Worksheet 5 Coarse-grained simulations with ESPResSo

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Important remarks

- Due date: **Tuesday, July 16th, 2013, 8:00**
- You can either send a PDF file to Jens Smiatek (smiatek@icp.uni-stuttgart.de) or submit a hand-written copy.
- If you have further questions, contact Jens Smiatek (smiatek@icp.uni-stuttgart.de)

The program package ESPResSo

The program package ESPResSo is developed and maintained at the Institute for Computational Physics and is mainly intended to perform coarse-grained simulations with Lattice-Boltzmann, Dissipative Particle Dynamics and Langevin Dynamics. It consists of a broad variety of electrostatic algorithms, analysis tools and various other features like the support of massively parallelized hardware architectures or GPU-platforms. In the following you will conduct coarse-grained simulations with the Lattice-Boltzmann and Dissipative Particle Dynamics method to learn how to work with ESPResSo. The package can be downloaded at

- ESPResSo-Homepage: http://espressomd.org/
- ESPResSo-Download: http://espressomd.org/wordpress/download/
- ESPResSo-Manual: http://espressomd.org/jenkins/job/ESPResSo/lastSuccessfulBuild/artifact/doc/ug/ug.pdf

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Important Remark: It is good to have a look inside the manual to understand how it works. This tutorial is mainly intended to understand how the coarse-grained methods and the simulation package works.

Coarse-grained simulations (20 points)

Download and install ESPResSo

Download the ESPResSo package version 3.2.0 (espresso-3.2.0.tar.gz) and install it in your home directory. You can follow the commands as given in the manual on p. 14. Before compilation and after using "./configure", please uncomment the macros in "myconfig-sample.h" for

- EXTERNAL_FORCES
- CONSTRAINTS
- DPD
- TUNABLE_SLIP
- LB
- LENNARD_JONES

and rename it to myconfig.h.

Lattice-Boltzmann simulations of a single particle in a fluid

Attached to this tutorial you will find the TCL-Script "lb_particle.tcl" which is intended to perform a Lattice-Boltzmann simulation of a single particle in a fluid. Have a look at the parameters in the script. What is their meaning? You can run the simulation with the command

- ./Espresso lb_particle.tcl

if your installation has been correctly conducted. Otherwise ask the tutors.

1 Single particle in a fluid

In the following the motion of a single particle in a Lattice-Boltzmann fluid will be considered. The coupling of the particle to the fluid will be performed by the scheme that was introduced in the lecture. Have look into the script file. Try to interpret the parameters of most importance. How is the system simulated? What are the interactions? Have a look into the manual to understand how it works. Visualize the corresponding trajectory.
Run the simulation. Calculate the mean square displacement of the particle by the equation

$$< (\vec{r}(t) - \vec{r}(t_0))^2 >= MSD \qquad (1)$$

and determine the Diffusion coefficient.
Hint: Remember Simulation Methods I how to calculate it.

Plane Poiseuille flow with Dissipative Particle Dynamics (DPD)

In the following, we will simulate a Plane Poiseuille Flow (PPF) in a confined microgeometry with Dissipative Particle Dynamics (DPD). The Poiseuille flow occurs for low Reynolds-numbers such that the Navier-Stokes equation can be reduced to the Stokes equation

$$\eta \frac{\partial^2}{\partial z^2} v_x(z) = -\rho F_x \quad (2)$$

with the shear viscosity η, the fluid density ρ, the fluid velocity $v_x(z)$ and the external force in x-direction F_x.

Plane Poiseuille flow equation

Solve the Stokes equation to get $v_x(z)$ with the boundary conditions

- $v_x(z_B) = 0$ where z_B denotes the position of the channel walls
- $\partial_z v_x(z)|_{z=0} = 0$ for the velocity derivative in the middle of the channel

DPD simulations

Look at the script "PPF.tcl". Try to interpret the parameters of most importance. How is the system simulated? What are the interactions? Have a look into the manual to understand how it works. Run the simulation with the command *./Espresso PPF.tcl*. Some parameters in the script are missing.

- We need a solvent density of $3.75\sigma^{-3}$. The effective box lengths are given by $(10 \times 10 \times 8)\sigma^{-3}$. To insert $\rho = 3.75\sigma^{-3}$ is therefore not correct. Have a look into the file!
- The DPD friction coefficient is given by $\gamma_{DPD} = 5.0$.

Run the warm up and the simulation.

Analysis of the Plane Poiseuille flow

After the simulations have finished, have a look at the output file. Try to understand the meaning of the different rows by having a look into the tcl-file. In order to analyze the flow profile, we have to calculate a histogram for several z-positions. Therefore we sort the particles according to their z-position to equidistant bins and sum up their velocities in x-direction. Having sorted all the particles, we average the summed velocities of the bin by taking into account the particle number within the bin to get the average velocity. Finally the average velocities will printed out according to their z-position which gives you the flow profile. Fit the corresponding flow profile and estimate the shear viscosity. Have a look at the PPF.tcl-file to estimate the external forces.