CS 5106 3D Modeling & Simulations in Bioinformatics

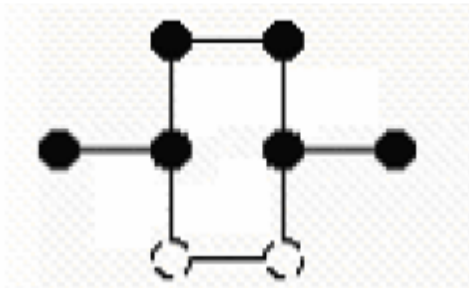
Assignment 1

Due Date: 19th March 2018, 10am

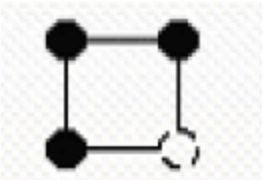
In the Hydrophobic-Polar (HP) model, the hydrophobic effect is assumed to be the driving force in protein folding. This greatly simplifies the interaction energies between non-bonded monomers by characterizing each amino acid in a peptide sequence as being either hydrophobic or polar. Thus, this model allows for the feasible simulation of protein folding by greatly reducing the degrees of freedom and simplifying the energy landscape. Considering a 2D grid for simulation with the scoring function only including non-bonded interaction (diagonals included) with H-H interaction having -1 score.

Implement the metropolis monte carlo algorithm using the following procedure

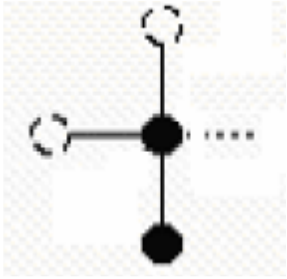
1. The monomer chains will be generated on a two-dimensional square lattice without periodic boundary conditions (make sure your lattice is significantly bigger than your protein sequence).
2. These chains will be grown to a desired length, n, using the "random walk" technique. Additionally, the use of a "self-avoidance" criterion will take into account the effects of excluded volume by forbidding any lattice point from being occupied by more than one monomer.
3. Following generation of the lattice chain, the energy of the conformation will be given by summing up contact energies of adjacent H-H monomers.
4. You have to design your own move set. Some examples are below



crank shaft



corner flip



end move

Use the following strings to report the minimum energy and the respective conformation found by your algorithm

ID	Length	Protein Sequence
		2D HP
S1-1	20	$(HP)_2PH_2PHP_2HPH_2P_2HPH$
S1-2	24	$H_2(P_2H)_7H$
S1-3	25	$P_2HP_2(H_2P_4)_3H_2$
S1-4	36	$P_3H_2P_2H_2P_5H_7P_2H_2P_4H_2P_2HP_2$
S1-5	48	$P_2H(P_2H_2)_2P_5H_{10}P_6(H_2P_2)_2HP_2H_5$
S1-6	50	$H_2(PH)_3PH_4PH(P_3H)_2P_4H(P_3H)_2PHPH_4(HP)_3H_2$
S1-7	60	$P_2H_3PH_8P_3H_{10}PHP_3H_{12}P_4H_6PH_2PHP$
S1-8	64	$H_{12}(PH)_2(P_2H_2)_2P_2HP_2H_2PPH_2P_2HP_2(H_2P_2)_2(HP)_2H_{12}$
S1-9	85	$H_4P_4H_{12}P_6(H_{12}P_3)_3HP_2(H_2P_2)_2HPH$
S1-10	100	$P_3H_2P_2H_4P_2H_3(PH_2)_2PH_4P_8H_6P_2H_6P_9HPH_2PH_{11}P_2H_3PH_2PHP_2HPH_3P_6H_3$
S1-11	100	$P_6HPH_2P_5H_3PH_5PH_2P_4H_2P_2H_2PH_5PH_{10}PH_2PH_7p_{11}H_7P_2HPH_3P_6HPH_2$