10.675 Computational Quantum Mechanics of Molecular and Extended Systems (Spring, 2001)
TR 11:00-12:30, 66-156

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Web address: http://web.mit.edu/10.675/www

Course Objectives:

• Learn a different approach to solving scientific and engineering problems: performing quantum mechanical calculations and understanding their scope, possibilities and limitations.
• Be able to perform calculations during your research at MIT, in Practice School, and in your future work.
• Gain a (partial) familiarity with the literature and be able to read it critically.
• Understand current research directions and possibilities.

Software:

Gaussian94 (Gaussian98): used to perform quantum mechanical calculations
Cerius2: GUI, used to create job files, run jobs, and visualize output
GaussView: GUI, used to create job files, run jobs, and visualize output

Hardware:

Project Athena: 46 SGI O2’s, 128 Mb memory
1-142 6
4-035* 20
66-080 10
W20-575 10

NCSA (National Computational Science Alliance):
SGI Origin 2000 (796 processors)

Your laboratory workstations, home PCs

Grading:

Homework 35%
Participation 25%
Final Project 40%