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WS 2010/2011

# 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.

**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 $U$.

**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.

**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

## 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 $\ddot{\vec{x}}$.

## 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 $\mu m$. 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