

# Molecular dynamics simulations in a nutshell

atomic-resolution structure

additional moieties  
(protons, H<sub>2</sub>O, counterions)

atomic positions  
(3D coordinates file)

atomic velocities  
(e.g. Maxwell distributed)

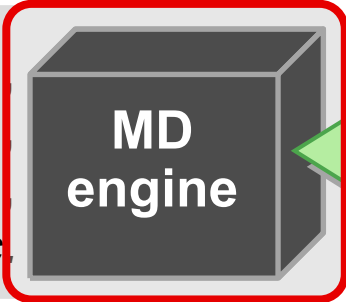
system description  
(PBC, ensemble, etc.)

covalent structure  
(topology file)

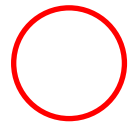
potential energy function  
(equations and parameter file)

force field

system PE  
system KE ( $T_{eff}$ )  
atomic forces  
etc.



**How does the black box work?**



⇒ Discretize time and integrate the classical equations of motion *via* a finite difference method...

$$-\nabla_i U$$

Typical form of the force field:

$$\begin{aligned}
 U(\mathbf{R}) = & \sum_{\text{bonds}} K_r (r - r_{eq})^2 \\
 & + \sum_{\text{angles}} K_\theta (\theta - \theta_{eq})^2 \\
 & + \sum_{\text{dihedrals}} \frac{V_n}{2} (1 + \cos[n\phi - \gamma]) \\
 & + \sum_{i < j}^{\text{atoms}} \frac{A_{ij}}{R_{ij}^{12}} - \frac{B_{ij}}{R_{ij}^6} \\
 & + \sum_{i < j}^{\text{atoms}} \frac{q_i q_j}{\epsilon R_{ij}}
 \end{aligned}$$