Molecular Dynamics Simulations: Final Report

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1 Molecular Dynamics Simulations code

1.1 Introduction

We consider an isolated system of $N = 125$ particles with density $\rho = 0.7m/\sigma^3$ trapped in a region with PBC. Initially, the particles are located at the vertices of a simple cubic lattice with a bimodal velocity distribution, with which the kinetic energy K is compatible with $k_B T = 100\epsilon$. Then, we let the system evolve through the action of an integrator (*Velocity Verlet* or *Euler*) for 10^4 time steps, and we analyze its thermodynamic properties.

The Lennard-Jones potential describes the interactions between particles:

$$u_{LJ}(r) = 4\left[\left(\frac{1}{r}\right)^{12} - \left(\frac{1}{r}\right)^6\right].$$

Here, it is written in reduced units since it is more natural to do simulations with dimensionless quantities. We introduce a *cutoff* parameter $r_c = L/4$ that establishes a distance above which interactions are ignored. This reduces the computational cost, but produces discontinuities in the potential that we must fix with truncation:

$$u_{LJ}(r) = \begin{cases} u_{LJ}(r) - u_{LJ}(r_c) & r \leq r_c, \\ 0 & r > r_c. \end{cases}$$

The Velocity Verlet integrator uses velocities to take the system to the next dynamic step:

$$r_i(t + \Delta t) = r_i(t) + v_i(t)\Delta t + \frac{f_i(t)}{2m_i}\Delta t^2,$$

$$v_i(t + \Delta t) = v_i(t) + \frac{f_i(t) + f_i(t + \Delta t)}{2m_i}\Delta t.$$

It is a fast and convenient algorithm to use when the system interacts with a thermal bath. On the other hand, the Euler integrator uses both distances and

velocities to update the state of the system:

$$r_i(t + \Delta t) = r_i(t) + v_i(t)\Delta t + \frac{f_i(t)}{2m_i}\Delta t^2 + \mathcal{O}(\Delta t^3),$$

$$v_i(t + \Delta t) = v_i(t) + \frac{f_i(t)}{m_i}\Delta t + \mathcal{O}(\Delta t^2).$$

Its disadvantages are the energy drift and the lack of symmetry under time reversal. In both equations, f_i is the force associated with the Lennard-Jones potential.

1.2 Results

Figure 1 shows the results obtained with the Velocity Verlet integrator. For $\delta t = 10^{-3}$, K and U fluctuate more intensely. However, in both cases the total energy and momentum are conserved.
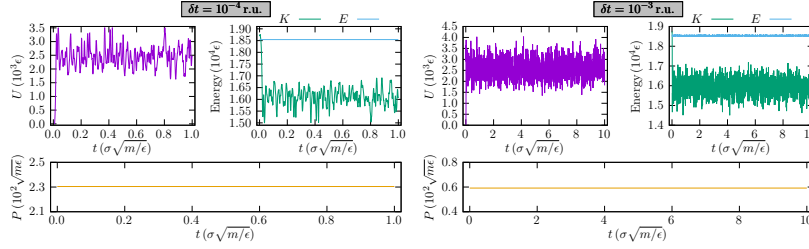

Figure 1: Energies and total momentum calculated with the Velocity Verlet integrator for different time increments δt.

On the other hand, Figure 2 shows the results obtained with the Euler integrator. For $\delta t = 10^{-4}$, the energies are reasonable even though the total energy is not preserved. For $\delta t = 10^{-3}$, however, the energies blow up which is a manifestation of the integrator's flaws. In both cases, the total momentum is a conserved quantity.
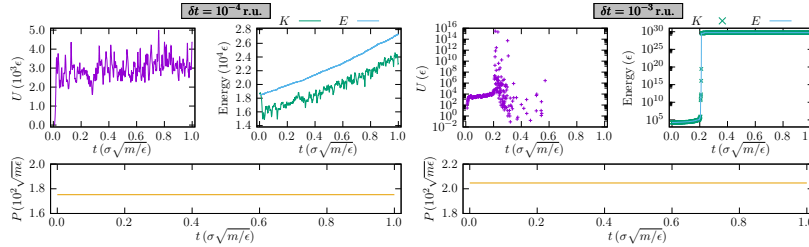

Figure 2: Energies and total momentum calculated with the Euler integrator for different time increments δt.

Finally, Figure 3 shows the initial and equilibrium velocity distributions of the particles obtained with the Velocity Verlet integrator for $\delta t = 10^{-4}$. The
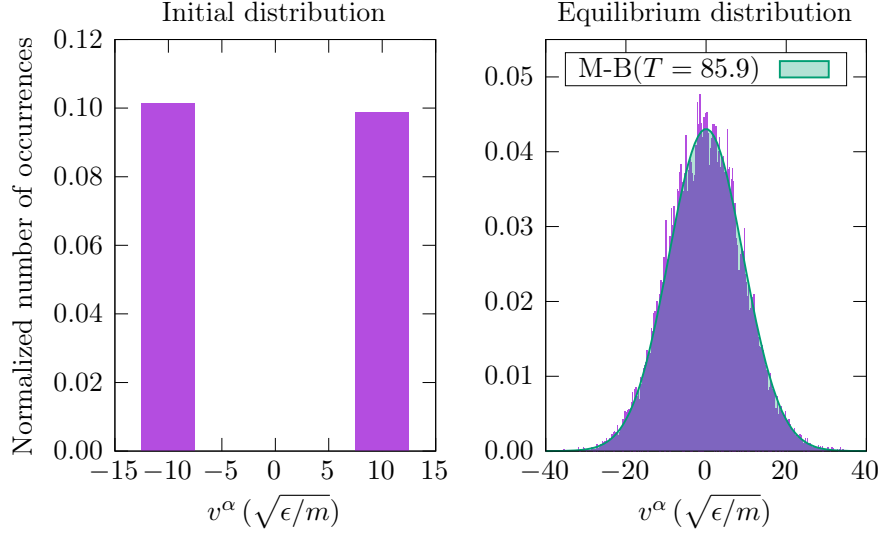
Figure 3: Initial and equilibrium velocity distributions of the particles obtained with the Velocity Verlet integrator for $\delta t = 10^{-4}$.

system leaves the initial bimodal distribution as it evolves and cools down, eventually reaching a Maxwell-Boltzmann equilibrium distribution

$$f(v_\alpha) = \frac{1}{\sqrt{2\pi T}} \exp\left(-\frac{v_\alpha^2}{2T}\right).$$

2   Properties of a Lennard-Jones liquid

2.1   Introduction

We consider a system of $N = 125$ argon atoms trapped in a region with PBC. Initially, the atoms are at rest at the vertices of a simple cubic lattice. After melting the crystalline structure, we put the system in contact with a thermal bath at $k_B T = 2\epsilon$ using an Andersen thermostat, and let it evolve with the Velocity Verlet integrator for 10^6 time steps. The objective is to obtain the thermodynamic properties of the system.

As in the previous section, the atoms interact through the Lennard-Jones potential and the simulation is carried out with reduced units. Once finished, we retrive the physical units multiplying the different quantities by an appropriate combination of parameters (Table 1).
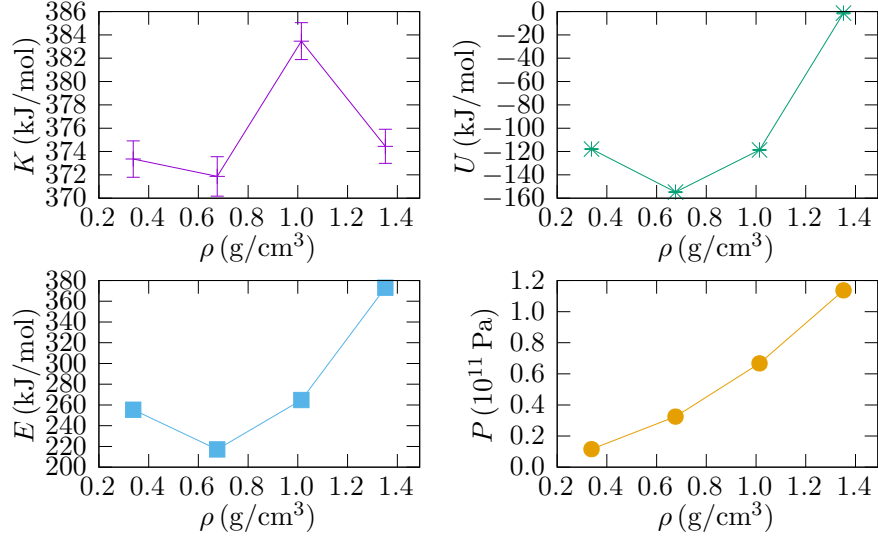
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Figure 4: Test.

Table 1: Test.

Physical quantity	Unit
Leght	σ
Energy	ϵ
Mass	m
Time	$\sigma(m/\epsilon)^{1/2}$
Velocity	$(\epsilon/m)^{1/2}$
Force	ϵ/σ
Pressure	ϵ/σ^3
Temperature	ϵ/k_B

Figure 5: Test.