DynamO Workshop

Tutorial Worksheet 3

In this tutorial, we will learn how to generate and modify a configuration file for a single molecule. This includes describing the properties that can be extracted from DynamO from a simulation run. Then, we will learn how to construct a configuration file where a single molecule configuration is arranged in a regular lattice and compressed to the desired density. This will enable us to use DynamO to perform bulk simulations of complex molecules.

1 Single chain simulations

We will perform a simulation of a single polymer chain composed of 16 linearly bonded hard spheres with diameter σ and bond length $l = \sigma$. First, we need to create the configuration file using `dynamod`:

```
dynamod --pack-mode 2 --i1 16 --f1 1 --thermostat 100 -o config.out.xml.bz2
```

The argument to the option `--i1` gives the number of spheres in the chain, and the argument of the option `--f1` gives the ratio of the sphere diameter to the bond length. The argument to the `-o` option gives the name of the file where the configuration is stored. For more details, consult `dynamod --help --pack-mode 2`.
Next, we perform a run of 10^6 events to equilibrate the configuration

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

The final configuration will be written to the file `config.out.xml.bz2`, the default.
Now run DynamO with the radius of gyration output plugin turned on:

```
dynarun --engine 1 -c 10000000 \
    -L RadiusGyration \
    config.out.xml.bz2
```

The output from this run will be written to the file `output.xml.bz2`.
Note that the `--L RadiusGyration` option will generate a histogram for the components of the radius of gyration tensor for the molecule. We can change the width of the bin that the radius of gyration is collected, by adding the following:

```
dynarun --engine 1 -c 10000000 \
    -L RadiusGyration:BinWidthGyration=0.1 \
    config.out.xml.bz2
```

Regular snapshots of the configuration can be obtained by including the `--snapshot` option.

```
dynarun --engine 1 -c 10000000 \
    --snapshot-events 100000 \
    config.out.xml.bz2
```

The configurations will be put in to a set of files `Snapshot.output.?e.xml.bz2`, where the `?` denotes the number of the snapshot configuration.

2 Packing molecules

Now we will consider simulations of molecules in bulk systems, where several molecules are packed in the simulation box. In order perform this sort of simulation, we first need to create the initial configuration file. In this portion of the tutorial, we will generate a packed configuration of linear chains of length $N = 16$. We start by creating a single chain configuration:

```
dynamod --pack-mode 2 --i1 16 --f1 1 --thermostat 100 -o config.out.xml.bz2
```

Arrange the configuration in a lattice:

```
dynamod --pack-mode 3 --density 0.001 \
    --i1 0 --xcell 3 --ycell 3 --zcell 3  \
    --s1 config.out.xml.bz2
```

If there are overlaps in the system, then decrease the density of the system. Once the lattice configuration is constructed, the bonding entry in the configuration file needs to be corrected, and the `ContactMap` entry needs to be removed.
In order to get the system to the target monomer density, we use the growth algorithm to compress the configuration:

```
dynarun --engine 3 --growth-rate 10 --target-density 0.1 \
    config.out.xml.bz2
```

This compression can cause the system to heat very rapidly. Consequently, the velocities need to be rescaled in order to make the kinetic temperature equal to the target (desired) temperature and zero the total momentum of the system

```
dynamod --zero-momentum --rescale-T 100 -o config.out.xml.bz2 \
        config.out.xml.bz2
```

Once this is complete, you have a configuration that can be used to run a simulation. If a different density is required, then this configuration can be further compressed.
Now run DynamO to determine the pressure of the system

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

3 Tutorial challenges

- Determine the variation of the mean-square radius of gyration of a linear hard-sphere chain as a function of the number spheres on the chain N.
- Determine the how pressure, radius of gyration, monomer-monomer pair correlation function, and viscosity vary as a function of the monomer density for chains of different lengths N.