Example 5: Simulating Divalent Ion Distributions around Nucleic Acid Duplexes

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# Solute all-atom coordinate files and electrostatic potentials

Uncompress the dna\_rna\_allatom\_coordinates\_potentials.tar.gz to extract the all-atom coordinate files (.pqr) and electrostatic potential maps (.dx) of four 25 base pair nucleic acid duplexes.

$ tar –zxvf dna\_rna\_allatom\_coordinates\_potentials.tar.gz

The folder names and files are listed in the table below. The PQR files were generated using PDB2PQR software, from PDB files provided by Alexey Onufriev and Igor Tolokh (from Virginia Tech). The electrostatic potentials (in .dx files) were approximated by solving the Poisson equation with the Adaptive Poisson Boltzman software (APBS) package. The input file used for the APBS calculations are also provided in the file folders.

|  |  |  |
| --- | --- | --- |
| File folder | 25 bp nucleic acid duplex | .pqr and .dx files |
| polyA\_polyT\_DNA\_model | poly(dA):poly(dT) | polyAT25.pqr, pot\_polyAT25\_npbe\_pdie2.dx |
| A-RNA\_model | A-RNA | rGCAU25\_cc.pqr, pot\_rGCAU25\_cc\_npbe\_pdie2.dx |
| mixed\_sequence\_DNA\_model | Mixed sequence DNA | dGCAT25\_cc.pqr, pot\_dGCAT25\_cc\_npbe\_pdie2.dx |
| DNA\_RNA\_hybrid\_model | DNA:RNA hybrid | hyb\_DNA\_RNA\_cc.pqr, pot\_hyb\_DNA\_RNA\_cc\_npbe\_pdie2.dx |

# Example Folders

Uncompress the files listed in the table below, using the command

$ tar –zxvf {filename}.tar.gz

|  |  |
| --- | --- |
| Simulation Examples | Compressed files |
| Example 5A: GCMC simulation with 25 bp poly(dA):poly(dT) DNA duplex in 100 mM SrCl2, using the unrestricted primitive model (UPM) | ./gibs/Simulation\_Examples/excess\_chempot\_SrCl2\_100mM\_PID\_UPM.tar.gz  ./gibs/Simulation\_Examples/SrCl2\_UPM\_PolyAT25.tar.gz |
| Example 5B: GCMC simulation with 25 bp poly(dA):poly(dT) DNA duplex in 100 mM SrCl2, using the SPM model with Lennard-Jones ion-water interactions | ./gibs/Simulation\_Examples/excess\_chempot\_SrCl2\_100mM\_PID\_SPM+LJ.tar.gz  ./gibs/Simulation\_Examples/SrCl2\_SPM\_LJ+IW\_PolyAT25.tar.gz |

Note: All input files are provided. For the solute simulations, due to the large file sizes associated with particle counts and acceptance rates, only the RDF output files and final simulation states are provided. However, for the equilibration runs, all output files are provided. In some cases (e.g, the excess potential calculations), only the input files may be available but the final chemical potential values can be checked by comparing the values to those listed in this document.

# Example 5A: GCMC simulation with 25 bp poly(dA):poly(dT) DNA duplex in 100 mM SrCl2, using the unrestricted primitive model (UPM)

In this example, we compute the cylindrical radial distribution and the total number of ions and water around a 25 bp poly(dA):poly(dT) DNA duplex in 100 mM SrCl2, using the UPM model.

Simulations are performed in the same way as in Example 4A.

Input files for the excess chemical potential calculation are provided in the folder: ./gibs/Simulation\_Examples/excess\_chempot\_SrCl2\_100mM\_PID\_UPM

The excess chemical potentials of Sr2+ and Cl- are -0.9237 and -0.2918, respectively.

Input files for the solute simulations are provided in the folder:

./gibs/Simulation\_Examples/SrCl2\_UPM\_PolyAT25

RDF output files are also provided.

# Example 5B: GCMC simulation with 25 bp poly(dA):poly(dT) DNA duplex in 100 mM SrCl2, using the SPM model with Lennard-Jones ion-water interactions

In this example, we compute the cylindrical radial distribution of ions and water around a 25 bp poly(dA):poly(dT) DNA duplex in 100 mM SrCl2 and water (solvent packing fraction 0.3 in 100 Angstrom cube box), using the SPM model with ion-water Lennard-Jones interactions. This example is different from example 5A in that, it includes Lennard-Jones interactions between the ion and water hard spheres.

Simulations are performed in the same way as in Example 4B.

Input and output files for the excess chemical potential calculation are provided in the folder: ./gibs/Simulation\_Examples/ excess\_chempot\_srcl2\_100mM\_PID\_SPM+LJ

The excess chemical potentials of Sr2+, Cl-, and water are -0.2611, 0.8527, and 1.0612, kcal/mol respectively.

Input files for the solute simulations are provided in the folder:

./gibs/Simulation\_Examples/SrCl2\_SPM\_LJ+IW\_PolyAT25

Run the simulations and plot the RDFs. Compare them to the RDFs files provided in the production run folder. Only use the data in columns 1 and 2 of the RDF output files. Ignore the other columns.

## RDF plots

The figure below shows plots of RDFs from the UPM (Example 5A) and SPM+LJ simulations for 100 mM SrCl2. The total and excess number of Sr2+ ions are also plotted.

