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

The second homework is due on **April 13th at 10PM**. CBB&CS students should complete all problems, while MCDB&MBB students should complete all problems except for ones denoted "CBB/CS only". The completed assignment should be emailed to cbb752@gersteinlab.org.

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,

$V_{lr}\left(r_{i,j}\right) = 4\varepsilon_h\left[\left(\dfrac{\sigma}{r_{i,j}}\right)^{12} + C\left(\dfrac{\sigma}{r_{i,j}}\right)^{6}\right]$ 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, $V_{bl}\left(r_{i,j}\right) = \dfrac{k_b}{2}\left(r_{i,j} - \sigma\right)^2$, k_b is the spring constant,

$V_{ba}\left(\theta_{i,j,k}\right) = \dfrac{k_\theta}{2}\left(\theta_{i,j,k} - \theta_0\right)^2$, k_θ is the bend spring constant, $\theta_{i,j,k} = \cos^{-1}\left(\dfrac{\vec{r}_{i,j}\bullet\vec{r}_{k,j}}{r_{i,j}r_{k,j}}\right)$, 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

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

Problem 2 (CBB/CS only):

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.

Problem 3:

During their growth season apples are frequently sprayed with pesticides to prevent damage by insects. By eating apples you accumulate these pesticides in your body.
An important factor determining the concentration of pesticides is their half life in the human body. An appropriate mathematical model is:

$dP/dt = \sigma - \delta P$

where σ is the daily intake of pesticides, i.e., $\sigma = \alpha A$ where A is the number of apples that you eat per day and α is the amount of pesticides per apple, and δ is the rate at which the pesticides decay in human tissues.

a. Sketch the amount of pesticides in your body, P(t), as a function of your age, assuming you eat the same number of apples throughout life.
b. How much pesticide do you ultimately accumulate after eating apples for decades?
c. Suppose you have been eating apples for decades and stop because you are concerned about the unhealthy effects of the pesticides. How long does it take to reduce your pesticide level by 50%?
d. Suppose you start eating two apples per day instead of just one. How will that change the model, and what is the new steady state? How long will it now take to reduce pesticide levels by 50% if you stop eating apples?
e. What is the decay rate (δ) if the half-life is 50 days?

Problem 4:

Consider a replicating population where most of the death is due to competition with other individuals, i.e., let $f(N) = cN$ in a model where $dN/dt = bN - f(N)N$.

a. Sketch the *per capita* death rate as a function of N.
b. Sketch the *per capita* net growth rate as a function of N
c. Compute the steady states.
d. Are the steady-states stable?

e. (CBB/CS only) Assuming N(0) = 1, simulate this model on the computer and find the parameter values that provide the best (i.e., least-squares) fit with the following experimental observations:

Time (hours)	N
0	1
3	1.22
6	1.27
12	2.09
24	2.45
36	2.22

Plot the predicted and observed values of N over 36 hours for these optimal parameters.