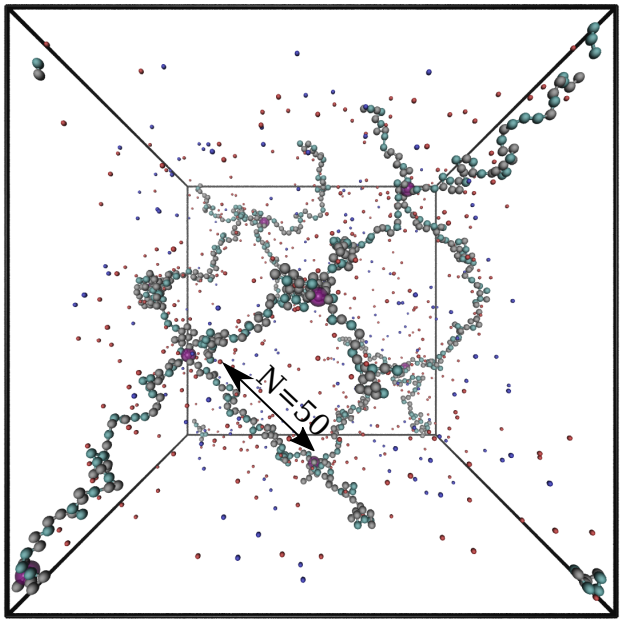
MCMD model. Langevin Molecular Dynamics (LMD).



The snapshot of the hydrogel model for Langevin dynamics

- Diamond network of point particles
- Lennard–Jones interaction

$$V_{\mathrm{LJ}}(r) = \begin{cases} 4\epsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right], & \text{if } r < r_{\mathrm{cutoff}} \\ 0, & \text{elsewhere} \end{cases}$$

σ = 0.35 nm

- FENE potential

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

Δr_{max}= 2σ

- Electrostatic interaction

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