Physics 514 – MD Exercise

Emanuel Gull

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1 Molecular Dynamcis

1.1 Code

Write a Lennard Jones simulation, either by downloading the sample code from the Canvas website and implementing the missing force calculation or by implementing a simulation yourself.

1.2 Integrator

Replace the forward Euler method with a velocity verlet algorithm:

- Calculate:

$$\vec{x}(t+\Delta t) = \vec{x}(t) + \vec{v}(t)\,\Delta t + \tfrac{1}{2}\,\vec{a}(t)\,\Delta t^2 \tag{1}$$

- Derive $\vec{a}(t+\Delta t)$ from the interaction potential using $\vec{x}(t+\Delta t)$
- Calculate:

$$\vec{v}(t+\Delta t) = \vec{v}(t) + \tfrac{1}{2}\,\left[\vec{a}(t) + \vec{a}(t+\Delta t)\right]\Delta t \tag{2}$$

Check that the total energy stays constant as a function of time, at least for short times.

1.3 Measurements

Examine the trajectories of your molecules. Find a region of phase space where the system is solid and another one where it is fluid. Don't forget to thermalize! Plot the positions as a function of time to show the difference between the fluid and the solid. Hint: changing the pressure or number of molecules in the box is an easy way to change the phase.

1.4 Measurements (II)

measure the angle integrated pair correlation function $g(r)$ in both cases, plot it as a function of r.