

Molecular dynamics for polymers

Consider an ensemble of particles interacting via the Lennard-Jones potential,

$$U_{LJ}(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (1)$$

where r is the distance between the two particles, σ is the interaction range and ϵ is the interaction strength.

The Lennard-Jones particles can be connected to form a polymer, by joining the i -th and $i+1$ -th potential by means of finitely extensible nonlinear elastic (FENE) springs, defined by the potential

$$U_{FENE}(r) = -\frac{KR_0^2}{2} \log \left[1 - \left(\frac{r}{R_0} \right)^2 \right] \quad (2)$$

where $r = |\mathbf{r}_{i+1} - \mathbf{r}_i|$ and R_0 is the bond length (take it equal to 1.6σ), and K is the bond strength (take it equal to $10 k_B T / \sigma^2$, or larger).

1. What do you think the typical states of a polymer made up by stringing together N particles (also called monomers) will be for ϵ small and large respectively?
2. Write a Java code to simulate an N -monomer polymer in the NVE ensemble, and to visualise the results. Try varying the value of ϵ , and confirm your previous guess for the typical states the polymer is in.
3. Generalise your code to simulate the polymer in the NVT ensemble, by using the Nose-Hoover algorithm.
4. Use your code to compute the average pair potential energy per monomer, together with its error (computed as the variance of this quantity), as a function of ϵ , for $N = 100$ and $N = 200$. Comment the results.