CB&B752/MCDB452/MB&B752/MCDB752/CPSC752
Homework 1

Problem 1:

For the BLN model protein discussed in class and in J. D. Honeycutt and D. Thirumalai, "The nature of folded states of globular proteins," Biopolymers 32 (1992) 695, which includes Lennard-Jones-like long-range (V_{lr}), bond length (V_{bl}), bond angle (V_{ba}), and dihedral angle (V_{da}) interactions, calculate analytical expressions for the x-, y-, and z-components of the force on a given monomer i for a chain of length N. The total potential energy is given by

$$V_{tot} = \sum_{i=1}^{N}\sum_{j=1}^{i-2} V_{lr}\left(r_{i,j}\right) + \sum_{i=1}^{N-1} V_{bl}\left(r_{i,i+1}\right) + \sum_{i=1}^{N-2} V_{ba}\left(\theta_{i,i+1,i+2}\right) + \sum_{i=1}^{N-3} V_{da}\left(\phi_{i,i+1,i+2,i+3}\right)$$, where $r_{i,j} = \left|\vec{r}_i - \vec{r}_j\right|$, $\vec{r}_i$ locates the center of monomer i, σ is the diameter of the monomer,

$$V_{lr}\left(r_{i,j}\right) = 4\varepsilon_h\left[\left(\frac{\sigma}{r_{i,j}}\right)^{12} + C\left(\frac{\sigma}{r_{i,j}}\right)^{6}\right]$$ with C=-1 and $\varepsilon=\varepsilon_h$ when i,j=B,B, C=1 and $\varepsilon=\varepsilon_L$ $=2/3\varepsilon_h$ when i,j=LL, LB, and C=0 and $\varepsilon=\varepsilon_h$ when i,j=NN, NL, NB, and ε_h is the Lennard-Jones energy scale, $V_{bl}\left(r_{i,j}\right) = \frac{k_b}{2}\left(r_{i,j} - \sigma\right)^2$, k_b is the spring constant,

$V_{ba}\left(\theta_{i,j,k}\right) = \frac{k_\theta}{2}\left(\theta_{i,j,k} - \theta_0\right)^2$, k_θ is the bend spring constant, $\theta_{i,j,k} = \cos^{-1}\left(\frac{\vec{r}_{i,j}\bullet\vec{r}_{k,j}}{r_{i,j}r_{k,j}}\right)$, and θ_0 is the equilibrium bend angle, $V_{da}(\phi_{i,j,k,l}) = A(1+\cos(\phi_{i,j,k,l})) + B(1+\cos(3\phi_{i,j,k,l}))$, where A and B constants and where $\phi_{I,j,k,l}$ is defined by

$\cos\left(\phi_{i,j,k,l}\right) = (\vec{r}_{i,j}\times\vec{r}_{k,j})\cdot(\vec{r}_{j,k}\times\vec{r}_{l,k}) / \left(\left|(\vec{r}_{i,j}\times\vec{r}_{k,j})\right|\left|(\vec{r}_{j,k}\times\vec{r}_{l,k})\right|\right)$ and

$\sin\left(\phi_{i,j,k,l}\right) = \vec{r}_{j,k}\cdot\left[(\vec{r}_{i,j}\times\vec{r}_{k,j})\times(\vec{r}_{j,k}\times\vec{r}_{l,k})\right] / \left(\left|(\vec{r}_{i,j}\times\vec{r}_{k,j})\right|\left|(\vec{r}_{j,k}\times\vec{r}_{l,k})\right|\right)$. Calculate the total potential energy V_{tot} for the configuration of the (N=46) polymer $B_9N_3(LB)_4N_3B_9N_3(LB)_5L$ in the file config.dat.

Download the file config.dat from the course website, which lists the positions of the 46 monomers corresponding to the ground state of the BLN model $B_9N_3(LB)_4N_3B_9N_3(LB)_5L$ in the following format:
r_{x1} r_{y1} r_{z1}
r_{x2} r_{y2} r_{z2}
…
r_{xN} r_{yN} r_{zN}

With these coordinates, calculate the total potential energy of the configuration in config.dat.