Physics 514 – MD Exercise

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Due 10:00 AM, Thursday September 28 2017

1 Molecular Dynamcis

1.1 Code

Write a Lennard Jones simulation, eithr by downloading the sample code lj_start.py from Canvas 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: Change the pressure of your systems by changing the size of the simulation box or the number of your particles, and then look at the trajectories of two particles (you don't have to choose the entire grid) over time. Then you should observe the differences of your solid-like system and gas-like system.

1.4 Measurements (II)

measure the angle integrated pair correlation function $g(r)$ in both cases, plot it as a function of r.
Hint: remember to include the rebox() function in your implementation of $g(r)$.

Homework Submission

Summarize your results and plots into one PDF file and also submit your codes to Canvas.