2. Molecular Dynamics: Modelling

July 2, 2012

2.1. Pair Potentials and Forces

Name	potential	force	attractive(-) / repulsive(+)
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	$4\epsilon \cdot \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right)$	$\frac{24\epsilon}{r}\epsilon \cdot \left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6\right)$	+ -

Pair Potentials and Forces – Homework Exercise

Example: Softsphere-, Van-der-Waals- and Lennard-Jones-Potential for Helium (He)

Helium is an inert gas, so it can be modelled very well with the single-center Lennard-Jones potential with parameters

- $\epsilon = 10.2$
- $\sigma = 2.28$

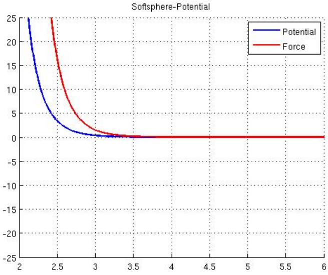

Figure: Softsphere-Potential

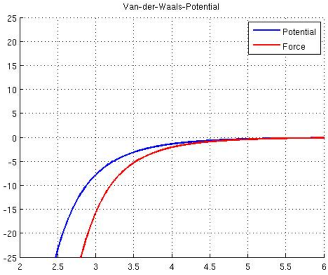

Figure: Van-der-Waals-Potential

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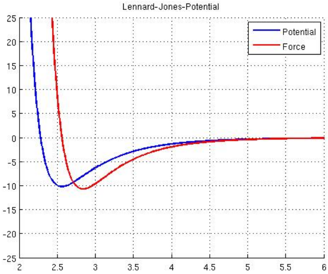
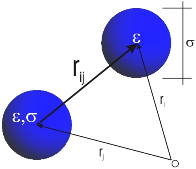


Figure: Lennard-Jones-Potential

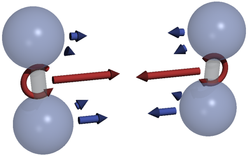
- Hard-sphere model not integratable
- Differences: model repulsive and / or attractive potentials
- All potentials decrease quickly $\Rightarrow$ so called short-range potentials (decrease faster in r than $\frac{1}{r^d}$ (d: Dimension)

2.2. Multi-Centered Molecules

- Up to now: assumption, that molecules are spheres and can be modelled by one Lennard-Jones-Center
- sensible for inert gases (He, Ar, Kr, etc...), Methan (CH_4)
- Force on molecule i: $\vec{F}_i = \sum_{j \neq i} \vec{F}_{ij}$



But how about elongate molecules (e.g. Ethan(C_2H_6), Carbon-Dioxyd (CO_2))?



2.2.1. Torque (Drehmoment)

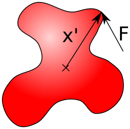


Figure: Force acting on object

- Let's assume to have a directed force $\vec{F}$ (e. g. created by a spring) exceeded on the point $\vec{x'}$ relative to the center of mass of an object.
- Then the torque is computed by

$$\vec{\tau} = \vec{x'} \times \vec{F}$$

Multiple Torques

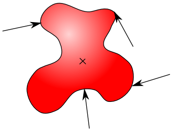
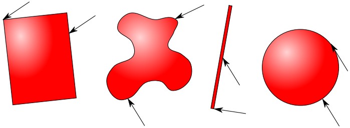


Figure: Multiple forces acting on an object

- We are not only interested in a single torque acting on an object
- When multiple forces are exceeded on an object, they have to be combined somehow
- According to the summation of angular velocities, we can just add them up:

$$\vec{\tau} = \sum_i \vec{x}_i' \times \vec{F}_i$$

2.2.2. Inertia



- Change of angular velocity due to torque clearly depends on the **shape of the object**!
- This information can be expressed in form of the **inertia tensor**.
- For spheres and boxes, these tensors are

$$I_{Sphere} = \begin{pmatrix} \frac{2}{3}mr^2 & . & . \\ . & \frac{2}{3}mr^2 & \\ . & . & \frac{2}{3}mr^2 \end{pmatrix} \quad I_{Box} = \begin{pmatrix} \frac{1}{12}m(w^2+d^2) & . & . \\ . & \frac{1}{12}m(h^2+d^2) & \\ . & . & \frac{1}{12}m(h^2+w^2) \end{pmatrix}$$

See `http://en.wikipedia.org/wiki/List_of_moments_of_inertia` for more inertia tensors

Inertia

- Similar to the translational force $\vec{F} = m \cdot \vec{a}$, we get a formula for the torque depending on the angular acceleration α and the inertia tensor:

$$\vec{\tau} = I\vec{\alpha}$$

- Since we are **interested in computing the change in the angular acceleration**, we are allowed to rewrite the equation:

$$\vec{\alpha} = I^{-1}\vec{\tau}$$

- Warning: This formula is valid only in object space!!!
  However, the forces exerted on the object might only be given in world space.

  $\Rightarrow$ convert to world space