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Scientific Computing II

Molecular Dynamics

Exercise 13: Pair Potentials and Forces

There are different potentials describing the interaction between two entities. Examples are the harmonic potential for two bodies which are connected by a spring or the gravitational potential for any pair of objects in our universe. For this exercise, you will need:

- Hard sphere potential: $U_{HS}(r) = \begin{matrix} \infty & \forall\, r \leq d \\ 0 & \forall\, r > d \end{matrix}$
- Soft sphere potential:$U_{SS}(r) = \epsilon \left(\frac{\sigma}{r}\right)^n$
- Van der Waals potential: $U_W(r) = -4\epsilon \left(\frac{\sigma}{r}\right)^6$
- Lennard-Jones potential: $U_{LJ}(r) = \alpha\epsilon \left(\left(\frac{\sigma}{r}\right)^n - \left(\frac{\sigma}{r}\right)^m\right)$

(a) From the formula for the pair potential, the force which acts upon the two bodies can be derived. Calculate the force for the given potentials.

(b) Draw an approximate graph of all potentials and forces.

(c) Examine the calculated force functions and try to find qualitative differences between them. Consider especially the following properties:

- attraction or repulsion
- influence of the distance
- usability on a computer

Exercise 14: Multi-Centered Molecules

For single-centered molecules, the force on molecule i equals the sum of all forces between molecule i and all other molecules: $\vec{F}_i = \sum_{j \neq i} \vec{F}_{ij}$.

Using the force, the acceleration of molecule i is given by the following formula:

$$\ddot{\vec{x}}_i = \frac{\vec{F}_i}{m_i} = \frac{\sum_{j \neq i} \vec{F}_{ij}}{m_i}$$

For multi-centered molecules, there are some more values to be considered to be able to represent rotations:

- values considered for single-centered molecules: force $\vec{F}$, mass m, acceleration $\ddot{\vec{x}}$.
- values only to be considered for multi-centered molecules: torque T, moment of inertia I, angular acceleration $\ddot{\omega}$.

Find the formula for the angular acceleration that is analogue to the formular for the acceleration $\ddot{\vec{x}}$.

Exercise 15: Internal degrees of freedom

Consider the following model of a molecular fluid:

- Molecules consist of two atoms, which interact via a harmonic potential:

$$U_{harmonic}(r_{ij}) = \frac{1}{2}k(r_{ij} - r_0)^2,$$

  where k models the bond strength and r_0 the equilibrium bond length between the two atoms.
- Atoms of different molecules interact by the Lennard-Jones potential.
- The time integration is carried out for each atom, based on the forces on that atom.

Set up the formulas to

(a) calculate the total potential in the computational domain for N molecules ($2N$ atoms).

(b) calculate the force on an atom due to the potential model,

(c) describe the system of differential equations that describes the movement of the atoms! Formulate the Velocity-Störmer-Verlet integration scheme in order to solve that system.

(d) To efficiently calculate the force, we use the truncated Lennard-Jones potential with a cut-off radius r_c.

Give the runtime complexity with respect to the number of particles, and explain shortly why this complexity is obtained.

(e) `Outlook`: Derive the Shake-algorithm to enforce fixed bond-lengths for the diatomic fluid under consideration.
How does it compare to rigid-body motion in exercise 14?