CB&B752/MCDB452/MB&B752/MCDB752/CPSC752
Homework 2

The second homework is due on Nov. 28 at 11:59pm. CBB&CS students should complete all problems, while MCDB&MBB students should complete problem 1. The complete assignment should be emailed to cbb752@gersteinlab.org

Problem 1 (MCDB/MBB & CBB/CPSC):

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 ε=ε_h when i,j=B,B, C=1 and ε=ε_L =2/3ε_h when i,j=LL, LB, and C=0 and ε=ε_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

$\sin\left(\phi_{i,j,k,l}\right) = \vec{r}_{j,k}\cdot\left[(\vec{r}_{i,j}\times\vec{r}_{k,j})\times(\vec{r}_{j,k}\times\vec{r}_{l,k})\right] / \left(\left|(\vec{r}_{i,j}\times\vec{r}_{k,j})\right|\left|(\vec{r}_{j,k}\times\vec{r}_{l,k})\right|\right)$. Use

$\vec{F}_i = -\left[\hat{x}\frac{\partial V_{tot}}{\partial x_i} + \hat{y}\frac{\partial V_{tot}}{\partial y_i} + \hat{z}\frac{\partial V_{tot}}{\partial z_i}\right]$ to calculate the total force on monomer i.

Problem 2 (CPSC/CBB):

Write a c++ function to calculate the N-3 dihedral angles for a polymer chain, assuming that the positions $\vec{r}_i$ of the i=1,N monomers are specified. Download the file positions.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}

Compare your results to the answers in file dihedral.dat, which can also be downloaded from course website.