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Scientific Computing II

Molecular Dynamics

Exercise 8: Dimensionless Formulation

We want to simulate Argon using the Lennard Jones model at a mass density $\rho = 1008kg/m^3$ and temperature $T = 215K$ as well as a time step $\Delta t = 10^{-15}s$. The atomic weight of Argon is 39.9u (i.e. 39.9g correspond to 1 mol). Derive the dimensionless form of the problem using the formulation and formulas from the lecture slides. You may further assume that the Boltzmann constant should be scaled to unity in the dimensionless form, i.e. $k_{B_c} = k_B$.

Exercise 9: Initial Conditions

Liquids are defined by high number densities $n = N/V$ and high volume fractions $f = \frac{Volume(molecules)}{V}$ where N is the number of molecules, V is the volume which contains the N molecules and $V(molecules)$ corresponds to the effective volume that is occupied by the molecules.
In order to provide initial conditions to a Molecular Dynamics simulation, a common approach consists in mapping the molecules onto a Cartesian grid, cf. Fig. 1. The mesh size Δx is chosen such that the total number of molecules $N := N_x \times Ny \times N_z$ and the (three-dimensional) volume under consideration V yield the required number density n. However, due to the strong repulsive forces in a (Lennard Jones) fluid, the mesh size should typically not be chosen smaller than the interaction depth σ.
What is the maximum volume fraction $f := \frac{Volume(spheres)}{V}$ that can be achieved by this method? $V(spheres)$ shall correspond to the volume that is occupied by spherical Lennard Jones particles with diameter σ. How can we extend the method to even higher volume fractions?

Exercise 10: Thermostat

Let $\overline{v} = \frac{1}{N}\sum_{i=1}^{N} v_i$ denote the average flow velocity in a Molecular Dynamics simulation and

$$T = \frac{m}{dNk_B}\sum_{i=1}^{N}(v_i - \overline{v})^2 \tag{1}$$

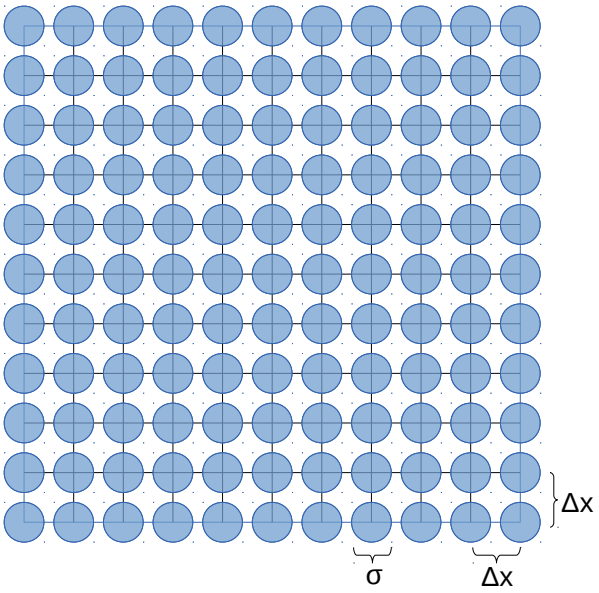

Figure 1: Particles (blue disks) are initialised on a grid with equidistant mesh size Δx in all spatial directions. For sake of simplicity, the two-dimensional case is shown.

a measure for the temperature fluctuations. All molecules are of same material and a mass m. Show that the thermostat

$$v_i^{new} := \overline{v} + \sqrt{\frac{T^{new}}{T}}(v_i - \overline{v}) \tag{2}$$

yields a temperature T^{new} and leaves the average flow velocity unchanged, i.e. $\overline{v}^{new} = \frac{1}{N}\sum_{i=1}^{N} v_i^{new} = \overline{v}$.

Programming Exercise 8: Two-Particle System

In the following, we want to consider the motion of a molecule A in proximity of another molecule B which is fixed in space. The interaction of the two molecules is modelled by the 12-6 Lennard Jones potential. The Lennard Jones parameters ϵ, σ and the mass of each molecule m are scaled to unity, $\epsilon = \sigma = m = 1$. Molecule B is fixed at $(0.0, 0.0)$ of our domain throughout the following experiments.

(a) Write a function `computeForce(xA,xB)` in Matlab which computes the force acting on molecule A due to molecule B. The arguments `xA` and `xB` correspond to the current positions of both molecules.
Write another function `timestep(xA,vA,FA,dt)` which computes the new position and velocity of molecule A. The time stepping should first compute the new velocity v^{new} using the explicit Euler method, $v^{new} = v_A + dt \cdot F_A$, and subsequently determine the new position x^{new} by the Heun-method, $x^{new} = x_A + \frac{dt}{2}(v_A + v^{new})$.

(b) Simulate the movement of molecule A for the following initial conditions using a time step $\Delta t = 0.0001$:

a) $x_A = (-2, 0)$, $v_A = (0, 0)$, 200 000 time steps

b) $x_A = (-2, 1)$, $v_A = (1, 0)$, 20 000 time steps

Measure the trajectory of molecule A.

(c) The total energy of the molecular system $E = E_{kin} + U$ is formed by the kinetic energy E_{kin} and the potential energy U of the system and is generally conserved in Molecular Dynamics simulations. Measure the kinetic, potential and total energy for the different cases in (b) by implementing a function `computeEnergy(xA,xB,vA,vB)`. Is the energy conserved over time?

(d) Re-run the simulations of (b) neglecting attractive forces in the Lennard Jones model. For this purpose, remove the power-6 term. Compare the arising trajectory of molecule A with the trajectories from (b).