CHEM 7711/8711: Approximate Chemical Modeling Methods

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Office hours: 8:30-9:30 am Tuesdays and Thursdays and by appointment.

Schedule: Tuesdays and Thursdays 9:40 am – 11:05 am

Textbook: Molecular Modeling. Principles and Applications, A. Leach, Addison Wesley Longman Ltd.
(Suggested) Computational Chemistry, G. H. Grant and W. G. Richards, Oxford Science Publications

Content: This course focuses on modeling techniques applicable to large chemical systems. The majority of these techniques are based on the molecular mechanics approximation. Techniques to be discussed include molecular mechanics, geometric optimization, conformational searching, solvation, molecular dynamics, free energy approximations and transition state modeling in the molecular mechanics formalism.

Grading: Grades will be based on application of methods discussed to individual projects (preferably related to an ongoing research project), quizzes, homework assignments, class participation and a final examination. The final examination will contribute 75 pts to the course total. The projects will be developed according to the following schedule.

Project Development	***Date Expected***	***Points***
Brief description of a research problem and its context w/literature – written (~1 page + references)	9/16	20
Discussion of computational approach to the research problem w/literature – written (~1 page + references)	10/7	20
Research update I – written (~1 page)	10/28	20
Research update II – written (~1 page)	11/18	20
Report – written (use good judgement) and oral (~30 min.)	12/2, 12/7	70

Course Total: 300

Grading scale*:		
	270-275/276-294/295-300	$A^-/A/A^+$
	250-255/256-264/265-269	$B^-/B/B^+$
	230-235/236-244/245-249	$C^-/C/C^+$
	210-224/225-229	D/D^+
	<210	F

Other:

- Noise-making electronic devices (cellular phones, pagers, etc.) should not be allowed to disrupt class sessions. Either turn them off or leave them elsewhere.
- Class email lists will be used. These lists will use your University of Memphis email account. If you do not regularly check that account, make sure your email is forwarded to the account you do use (go to iam.memphis.edu to set up email forwarding).
- Documents will be made available to students via the WWW (http://www.chem.memphis.edu/parrill/chem8711/index.htm).
- It is expected that every student will submit evidence of his or her own individual understanding and effort. Students are encouraged, however, to discuss their individual

projects with other students and other professors. Any type of academic dishonesty will be met with severe penalties, and will be handled on an individual basis.

Course Topics

CHEM 7711/8711 will include the following topics:

Molecular Mechanics
- Overview
- Functional Form
- Forcefields
- Parameterization
- Limitations
- Overcoming Limitations

Geometry Optimization
Conformational Search Methods (with and without experimental restraints)
- Multiple Minimum Problem
- Dihedral Driving
- Monte Carlo
- Distance Geometry
- Simulated Annealing
- Poling

Ensembles
- Molecular Dynamics
- Monte Carlo
- Brownian/Langevin Dynamics

Solvation Treatments
- Explicit inclusion of solvent molecules (dynamics)
- Constant dielectric
- GB/SA
- Poisson-Boltzmann

Transition State Modeling
- Parameterization of TS as a minimum
- PES crossing

Free Energy Difference Determination
- Statistical Perturbation Energy (SPE a.k.a. Free Energy Perturbation, FEP)
- Thermodynamic Integration

CHEM 7711/8711 will also include some of the following topics: (depending on class interests/needs)

Visualization
Docking (intermolecular complex geometry modeling)
Quantitative Structure-Activity Relationships
Structural Descriptors
DNA modeling
Carbohydrate modeling
Lipid modeling
Protein modeling – general
Homology modeling of proteins
Modeling inorganic compounds in the MM formalism
Artificial intelligence in chemistry
De novo molecular design
Combined methods (QM/MM)

CHEM 7711/8711 Reading List

Journals

Advances in Molecular Modeling
Journal of Computational Chemistry
Journal of Chemical Information and Computer Sciences
Journal of Molecular Graphics and Modeling
Journal of Molecular Structure-Theochem
Journal of Physical Chemistry
Journal of Chemical Physics

Books

Reviews in Computational Chemistry, Lipkowitz and Boyd, eds.
Molecular Mechanics, Burkert and Allinger, ACS Monograph, 1982.
Molecular Modeling, Comba and Hambley, Weinheim, 1995.
Quantitative Structure-Activity Relationships of Drugs, J. Topliss, ed. 1983.

Articles

Specific articles will be distributed and/or suggested for some topics included in the course as we reach them.