DynamO Workshop

Tutorial Worksheet 4

This tutorial will examine the structural phase transitions exhibited by an isolated square-well homopolymer. First, the contact map output plugin within DynamO will be described. Then, the tutorial will introduce the replica exchange engine in DynamO, which helps the system overcome free energy barriers to equilibration. Finally, it will discuss the histogram reweighting tool, which can be used to combine data from simulations performed at different tempertures.

1 Contact map

First, let's create a low temperature configuration file for a square-well homopolymer consisting of 20 spheres:

```
dynamod -m 2 --i1 20 --f1 1 -T 0.15 -o config.out.xml.bz2
```

Now, perform a quick equilibration run

```
dynarun --engine 1 -c 1000000 --equilibrate config.out.xml.bz2
```

The contact map can be generated by adding the command line option `-L ContactMap` to `dynarun`. To perform the production run, we execute:

```
dynarun --engine 1 -c 1000000 -L ContactMap config.out.xml.bz2
```

The output of the run is contained in the file `output.xml.bz2`.

2 Replica exchange

construct a square-well homopolymer of length $N = 20$, $\sigma/l = 1$... plot the average radius of gyration as a function of temperature... plot the histogram of the energy at different temperatures
Create a series of configuration files at different temperatures:

```
dynamod -m 2 --i1 20 --f1 1 -T 0.15 -o config.0.start.xml.bz2
dynamod -m 2 --i1 20 --f1 1 -T 1.5  -o config.1.start.xml.bz2
dynamod -m 2 --i1 20 --f1 1 -T 1    -o config.2.start.xml.bz2
```

A replica exchange simulation can be run using DynamO with the configuration files by executing

```
dynarun config.*.start.xml.bz2 --engine 2 -i 1 -f 100
```

Note that the final configurations will be put in the files `config.*.end.xml.bz2`. The respective output files for each of the simulated temperatures will be in the files `output.*.xml.bz2`.
Now run the configuration with the energy histogram turned on

```
dynarun config.*.end.xml.bz2                          \
    --engine 2 -f 1000 -i 1                            \
    -L ContactMap                                      \
    -L RadiusGyration                                  \
    -L IntEnergyHist:BinWidth=0.01
```

Information regarding the replica exchange run is given in the files `replex.dat` and `replex.stats`. Note that in order for the replica exchange moves to be effective, the energy histograms of systems with "adjacent" temperatures must overlap. If this is not the case, then add intermediate temperature systems to your simulations and rerun.

3   Histogram reweighting

The energy histograms from simulations performed at different temperatures can be combined using histogram reweighting by using the tool `dynahist_rw`:

```
dynahist_rw output.*.xml.bz2
```

The energy histograms are contained in the files `output.?.xml.bz2.ReweightedEnergyHist`. An estimated heat capacity curve is in the file `Cv.out`. Estimates for the temperature variation of the mean energy and the mean square energy are in the files `Energy.out` and `Energy2.out`, respectively.

4   Tutorial challenges

- Analyze the transitions in a square-well homopolymer of length $N = 20$ and sphere diameter $\sigma/l = 1.6$. The large diameter of the spheres leads to local stiffening of the polymer chain.

- Create a block co-polymer using the HP model and develop a bulk system using this molecule. Perform a replica exchange simulations to look for microphase separation.