

## ISC 5225 Spring 2011

# Molecular Dynamics: Algorithms and Applications

## SYLLABUS

**Instructor** Sachin Shanbhag

488, Dirac Science Library (TR)

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**Class** DSL 152 (TR: 2.00-3:15)

**Text** None required. Class notes + web resources will suffice.

**References** “Understanding Molecular Simulation”, by Frenkel and Smith  
“The Art of Molecular Dynamics Simulation”, by D.C. Rapaport  
“Computer Simulation of Liquids”, Allen and Tildesley

**Resources** “Lectures in Molecular Simulation”, by David Kofke

<http://www.eng.buffalo.edu/~kofke/ce530/index.html>

“Molecular Simulation”, by Cameron Abrams

<http://www.pages.drexel.edu/~cfa22/msim/msim.html>

### Broad Course Outline

1. Introduction to Molecular Simulation
2. Simple MD (NVE)
3. Statistical Mechanics
4. Measurement, Statistics, Ensembles
5. Using molecular dynamics and visualization software
6. Molecular modeling (polymers, three-body potentials)
7. Advanced topics (free energy methods, parallelization, electrostatics and Ewald Summation)

**Grading** Assignments = 65% (equally weighted)

Mid-Term = 15%

Project = 20%

**Pre-requisites:** Instructor permission. Some programming or scripting experience (in any language) is assumed.

**University Attendance Policy:** Excused absences include documented illness, deaths in the family and other documented crises, call to active military duty or jury duty, religious holy days, and official University activities. These absences will be accommodated in a way that does not arbitrarily penalize students who have a valid excuse. Consideration will also be given to students whose dependent children experience serious illness.

**Academic Honor Policy:** The Florida State University Academic Honor Policy outlines the University's expectations for the integrity of students' academic work, the procedures for resolving alleged violations of those expectations, and the rights and responsibilities of students and faculty members throughout the process. Students are responsible for reading the Academic Honor Policy and for living up to their pledge to ". . . be honest and truthful and . . . [to] strive for personal and institutional integrity at Florida State University." (Florida State University Academic Honor Policy, found at <http://dof.fsu.edu/honorpolicy.htm>.)

**Americans With Disabilities Act:** Students with disabilities needing academic accommodation should:

- register with and provide documentation to the Student Disability Resource Center; and
- bring a letter to the instructor indicating the need for accommodation and what type. This should be done during the first week of class.

This syllabus and other class materials are available in alternative format upon request. For more information about services available to FSU students with disabilities, contact the:

Student Disability Resource Center  
874 Traditions Way  
108 Student Services Building  
Florida State University  
Tallahassee, FL 32306-4167  
(850) 644-9566 (voice)  
(850) 644-8504 (TDD)  
[sdrc@admin.fsu.edu](mailto:sdrc@admin.fsu.edu)

<http://www.disabilitycenter.fsu.edu>

**Syllabus Change Policy:** Except for changes that substantially affect implementation of the evaluation (grading) statement, this syllabus is a guide for the course and is subject to change with advance notice.