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Scientific Computing II

Exercise B

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Tutorial: 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:

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

Now consider multi-centered molecules. There are some more values to be considered to be able to represent rotations:

- values already 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 $\ddot{\omega}$.

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

Homework: Pair Potentials and Forces

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

- 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