2. Molecular Dynamics: Modelling

July 2, 2012
### 2.1. Pair Potentials and Forces

<table>
<thead>
<tr>
<th>Name</th>
<th>potential</th>
<th>force</th>
<th>attractive(-) / repulsive(+)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hard Sphere</td>
<td>$\infty \quad \forall r \leq d$</td>
<td>$0 \quad r \neq d$</td>
<td>+</td>
</tr>
<tr>
<td></td>
<td>$0 \quad \forall r &gt; d$</td>
<td>$\infty \quad r = d$</td>
<td></td>
</tr>
<tr>
<td>Soft Sphere</td>
<td>$\epsilon \cdot \left( \frac{\sigma}{r} \right)^n$</td>
<td>$\frac{n \cdot \epsilon \cdot \left( \frac{\sigma}{r} \right)^n}{r}$</td>
<td>+</td>
</tr>
<tr>
<td>Van der Waals</td>
<td>$-4 \epsilon \cdot \left( \frac{\sigma}{r} \right)^6$</td>
<td>$-\frac{24 \epsilon \cdot \left( \frac{\sigma}{r} \right)^6}{r}$</td>
<td>-</td>
</tr>
<tr>
<td>Lennard-Jones-12-6</td>
<td>$4 \epsilon \cdot \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right)$</td>
<td>$\frac{24 \epsilon \cdot \left( \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right)}{r}$</td>
<td>+ -</td>
</tr>
</tbody>
</table>
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
Helium is an inert gas, so it can be modelled very well with the single-center Lennard-Jones potential with parameters

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

- 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))

**Figure:** Lennard-Jones-Potential
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)

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

• 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

\[
I_{\text{Sphere}} = \begin{pmatrix}
\frac{2}{3} m r^2 & \cdot & \cdot \\
\cdot & \frac{2}{3} m r^2 & \cdot \\
\cdot & \cdot & \frac{2}{3} m r^2
\end{pmatrix}, \quad I_{\text{Box}} = \begin{pmatrix}
\frac{1}{12} m (w^2 + d^2) & \cdot & \cdot \\
\cdot & \frac{1}{12} m (h^2 + d^2) & \cdot \\
\cdot & \cdot & \frac{1}{12} m (h^2 + w^2)
\end{pmatrix}
\]

Inertia

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

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

- 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