Computer Simulations

3^{rd} problem set

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Submission deadline:

Schedule A: week of May 12
Schedule B: week of May 19

Please upload your files in the Teach Center before the assessment discussion with your tutor.

Molecular dynamics simulations of a Lennard-Jones-like liquid

In a classical approximation, interactions between atoms consist of a repulsive term due to electron shell overlap and an attractive term due to dipole-dipole interactions. These terms are typically parameterized by the Lennard-Jones potential. For computational convenience, we use the Wang-Frenkel interaction potential between particles i and j instead

$$U_{ij}^{\mathrm{WF}} = \begin{cases} \epsilon \left[\left(\frac{\sigma}{r_{ij}} \right)^2 - 1 \right] \left[\left(\frac{r_c}{r_{ij}} \right)^2 - 1 \right]^2 & \text{if } r_{ij} < r_c \\ 0 & \text{otherwise.} \end{cases}$$

with σ and ϵ being phenomenological constants and r_c being the cutoff distance. The distance between molecules is denoted r_{ij}. We consider a two-dimensional system of spherical molecules with periodic boundary conditions. The molecules all have the same mass m.

1. Initialization

(a) Write a script to generate the positions of a two-dimensional system of molecules with a packing fraction ϕ, which is defined as

$$\phi = \frac{N\pi\sigma^2}{A},$$

with N being the number of molecules and A being the total surface area of two-dimensional system. Make sure that the molecules do not overlap because that would lead to very large energies.

(b) Generate initial velocities for all particles by drawing independent velocities in every dimension from a Gaussian distribution corresponding to an initial temperature T. Make sure that the velocity of the center of mass of the system vanishes.

2. Force calculation

The force between the molecules is given as usual by $\boldsymbol{f}_{ij} = -\nabla U_{ij}$. The forces are assumed to be pairwise additive.

(a) Write a script to calculate the force on all particles from the positions of the particles. Take care that periodic boundary conditions are used.

(b) Include a calculation of the total potential energy of the system in the calculation of the forces.

(c) Evaluate the scaling of computational cost of the force calculation with the number of particles N.

3. **Integration of the equations of motion**

(a) Nondimensionalize the equations and pick a sensible time step in terms of σ, ϵ and the particle mass m.

The velocity-Verlet algorithm for positions $\boldsymbol{r}$, velocities $\boldsymbol{v}$ and forces $\boldsymbol{f}$ consists of the following steps:

$$\boldsymbol{v}(t+\tfrac{\Delta t}{2}) = \boldsymbol{v}(t) + \tfrac{\boldsymbol{f}(t)}{2m}\Delta t$$
$$\boldsymbol{r}(t+\Delta t) = \boldsymbol{r}(t) + \boldsymbol{v}(t+\tfrac{\Delta t}{2})\Delta t$$
$$\boldsymbol{f}(t+\Delta t) = \boldsymbol{f}(r(t+\Delta t))$$
$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t+\tfrac{\Delta t}{2}) + \tfrac{\boldsymbol{f}(t+\Delta t)}{2m}\Delta t$$

(b) Implement the velocity-Verlet algorithm to solve the equations of motion.

(c) Calculate the kinetic energy at every integer time step and plot the total energy and the temperature as a function of time.