Outline, Chemistry 5021/8021

Computational Chemistry

Spring, 2005
(Schedule is tentative)

I. Introduction

II. Molecular Mechanics and Force Fields.

A. Force fields, potential energy functions, inter and intramolecular interactions, empirical parameters. (CJC, Chapter 2; ref. ARL, Chapter 4)
B. Lab. InsightII and VMD.
C. Molecular mechanics calculations, energy minimization, conformational analysis, vibrational frequencies, and normal mode analysis.
D. Lab. CHARMM and InsightII.
E. First Project Assignment.

III. Molecular Simulations.

A. Monte Carlo Simulations
    a. Importance sampling and Metropolis sampling
    b. Basic algorithms and technical details
    c. Moves
B. Molecular Dynamics Simulations
    a. Equations of motion and force calculations
    b. Diffusion
    c. Integration schemes
C. Liquid Water
    a. Models
    b. Properties
D. Ensembles
    a. Canonical and microcanonical Monte Carlo
    b. Isothermal-isobaric Ensemble Monte Carlo
    c. Grand-Canonical Ensemble Monte Carlo
    d. Constant T and P molecular dynamics

III. Liquids.

A. Solvents (Polar and nonpolar)
B. Solutions
C. Acidity and Basicity, and Computation of pKa
D. Continuum Solvation Models

IV. Structure and Dynamics of Proteins.

A. Protein Structure and PDB

B. Building Models for Protein Structure and Energy Calcultions
C. Normal Mode Analysis
D. Molecular Dynamics of Proteins
E. Solvation

V. Free Energy Simulations.

A. Free Energy Perturbation
    a. Free energy of solvation
    b. Partition coefficients
B. Thermodynamic Integration and Umbrella Sampling
C. Potential of Mean Force for Condensed Phase Reactions
D. Hydrophobic Effects and Ion-Pair Interactions in Water

VI. Quantum Mechanics.

A. Gaussian and GaussView
B. Hartree-Fock Theory and Basis Sets
C. Semiempirical Methods
D. Electron Correlations
E. Density Functional Theory

VII. Combined QM/MM Methods.

A. Why and How to Combine QM and MM
B. Solvation and Solvent Effects
    a. Polarization
    b. Reaction profiles in soluton
C. Protein-Ligand Interactions
D. Modeling Enzymatic Reactions

Final Exam: presentation of a critical analysis of selected papers. (to be determined.)