Scientific Computing II

Exercise B
July 2, 2012

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:

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

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 $\ddot{x}$.
- 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 $\ddot{x}$.
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:** $U_{HS}(r) = \begin{cases} \infty & \forall \ r \leq d \\ 0 & \forall \ r > d \end{cases}$
- **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:** $U_{LJ}(r) = 6\epsilon \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right)$

**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