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# Algorithms of Scientific Computing II

Exercise 3 - Discretization, Short-Range Potentials

## 1) Time Discretisation

The movement of the molecules is being described by the following ordinary differential equation: $F_i = m_i \ddot{r}_i$.

In the lecture different methods for the discretization of that ODE have been introduced. In this exercise we will deal with those methods in more detail.

**a)** Use the Taylor-Series to derive the position equation of the *Explicit- Euler*-method

**b)** The "Störmer Verlet"-method is given by the following formulas:

$$\vec{r}(t+\Delta t) = 2 \cdot \vec{r}(t) - \vec{r}(t-\Delta t) + \Delta t^2 \cdot \vec{a}(t) \quad (1)$$

$$\vec{v}(t) = \frac{\vec{r}(t+\Delta t) - \vec{r}(t-\Delta t)}{2\Delta t} \quad (2)$$

Use the Taylor-Series to derive the position equation of the *Störmer-Verlet*-method

**c)** What are the drawbacks of the *Störmer-Verlet*-method?

**d)** In exact arithmetics, the *Störmer Verlet*- and the *Velocity-Störmer-Verlet*-method are equivalent. Prove the equivalence of the two schemes by starting from the *Störmer Verlet*-method and derive the *Velocity-Störmer-Verlet*-method:

$$r(t+\Delta t) = r(t) + \Delta t \cdot v(t) + \frac{\Delta t^2}{2} \cdot a(t) \quad (3)$$

$$v(t+\Delta t) = v(t) + \frac{\Delta t}{2} \cdot (a(t) + a(t+\Delta t)) \quad (4)$$

**e)** The Euler discretisation scheme is not time reversible. Analyse the *Velocity-Störmer-Verlet*-method to find out whether it is time reversible.

**(f)** For the derivation of the Euler method, which is a first order method, all terms of second or higher order were neglected. In the derivetion of the Störmer Verlet method, all terms of fourth or higher order were neglected. Yet, the Störmer Verlet method is not a third order, but only a second order method. Show why this is the case.

## 2) Short-range Potentials

**a)** Assume we simulate a molecular dynamics scenario with N molecules. If we explicitely compute the forces between all pairs of molecules, O($N^2$ ) operations are necessary. For short-range potentials, we neglect interactions between particles that have a mutual distance bigger than a certain cut-off radius. This reduces the number of required operations to O(N).

Someone tries to convince you that this is not true:

*Assume that a simululation with N molecules requires C operations for the force calculations. Double the number of molecules in the domain. Then we of course have to compute forces for twice as many molecules. But, in addition, the number of molecules within the cut-off radius of a certain molecule doubles, too. Such, we need 4C operations, which means that the number of operations behaves like O($N^2$).*

**b)** For short-range potentials it is sufficient to consider only neighbouring particles for the force calculation. That means that all particles which are farther away as the cutoff-radius are neglected. But this is only allowed when the integral over the cut-away potential (from $r_c$ to inf is finite.

Now let's consider potentials of the form

$$U(r) = c \cdot r^{-p}$$

For which values of $p$ is this potential short-range in 1D / 2D (or 3D)?

## 3) Linked Cells

**a)** The linked cell datastructure is used to access neighbouring molecules. In the most simple case, the cells are cubic and the side length of a cell equals the cutoff radius. In 3D, apart from the cell itself, 26 additional cells have

to be examined (8 cells in 2D). By reducing the size of the cells, more cells have to be used, but the volume covered by these cells is smaller. As the covered volume corresponds to the number of distance calculations, smaller cell sizes can increase the performance. Calculate the covered volume for $l = rc$, $l = \frac{rc}{2}$, $l = \frac{rc}{4}$ and $l \to 0$ in 2D and 3D.

| | $l = rc$ | $l = \frac{rc}{2}$ | $l = \frac{rc}{4}$ | ... | $L \to 0$ |
|---|---|---|---|---|---|
| $2D$ | | | | | |
| (% unnecessary) | | | | | |
| $3D$ | | | | | |
| (% unnecessary) | | | | | |

**b)** As investigated in part a), the computational time to evaluate the force on one particle depends on the size of the cells of the linked-cells datastructure. Try to determine further factors which influence the computational time and construct a formula!