1 Introduction to Molecular Dynamics

- The interaction between molecules is represented by the interaction law specified by the potential $U(r_1, \ldots, r_N)$ (aka force field) representing the potential enery of N interacting atoms as a function of their positions in 3D space $r_i = (x_i, y_i, z_i)$ [**?**].

$$
\begin{aligned}
U(\mathbf{r}_1, \cdots, \mathbf{r}_N) = & \sum_{\text{bonds}} \frac{a_i}{2}(l_i - l_{i0})^2 + \sum_{\text{angles}} \frac{b_i}{2}(\theta_i - \theta_{i0})^2 \\
& + \sum_{\text{torsions}} \frac{c_i}{2}[1 + \cos(n\omega_i - \gamma_i)] \\
& + \sum_{\text{atom pairs}} 4\varepsilon_{ij}\left[\left(\frac{\sigma_{ij}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}}\right)^{6}\right] \\
& + \sum_{\text{atom pairs}} k\frac{q_i q_j}{r_{ij}}
\end{aligned}
$$

Typical force-field used in biosystem simulations

- Another set of equations used in MD simulate Potential Enenergy

$$E_P(x) = E_{bonded} + E_{non-bonded} \tag{1}$$

- *ab initio* (from the beginning) Born-Oppenheimer:
  In quantum chemistry, the computation of the energy and the wavefunction of an average-size molecule is a formidable task that is alleviated by the Born–Oppenheimer (BO) approximation, named after Max Born and J. Robert Oppenheimer[from wikipedia]

- van-der-Waals

- Energy minimazation
- Schrodinger Equation One dimensional wave-function mathematical representation

$$\psi(x,t) = A\,\cos(\phi + k\,x - \omega\,t), \tag{2}$$