



INSTITUTE OF MICROELECTRONICS

NSSC2 - EXERCISE 1

Group 9

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1 Task 1: Questions

- (a) Is the fourth-order Runge-Kutta method a good integrator in the context of molecular dynamics? Why? Give at least two reasons.

This method is not a good idea. For example, assume a system of 10000 particles for which we have to integrate 10000 ODEs per axis, 30000 in total (3D-space: x,y,z) \Rightarrow the dimension of the matrix. For second order ODEs we also have to rewrite the equations into multiple ODEs of first order. So the number of equations doubles (2 consecutive ODEs of first order instead of one second order ODE) to 60000. The Runge-Kutta method is defined as:

$$\begin{aligned}\Phi(t, y, h) &:= \frac{1}{6}[k_1 + 2k_2 + 2k_3 + k_4] \\ k_1 &:= f(t, y) \\ k_2 &:= f\left(t + \frac{h}{2}, y + \frac{1}{2}hk_1\right) \\ k_3 &:= f\left(t + \frac{h}{2}, y + \frac{1}{2}hk_2\right) \\ k_4 &:= f(t + h, y + hk_3)\end{aligned}$$

The Runge-Kutta method has a high computational cost that is paid at every time step of a simulation. However, it is often used for equations with a lower dimension matrix. Another big disadvantage is that they do not easily yield good global estimates of the truncation error. Additionally, it does not guarantee conservation of energy and momentum in the system.

- (b) Describe the advantages of automatic differentiation as a method to calculate forces.

Instead of using finite differences to calculate the derivatives of our functions we could use the Automatic differentiation (AD). Assume we have a system with a Lenard-Jones Potential

$$\begin{aligned}V_{LJ}(R) &= 4\epsilon \left[\left(\frac{\sigma}{R} \right)^{12} - \left(\frac{\sigma}{R} \right)^6 \right] \\ f &= -\nabla V_{LJ}(R)\end{aligned}$$

The way to go is now to separate the terms with an R dependency and differentiate them separately. After that we could insert R and calculate the force on that coordinate.

A big advantage of Automatic differentiation(AD) is its exactness in contrast to using finite differences. AD is very efficient, to derive a derivative, less computations have to be done than compared to a numerical differentiation. And AD is robust.

- (c) When the potential energy of a system is described using the Lennard-Jones model, how does the number of calculations per time step scale with the number of particles? Why?

To determine the potential energy of a particle when the Lenard-Jones potential is used, you need the (pair wise) distances to all other particles. Assume a system with M particles, so we need to calculate $M - 1$ distances for the first particle, $M - 2$ for the second, and so on. To calculate the energy of the whole system, we end up having to calculate $\frac{M^2 - M}{2}$ different distances and therefore the number of calculations scales with $O(M^2)$.

- (d) Describe a strategy to make that number of calculations proportional to the number of particles.

If the potential of the system is described by the Lennard-Jones potential, it is possible to define a cut-off radius and only include the particles in that radius for the calculations. This ensures also that the number of calculations in that area is now $m \ll M$ and scales also with $O(m^2 * M) \Rightarrow m^2 * O(M)$.

2 Task 4: Post-processing

We studied the conservation of energy as a function of the time (=iterations) for a system with 200 particles, an average density of 0.8 and a sigma of 1. We started with a step length of 0.1. As one can see, our calculations only start making sense after we use a step length smaller than 0.05. When using a time step of $\delta t = 0.01$, it takes approximately 10 iterations until the potential and kinetic energies start to converge. When using a time step of $\delta t = 0.001$, it takes approximately 80 iterations until the potential and kinetic energies start to converge. In general, the smaller the time step is chosen, the longer it takes for the energies to converge.

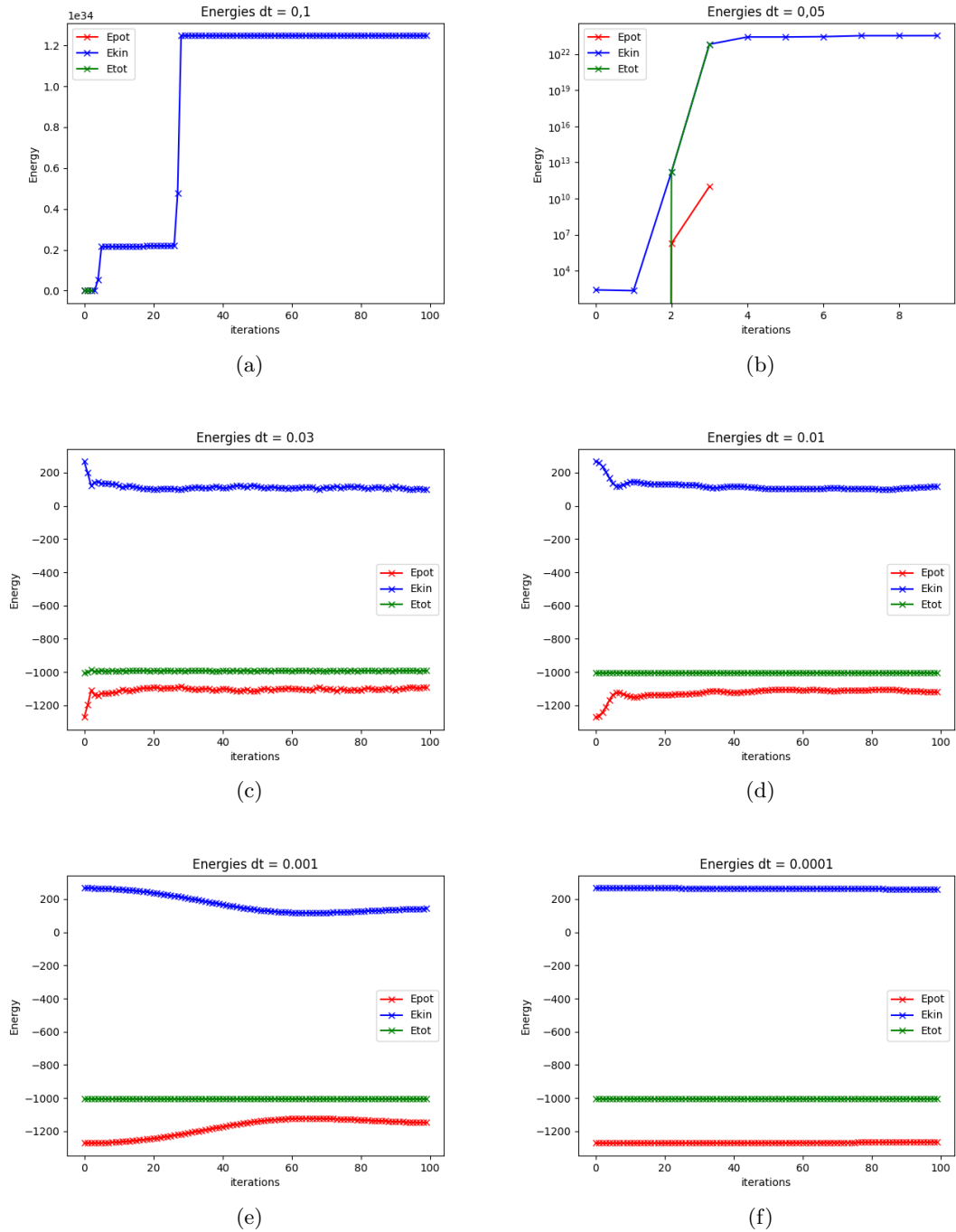


Figure 1: Conservation of energy for different step sizes

Next we calculated the averaged density of particles in a system described as above after 100 time steps.

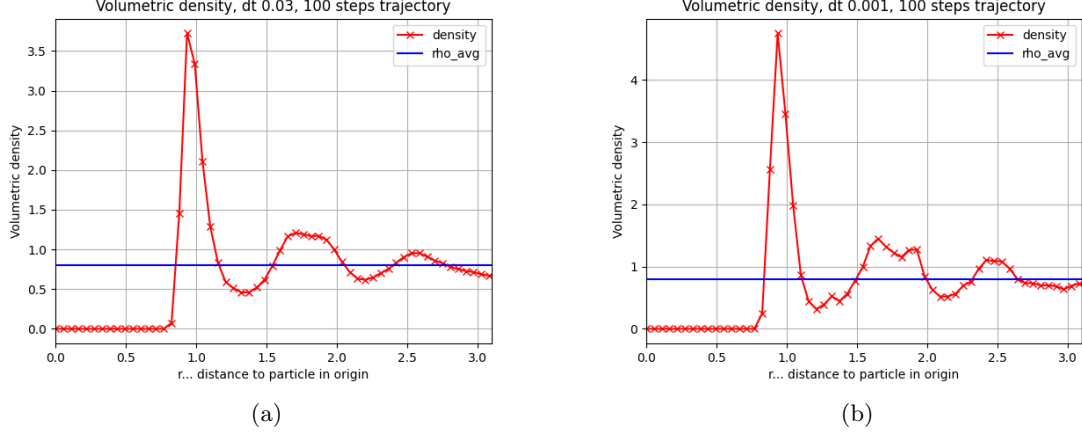


Figure 2: Volumetric density

What is striking in both figures, is a peak in density around 1. This can be explained by the potential $V_{LJ}(r)$ having its minimum exactly at 1 in our system of units, which reflects the expected distance of two interacting particles. It therefore is convenient for particles to be around this position (minimization of energy), and the density peaks there.

We have to mention, that we had some problems finding the right scaling, or normalization of the averaged density, in y-direction for this representation. We had to multiply with an additional factor of 2.2 (in addition to the expected normalization factors), but we honestly do not know where this factor would come from or where our calculations go wrong - although there should be a proper way to derive this from system parameters.

If there were no interactions between the particles, the density curve would flatten as the particles would be distributed evenly and we would end up with a constant particle distribution of around 0.8 particles per unit volume. In general, the volumetric density distribution reflects the potentials spatial symmetries, periodicity and the structure it gives to the particles in the simulation box (e.g. average distance between particles).