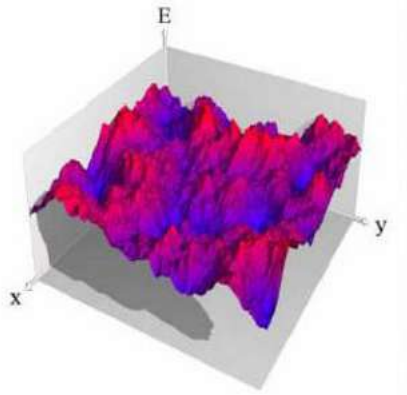
Molecular Dynamics

$E_T = E_c + V = cste$ $E_c = 3/2\ NkT = \frac{1}{2}\ mv^2$

Empirical Force Fields & programs

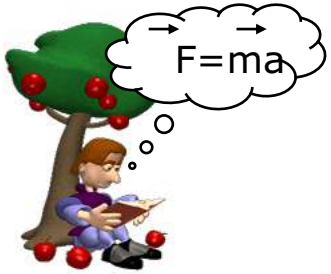
(Gromos, NAMD, Amber, Charmm…)



$$V = \sum_{\text{bonds}} k_b (b - b_0)^2 + \sum_{\text{angles}} k_\theta (\theta - \theta_0)^2 + \sum_{\text{dihedrals}} k_\phi [1 + \cos(n\phi - \delta)]$$

$$+ \sum_{\text{impropers}} k_\omega (\omega - \omega_0)^2 + \sum_{\text{Urey-Bradley}} k_u (u - u_0)^2$$

$$+ \sum_{\text{nonbonded}} \epsilon \left[\left(\frac{R_{\min_{ij}}}{r_{ij}} \right)^{12} - \left(\frac{R_{\min_{ij}}}{r_{ij}} \right)^{6} \right] + \frac{q_i q_j}{\epsilon r_{ij}}$$

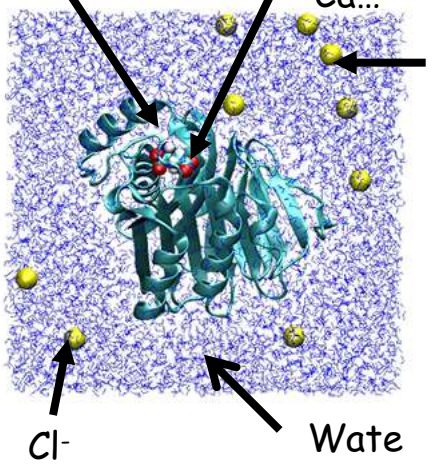


$\mathbf{r}_i(t) \rightarrow \mathbf{r}_i(t + \delta t)$

10^{-15}s ➔7-10 orders of magnitude

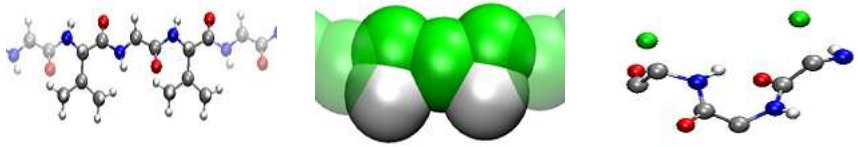
➔N atoms, N^2 Memory, N^3 time ➔ CPU & GPU

➢ **Local motion of peptides and proteins**



Coarse-grained

OPEP, Martini



➢ **Longer simulations and larger systems, but simplified !**