Introduction to computational biophysics (CS 428) (3 credit points)
Instructor: Ron Elber (ron@cs.cornell.edu) 5-7146

Pre-requisites: CS 100, MATH 293,294, Physics 112,213 CHEM 211 or equivalent.
BioBM 330 recommended

Tuesday and Thursday , lecture: 1:25-2:15 Olin Hall 245
Thursday, section: 2:30-3:20 Hollister Hall 306

Water:

1. Atomistic simulations. Fixed charge models. TIP3P and TIP4P. Energy minimization (steepest descent, conjugate gradient, Newton Raphson) and the geometry of the water dimer.
2. Water entropy and free energy. Calculation of partition functions. (Stochastic sampling, randomized algorithms, Metropolis algorithm. and Markov chains).
3. Hydrophobic effects and solvation of apolar molecules. (Enhanced sampling, multi-tempering, and multi-ensemble approaches).

Protein Folding:

1. Reduced representation of polymers and simulations of polymer collapse. (Lattice and continuous Monte Carlo simulations).
2. Simulation of kinetics and equilibrium –Brownian dynamics.
3. Global optimization techniques, randomized algorithms, protein design

Molecular dynamics:

1. Solving initial value problems. Extracting kinetic and thermodynamic properties.
2. Molecular dynamics with holonomic constraints (SHAKE).
3. Solvent and solutes, Periodic boundary conditions, pressure and temperature controls,
4. Computing long-range forces (Ewald sum).
5. Correlation functions and experiments
6. Transition state theory in the condensed phases

Statistics:

1. Estimators: Mean, standard deviation
2. Maximum likelihood
3. Confidence interval
4. chi-2 statistics
5. Regression
6. Goodness of fit

The students in the class must follow the code of academic integrity
http://www.cs.cornell.edu/degreeprogs/ugrad/CSMajor/index.htm#ai