

Langevin dynamics.

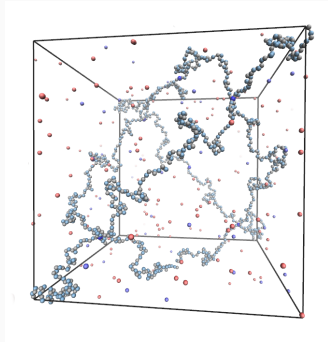


Figure 2: The snapshot of the hydrogel model for Langevin dynamics

- Diamond network of point particles
- Lennard–Jones interaction

$$V_{LJ}(r) = \begin{cases} 4\varepsilon \left(\left(\frac{\sigma}{r-r_c} \right)^{12} - \left(\frac{\sigma}{r-r_c} \right)^6 \right) & , r < r_c \\ 0 & , r > r_c \end{cases}$$

- FENE potential

$$V_{FENE}(r) = -\frac{1}{2}\Theta\Delta r_{max}^2 \ln \left[1 - \left(\frac{r-r_0}{\Delta r_{max}} \right)^2 \right]$$

- Electrostatic interaction

$$V_{EL} = l_B k_B T \cdot \frac{q_1 q_2}{r}$$