Spring Term 2002
Honors College Course
Introduction to Computational Science
(Chemistry 1460, MWF, 2:00-2:50)

Syllabus

Week 1 – Lectures 1,2 - goals of course, general overview of scientific computing illustrated by examples. Introduction to Mathcad.
Lecture 3 - Integration - as an introduction to Monte Carlo methods.

Week 2 – Lectures 1 - Random numbers and sampling methods.
Lectures 2,3 - Examples of Monte Carlo simulations in Chemistry and Biology

Week 3 - Lecture 1 - Ordinary differential equations (ODE).
Lecture 2 – Guest lecturer - Prof. Jeffry Madura, Duquesne Univ. "Modeling Fish Antifreeze Proteins with Monte Carlo Methods"

Week 4 – Systems of ODE's, kinetics, non-linear dynamics, molecular dynamics; Guest lecturer - Prof. Bard Ermentrout, Univ. Pittsburgh, "Oscillatory Reactions".

Week 5 – Optimization methods (steepest descent, Newton-Raphson, conjugate gradient, etc. Strengths and weaknesses of these methods). Why optimization is important in throughout the sciences and other disciplines.

Week 6 - Lectures 1,2 - Introduction to computational chemistry software - MOE or Materials Studio. Build structures for simple molecules, polymers, solids. Optimize structures, animation of normal modes.
Lecture 3 - Guest lecturer (to be announced).

Week 7 - Introduction to linear algebra - systems of equations, matrices, determinants. Least squares fitting.

Week 8 – Lectures 1, 2 -, eigenvalue problems, Huckel theory.
Lecture 3 - Guest lecturer (to be announced).

Week 9 - Lectures 1,2 - Boundary value problems - the quantum mechanical harmonic oscillator problem – example of the use of "shooting" methods.
Lecture 3 - visit to Pittsburgh Supercomputing Center and discussion of parallel computing.

Week 10 - Minimization on complex landscapes: simulated annealing, genetic algorithms, etc.

Week 11 - Fourier series, Fourier transforms, FFT's.

Week 12 – Lectures 1, 2 - Partial Differential Eqs. and their solution by finite-difference methods. Applications to: electrostatics, kinetics, theory of ion transport through biological channels.
Lecture 3 – Guest lecturer – tentatively, Prof. Robert Swendsen, CMU, "Computer Simulations of Phase Transitions"

Weeks 13-14 - Special Topics - protein folding, neural networks, economics, etc.
Guest lecturer, Prof. Ivet Bahar, UPMC, "Bioinformatics".

Comments on grading: Class participation (10%), weekly assignments (55%), project (35%). Students will choose their own project topic, about midway through the term.

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