration. GIBS uses a cavity-bias algorithm to achieve high sampling acceptance rates for inserting ions and solvent hard spheres when simulating dense ionic systems. In the current version, ion-ion interactions can be described using Coulomb, hard-sphere, or Lennard-Jones (L-J) potentials; solvent-ion interactions can be described using hard-sphere, L-J and attractive square-well potentials; and, solvent-solvent interactions are described using hard-sphere repulsions. GIBS can be used as a platform to evaluate new implicit solvent and coarse-grained models for predicting the thermodynamics properties of ionic solutions. GIBS is written in C++ and is available freely for the community to use as an educational and as a research tool.

The GIBS program was written by Dr. Dennis G. Thomas in collaboration with Dr. Nathan A. Baker, at the Pacific Northwest National Laboratory. The program was developed as part of projects funded by the National Institutes of Health through R01 Grant Nos. GM076121-04S1 and GM099450.

# Main Features

1. Automated excess chemical potential calculations for bulk electrolyte solutions.
2. Fast and efficient GCMC sampling of ion distributions in bulk electrolyte solutions and around fixed molecular solutes.
3. Models for Ion-Ion interactions using `Coulomb`, `hard-sphere`, `Lennard-Jones` potentials.
4. Models for Ion-Solvent interactions using `hard-sphere`, `Lennard-Jones`, `attractive square well` potentials.
5. Models for Solvent-Solvent interactions using `hard-sphere` repulsions.
6. Solvent representation as dielectric continuum (primitive model) or as hard spheres (solvent primitive model or SPM).
7. Ion representation as charged hard spheres.

# Download instructions and code compilation

## Files and folders to download

|  |  |
| --- | --- |
| Files and Folders | Contents |
| src | Contains source code (.cpp, .hpp, .h) files. |
| Simulation\_Examples | Contains example applications of GIBS. |
| CMakeLists\_Examples | Contains CMakeLists.txt file templates for mac, linux, and windows. These can be modified to suit the user’s choice of the operating system and computing platform. |
| inputfiles.docx | Contains descriptions and usage information of simulation input files and keywords used to set up the GCMC simulations |
| example\_1.docx,example\_2.docx, example\_3.docx, example\_4.docx, example\_5.docx, example\_6.docx | Contains examples to learn how to run GCMC simulations, using GIBS. |

## Compiling code

To compile the code, first create a build directory in the **gibs** directory, e.g.,

* mkdir build

In the build directory, generate a **Makefile** using *CMake*. Examples of CMakeLists.txtfiles are provided in the CMakeLists\_Examples directory. These files can be modified to suit the user's choice of C++ compiler and platform. The following examples show how to compile the code on a Mac and on a Windows OS.

1. Using GNU C++ compiler on Mac

$ cd CMakeLists\_Examples

$ cp CMakeLists\_mac.txt ../CMakeLists.txt

$ cd build

$ cmake –DCMAKE\_BUILD\_TYPE=RELEASE ../

$ make

2. Using a 32-bit MINGW compiler for Windows. Run cmake and make in the Windows command prompt window.

> copy CMakeLists\_WindowsMINGW.txt ../CMakeLists.txt

> cd build

> cmake –G “MinGW Makefiles” –DCMAKE\_BUILD\_TYPE=RELEASE ../

> mingw32-make

Running cmake will generate the Makefile. Running make will create the executable file, gibs.exe.

# Setting up and running simulations

1. Create a simulation *run folder* (e.g., run\_1)**.**
2. Create 2 folders in the *run folder*, inputfiles and outputfiles.
3. Example input files can be obtained from Simulation\_Examples.
4. Set the parameter values for the simulation (See inputfiles.docx).
5. Copy the executable file (gibs.exe) to *run folder*.

To execute a run on a mac or linux, and to save the screen output to a file (e.g. run\_1.out), do

$ ./gibs.exe > run\_1.out &

To execute a run in a Windows Command Prompt window, do

* start /B gibs.exe > run\_1.out

## Simulation files and examples

The following files have been provided to help understand how to set up a GCMC simulation using GIBS.

|  |  |
| --- | --- |
| Files | Description |
| inputfiles.docx | Contains descriptions and usage information of simulation input files and keywords used to set up the GCMC simulations |
| example\_1.docx,example\_2.docx, example\_3.docx, example\_4.docx, example\_5.docx, example\_6.docx | Contains examples to learn how to run GCMC simulations. |

# Citing GIBS

To acknowledge the use of GIBS, please cite:

(This section will be completed as soon as the GIBS paper is published.)

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