Spring Term 2002

Introduction to Modern Computational Chemistry

Chem. 3430, Tu., Th. 9:30 – 10:45

Lecture	**Topic**
	Electronic Structure Theory – Part I
1.	Hartree-Fock method; Gaussian basis sets
2.	Locating minima and transition states; vibrational frequencies
3.	Perturbation and coupled cluster theory; size extensivity, thermochemistry,
4.	Molecular properties – atomic charges, dipole and quadrupole moments, polarizabilities, IR and Raman intensities
5.	CASSCF, CASPT2, CI – applications to diradicals, bond breaking, and intro. to excited states
6.	Density functional theory – functionals, when appropriate?
7.	Locating transition states; minimum energy pathways
	Molecular Dynamics
8.	Systems of ODE's and general purpose ODE solvers; the Verlet algorithm for propagating MD trajectories.
9.	Periodic Boundary Conditions and the minimum image convention; treating Coulomb potentials via Ewald summation.
10.	Constraints on mechanical degrees of freedom; thermostats and barostats.
11.	Introduction to AMBER
12.	Extracting thermodynamic properties from MD: the ergodic hypothesis, the virial theorem (calculations of pressure and equations of state); calculation of free energies (thermodynamic integration) and chemical potentials (Widom insertion method).
13.	Extracting dynamical properties from MD: correlation functions and the calculation of transport properties and spectra.

Monte Carlo Simulations

14. Basic ideas (random number generators, etc.); dumb Monte Carlo (throwing darts to calculate integrals, etc.).

15. Smart Monte-Carlo: the Metropolis algorithm; practical issues in MC simulation: error bars, statistical independence of data (decorrelation times, etc.).

16. Applications to spin systems: the Ising model (phase transitions, critical slowing down, umbrella sampling).

17. Applications to continuous systems: equations of state of atomic and molecular systems.

18. Path Integral Monte Carlo for quantum thermodynamics

Finite Difference Methods for PDE's

19. Basics: discretization of PDE's into finite difference equations and their solution by relaxation methods.

20. Examples from electrostatics: Laplace Eq., Poisson Eq. And Poisson-Boltzmann Eq.

21. Advanced relaxation methods: critical slowing down and its solution by multigridding.

Electronic Structure Theory – Part II

22. Weak interactions - BSSE problem, paramaterizing force fields

23. Localized orbital MP2 (LMP2) method and other recent advances

24. Methods for treating excited states (CIS, CI, CASSCF, CASMP2, TDDFT)

25. Overview of various codes available at Pitt, and degree of parallelization

26. Excited states continued; continuum approaches to solvation

27. Using different levels of theory for primary and secondary systems: QM/MM methods

28. Methods for treating periodic systems; modeling surfaces - slab vs. cluster models