Free-Solution DNA electrophoresis

You are to investigate the motion of polyelectrolytes in bulk solution. Hydrodynamic interactions cannot be neglected here so you will use a Lattice Boltzmann fluid coupled to explicit ions which are represented by charged Week-Chandler-Anderson spheres. The salt/counter-ions as well as the charges on the polyelectrolyte backbone are subject to an external electrical field. Electrostatics should be handled by the P3M algorithm. A set of realistic parameters and a more in detail description of the system can be found in the attached papers. You should measure the DNA mobility from its total displacement from being driven by a weak external field. Verify how the mobility changes with DNA length (N) for very small chains and compare the results with the published simulation and experimental results. You will also use a separate set of simulations to obtain the zero-field mobility from the Green-Kubo relation. Compare your results between the two approaches.

Tasks

Theory

You should explain the difference between free-draining and non-free draining polymer. You should explain the Einstein–Smoluchowski relation in the context of electrophoretic mobility. Know when/if is applicable to charged polyelectrolytes.

Simulations

You will build a simulation script using ESPResSo to simulate charged polyelectrolytes of different lengths and measure the response to weak external electric fields. In general it is a good idea to start with a simple system first and incrementally increase the complexity of the system. This approach makes it easier to spot mistakes and allows for verification during the development process. While building your system, you should be careful about keeping the simulation time short (development stage). Once you are satisfied with your script you can then try better (more expensive) simulations (production stage).

1. create a real polymer of length N and equilibrate
2. add the counterions and equilibrate
3. include electrostatics with P3M and equilibrate
4. include hydrodynamic interactions with Lattice Boltzmann and equilibrate

From this point on you should measure the zero-field mobility and the mobility by applying a weak external electric field.
A good starting point for your simulation scripts are the ESPResSo Tutorials `https://espressomd.github.io/tutorials4.1.4.html` and the ESPResSo Documentation `https://espressomd.github.io/doc4.1.4/index.html`. For this simulation setup the *Part 3 of the Lattice Boltzmann tutorial* is a good staring point. The tutorials provide a good insight on how to set-up your system to use specific algorithms. A detailed explanation of the parameters for the algorithms can be found the documentation. Sometimes it might also be useful to have a look in the ESPResSo Samples `https://github.com/espressomd/espresso/tree/4.1/samples` folder. Parameters for your simulations can be found in [1].

Common pitfalls

- Do NOT try to build your script in one go. Take small steps and validate as often as possible
- To get good statistics you need a lot of data, so think ahead. File sizes can become quite large, therefore reduce the output to only include necessary information.
- Make use of the online analysis tools: velocity autocorrelation and center-of-mass position
- Save the quantities of interest and analyze it after the simulations. If you dont and your analysis script is wrong you will have to rerun your entire simulation.

There are many parameters to choose, many will seem arbitrary but they can make or break your simulations. In the following some hints are given which also include simulation parameters. Be aware that changing those can break your simulaiton.

Integrators

```
system.time_step = 0.01
system.cell_system.skin = 0.4
```

Thermostats

- when you use the Langevin thermostat, keep gamma to unity

  ```
  system.thermostat.set_langevin(kT=kT, gamma=1.0)
  ```

- when you want to switch from Langevin thermostat to LB

  ```
  # turn off Langevin thermostat
  system.thermostat.turn_off()
  # remove existing particle motion
  system.galilei.kill_particle_motion()
  # remove existing center of mass momentum
  system.galilei.galilei_transform()
  ```

- when you want to use LB

  ```
  # for CPU
  lbf = lb.LBFluid(agrid=1.0, dens=1.0, visc=1.0,
                   tau=0.01, kT=kT, seed=seed)
  # for GPU
  lbf = lb.LBFluidGPU(agrid=1.0, dens=1.0, visc=1.0,
                      tau=0.01, kT=kT, seed=seed)
  # remember to activate the friction coupling
  system.thermostat.set_lb(kT=kT, seed=seed, gamma=20.0)
  ```

Electrostatics

- start with a low bjerrum length in simulation units

  ```
  l_bjerrum = 2.0
  ```

- when you use P3M don't set the accuracy too small

  ```
  p3m = electrostatics.P3M(prefactor=l_bjerrum, accuracy=1e-4)
  ```

- warmup (integrate a few timesteps) your system when adding a new actor

Correlators

- When computing Green-Kubo-based mobility, consider the observable

  `espressomd.observables.FluxDensityProfile`

Potentially useful reading material

Lattice Boltzmann

- ESPResSo Documentation: `https://espressomd.github.io/doc4.1.4/lb.html`
- ESPResSo Tutorials *Lattice Boltzmann*: `https://espressomd.github.io/tutorials4.1.4.html`
- For further details on the Lattice Boltzmann Method: [3]

Electrostatic Methods

- ESPResSo Tutorials *Charged systems*: `https://espressomd.github.io/tutorials4.1.4.html`
- ESPResSo Documentation: `https://espressomd.github.io/doc4.1.4/electrostatics.html`

Polyelectrolyte Electrophoresis

- Paper: [1]
- PhD-Thesis: [2]
- Poster `https://www2.icp.uni-stuttgart.de/~icp/mediawiki/images/a/ad/MMSD07-poster.pdf`

References

[1] Kai Grass et al. "Importance of Hydrodynamic Shielding for the Dynamic Behavior of Short Polyelectrolyte Chains". In: *Physical Review Letters* 100 (2008), p. 096104. DOI: 10.1103/physrevlett.100.096104.

[2] Kai Christian Grass. "Towards realistic modelling of free solution electrophoresis: a case study on charged macromolecules". PhD thesis. Goethe-Universität Frankfurt am Main, 2008.

[3] Timm Krüger et al. *The Lattice Boltzmann Method: Principles and Practice*. Cham: Springer, 2017. isbn: 9783319446479. doi: 10.1007/978-3-319-44649-3.