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Algorithms of Scientific Computing II

Exercise 2 - Modelling

1) Potentials from Other Applications

Everybody knows potentials from other applications than molecular dynamics. In this tutorial, we consider the following two examples:

- Interaction of two bodies connected by a spring:

According to Hooke's Law

$$F(r) = -k(r - r_0)$$

holds for the force F between the two bodies at the ends of a spring stretched from its original (unloaded) length r_0 to r.

- Gravity between earth and moon:

According to Newton's laws, the gravity force between two bodies is given as

$$F(r) = -\frac{m_1 m_2 g}{r^2}.$$

a) The relation between the force F and the potential U in a two-body system is given by the formula

$$F(r) = -U'(r).$$

Derive the potential for each of the two examples. In the case of the spring, the result is called a harmonic potential, in case of earth and moon, it's the gravitational potential.

Sketch F and U as functions of r, shortly explain the connection (steepness versus force value) of the two functions.

ANSWER:

For the spring, we get the potential energy

$$U_{harm}(r) = -\int F(r)\, dr = -\int -k(r - r_0)dr = \frac{1}{2}k\left(r - r_0\right)^2.$$

For earth and moon, we get the potential energy

$$U_{grav}(r) = -\int F(r)dr = -\int -\frac{m_1 m_2 g}{r^2}dr = -g\frac{m_1 m_2}{r}.$$

caused by a mass attraction of two bodies (planets, e.g.)

b) The energy to be done for a change of the distance between the two bodies of a system from r_1 to r_2 is given by the formula

$$E = \int_{r_1}^{r_2} F(r)dr.$$

Transform this formula into a form that gives the energy E in dependence on the potential U.

ANSWER:

$$E = \int_{r_1}^{r_2} F(r)dr = U(r_2) - U(r_1).$$

c) What indicates a high attraction force between two bodies?

- a steep descent of the potential,
- a steep ascent of the potential,
- a high positive value of the potential,
- a high negative value of the potential,
- a slow descent of the potential,
- a slow ascent of the potential.

Remark: As can be seen from the examples above, negative forces are attraction forces and positive forces are repulsion forces.

2) 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.

ANSWER:

Name	potential	force	repulsive (+) / attractive(-)
Hard Sphere	$\infty \quad \forall r \leq d$ $0 \quad \forall r > d$	$0 \quad r \neq d$ $\infty \quad r = d$	+
Soft Sphere	$\epsilon \cdot \left(\frac{\sigma}{r}\right)^n$	$\frac{n \cdot \epsilon}{r} \cdot \left(\frac{\sigma}{r}\right)^n$	+
Van der Waals	$-4\epsilon \cdot \left(\frac{\sigma}{r}\right)^6$	$\frac{-24\epsilon}{r} \cdot \left(\frac{\sigma}{r}\right)^6$	-
Lennard-Jones-12-6	$4\epsilon \cdot \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right)$	$\frac{24\epsilon}{r} \cdot \left(2 \cdot \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right)$	+ -

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

ANSWER:

- Hard-Sphere: not integratable, therefore not usable on a computer

- Modell attractive / repulsive forces or both
- One thing in common: force and potential decrease very quickly with increasing distance, therefor called short-range potentials (as opposed to long-range potentials like gravitation)

3) 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 $\ddot{\vec{x}}$.

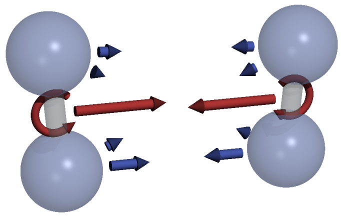
ANSWER:

A multi-centered molecule is composed of multiple centers (sites). The force between two molecules i and j on the center of molecule is calculated as the sum of the pairwise forces between the single sites:

$$F_{ij} = \sum_{sites_i} \sum_{sites_j} F_{sites}$$

The forces on the sites cause a torque on the molecule. The torque resulting from one site can be calculated as

$$\vec{\tau} = (\vec{r}_{site} - \vec{r}_{center}) \times \vec{F}_{site}.$$



where $\vec{r}_{site}$ denotes the position of the site and $\vec{r}_{center}$ is the position of the center of the molecule.

Thus the torque on the whole molecule i can be calculated as

$$\vec{\tau}_i = \sum_{sites} (\vec{r}_{site} - \vec{r}_{center}) \times \vec{F}_{site}$$

The relation between torque τ, angular acceleration $\frac{\delta\omega}{\delta t}$ and moment of inertia θ is given by

$$\vec{\tau} = \vec{\theta} \cdot \frac{\delta\omega}{\delta t}$$

Consequently, the angular acceleration for molecule i can be computed as

$$\frac{\delta\omega_i}{\delta t} = \frac{\vec{\tau}_i}{\vec{\theta}_i} = \frac{\sum_{sites}((\vec{r}_{site} - \vec{r}_{center}) \times \vec{F}_{site})}{\vec{\theta}_i}$$

4) Dimensionless formulation

a) What is the rationale of dimensionless formulations?

b) In order to simulate the inert gas Argon we have to create an initial configuration. The length of a timestep is 2.17 `fs`. The simulation domain is a cube of sidelength 1 μm. Initially, the gas should be subject to normal conditions, i.e. the pressure is 1 bar at a temperature of 273,5 `K`. Further we assume, that all atoms have the same velocity.

Calculate the following values (give the values which are marked with (*) dimensionless!):

- N: Number of atoms within the domain
- L*: side lenght of the domain
- dt*: timestep length
- v*: velocity of an atoms

– T*: temperature

ANSWER:

For the following calculation we use σ, ϵ and the mass of argon:

$$\begin{aligned}\sigma &= 3.41 \cdot 10^{-10} m \\ \epsilon &= 119.8 \cdot 1.38066 \cdot 10^{-23} J \\ &= 1.654 \cdot 10^{-21} J\end{aligned}$$

The molar mass of argon is $39.948 \frac{g}{mol} = 3.9948 \cdot 10^{-2} \frac{kg}{mol}$ and a mol of gas under normal conditions contains $6.0221415 \cdot 10^{23}$ molecules, (Avogadro constant), therefor follows for the mass of an atom:

$$\begin{aligned}m &= \frac{3.9948 \cdot 10^{-2}}{6.0221415 \cdot 10^{23}} kg \\ &= 6.6335 \cdot 10^{-26} kg\end{aligned}$$

The Loschmidt number corresponds to the number of molecules of an ideal gas under normal conditions contained in $1cm^3$. The volume of the simulation domain is $(1\mu m)^3 = 10^{-12} cm^3$.

Thus the number N of atoms is:

$$N = 2.687 \cdot 10^{19} \frac{1}{cm^3} \cdot 10^{-12} cm^3 = 2.687 \cdot 10^7$$

With the formulas for dimensionless position and time we obtain

$$\begin{aligned}L^* &= \frac{1}{\sigma} \cdot L = \frac{1}{3.41 \cdot 10^{-10} m} \cdot 10^{-6} m \\ &= 2932.6 \\ dt^* &= \frac{1}{\sigma} \cdot \sqrt{\frac{\epsilon}{m}} \cdot dt = \frac{1}{3.41 \cdot 10^{-10} m} \cdot \sqrt{\frac{1.654 \cdot 10^{-21} J}{6.6335 \cdot 10^{-26} kg}} \cdot 2.17 \cdot 10^{-15} s \\ &= 0.001\end{aligned}$$

Bevor calculating the dimensionless formulation of the velocity, we have to calculate the “real” velocity first. The temperature of matter is defined by the kinetic energy of its molecules. The kinetic energy can be calculated from the mass and velocity of the atoms:

$$T = \frac{2}{3 \cdot N \cdot k_B} \cdot E_{kin}$$
$$E_{kin} = \frac{1}{2} \cdot \sum_i m_i \cdot v_i^2$$
$$= \frac{1}{2} \cdot N \cdot m \cdot v^2$$

Those formulas can be reformulated:

$$E_{kin} = \frac{3}{2} \cdot N \cdot k_B \cdot T = \frac{3}{2} \cdot 2.687 \cdot 10^7 \cdot 1.38066 \cdot 10^{-23} \frac{J}{K} \cdot 273.15K$$
$$= 1.52 \cdot 10^{-13} J$$
$$v = \sqrt{\frac{2 \cdot E_{kin}}{N \cdot m}}$$
$$= \sqrt{\frac{2 \cdot 1.52 \cdot 10^{-13} J}{2.687 \cdot 10^7 \cdot 6.6335 \cdot 10^{-26} kg}}$$
$$= 412.98 \frac{m}{s}$$

From that we can calculate the dimensionless form of the velocity:

$$v^* = \frac{dt}{\sigma} \cdot v = \frac{2.17 \cdot 10^{-15} s}{3.41 \cdot 10^{-10} m} \cdot 412.98 \frac{m}{s}$$
$$= 0.0026281$$

Last we have to determine the dimensionless value for the temperature:

$$T^* = T \cdot \frac{k_B}{\epsilon} = 273.15K \cdot \frac{1.38066 \cdot 10^{-23} \frac{J}{K}}{1.654 \cdot 10^{-21} J}$$
$$= 2.2801$$