Computational Nanoscience
Course Syllabus

2 Credits
Course (cross-listed): Physics C203 (CCN 69735) / NSE C242 (CCN 61011)

Spring Semester, 2008: Tuesdays & Thursdays, 9:30-11:00 AM
Location: LeConte Hall, Room 325

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Course Description: This course will provide students with the fundamentals of computational problem-solving techniques that are used to understand and predict properties of nanoscale systems. Emphasis will be placed on how to use simulations effectively, intelligently, and cohesively to predict properties that occur at the nanoscale for real systems. The course is designed to present a broad overview of computational nanoscience and is therefore suitable for both experimental and theoretical researchers. Specific examples of topics the course will cover are:

1) The central ideas behind a wide range of nanomaterials simulations methods
2) How to break down a nanoscale problem into its "simulatable" constituents, and then piece it back together
3) How to simulate the same thing in two different ways
4) How to know what you're doing and why thinking is still important
5) The importance of connecting simulation directly with experiment
6) What to do with all of that data, and how to judge its accuracy and validity
7) Why the "multi-scale" modeling picture is critically important and also nonsense

While some aspects of the simulation methods such as numerical algorithms will be presented, there will be little if any programming required. Rather, we will emphasize the intelligent application (as opposed to "black box" use) of codes and methods, and the connection between the computer results and the physical properties of the problem.

Class time will be spent predominantly on lectures and discussion, to some extent on in-class simulation, and at the end of the semester on student presentations. Homework assignments will be assigned roughly every two weeks, most of which involve the use of on-line simulation tools developed for this class on the NanoHUB. Students are encouraged to explore www.nanhub.org, create a user account, and become familiarized with the nanoHUB project.

Required Textbooks: Due to the wide-ranging nature of material covered in this class, there will be no specific required textbooks. A combination of published review articles and relevant books will be encouraged as reading material. In addition, Powerpoint and

Breeze presentations will be posted on the course web site.

Grading: There are no exams. The breakdown of a final grade for this course is as follows:

- 20% class participation: your active participation during class is important, as is simply showing up.
- 40% homework: homework will consist mostly of numerical experiments with existing codes and at times of derivations related to the lectures. An in-class pop-quiz counts as one homework assignment. Working together on homework assignments is fine.
- 40% class project: class projects will consist of a written report based on simulations you carry out to solve a scientific problem of interest. This can be something directly related to your own research, or something that allows you to explore a certain realm of computational nanoscience more detail, or simply a topic of general interest to you. It is required that you submit a 1-page maximum description of your project no later than April 10.

Class Etiquette: A few important items regarding etiquette:

- Be on time. We will begin class at 9:30 AM.
- Come to class prepared, and expect to be called on periodically.
- Beverages are permitted in class, but food is not.
- If you cannot make a class meeting, or if you will be late for class, send both instructors an e-mail advising us of this in advance.
- Laptops, PDAs, cell phones and similar electronic devices will be turned off during class and left in your backpack or briefcase. The only exception to this is for in-class simulation days.

Course Website: http://mint.physics.berkeley.edu/compnano
Please check this website for the syllabus and any changes to it, pdfs of the class lectures (posted before each class), homework assignments, a general discussion forum for the class, and possibly other useful information.

Class Discussion Forum: http://mint.physics.berkeley.edu/Vanilla-1.1.4
This forum is meant to facilitate discussion among the class, a place where you can trade questions/answers with one another about homeworks, post questions to the instructors, and share helpful information regarding any other aspect of the class or computational nanoscience in general.

Tentative Schedule of Class Lectures:

- **Introduction**
  1/22 Introduction: Organization of Class, Historical Perspective, "Computer Experiments"
- **Molecular Dynamics**
  1/24 Introduction to Molecular Dynamics
  1/29 Computing Physical Quantities

1/31 Energy Minimization, Geometry Optimization, and Seeing What You're Doing
2/5 A Whole Lecture on Intra- and Intermolecular Potentials
2/7 A Day of Class Simulation: MD of Carbon Nanotubes

- **Monte Carlo Methods**
  2/12 Introduction to Monte Carlo Methods (Metropolis and Random Numbers)
  2/14 Monte Carlo and Kinetic Monte Carlo
  2/19 Monte Carlo Simulation of a Classical Liquid
  2/21 A Day of Simulation
- **Phase Transitions**
  2/26 Magnetism with a Toy Model: Ising
  2/28 Phase Transitions, Critical Slowing Down
- **Computational Quantum Mechanics**
  3/4 Introductory Concepts
  3/6 Quantum Chemistry - Molecular Orbital Calculations, Hartree-Fock, Basis Sets
  3/11 Quantum Chemistry - A Day of Class Simulation: Hartree-Fock Calculations
  3/13 Density Functional Theory
  3/18 Density Functional Theory - A Day of Class Simulation
  3/20 Modeling Solids with DFT - Density of States, Band Structure
  3/25 & 3/27 SPRING BREAK
  4/1 Beyond Density Functional Theory - Excited State Properties (GW, BSE), Transport Properties - guest lecture: Dr. Jeff Neaton
  4/3 Quantum Monte Carlo - guest lecture: Dr. Lucas Wagner
  4/8 Quantum Monte Carlo - guest lecture: Dr. Lucas Wagner
- **Other Topics**
  4/10 Survey of Computational Biology - guest lecture
  4/15 Computing the Mechanical Properties of Materials - guest lecture: Dr. Alex Greaney
  4/17 Modeling Growth and Synthesis of Materials
  4/22 Capturing Rare Events - guest lecture: Dr. Yosuke Kanai
- **Verification and Validation**
  4/24 How you know you're computing what you think you are, and how to assess whether it means anything
- **Connecting with Experiment**
  4/29 Ten Examples
  5/1 Simulating Liquids - Water
  5/6 Mystery Day
- **Final Projects**
  5/8 Class presentations: final projects
  5/13 Class presentations: final projects
  5/15 Class presentations: final projects