ME891 Molecular Modeling in Engineering: Methods and Applications

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Instructor: Prof. Nikolai Priezjev, EB2465, 432-9132, priezjev@egr.msu.edu;

Tu Th 4:10 PM - 5:30 PM, room# 1300 Engineering Building

Office Hours: Nikolai Priezjev (EB2465) Tu Th 5:30-6:30

Textbook: "Understanding Molecular Simulation: From Algorithms to Applications" by Daan Frenkel and Berend Smit, 2nd edition, Academic Press, San Diego, 2002. ISBN 0122673514. Two copies of the book are on reserve in the Engineering Library.
Suggested Reference Books:
"Computer Simulations of Liquids" by M. P. Allen and D. J. Tildesley, Clarendon, Oxford, 1987. Fortran Source Code
"The Art of Molecular Dynamics Simulation" by D. C. Rapaport, 2nd ed. Cambridge University Press, 2004.

Course Objective: This is an interdisciplinary, special topics graduate (and advanced undergraduate) level course aimed at students from engineering and materials science as well as physics and biochemistry. The objective of the course is to get experience in performing computer simulations and to apply numerical methods for sample problems.

Course Description: The course is an introduction to the theory and methods of classical molecular modeling as applied to contemporary research in engineering, physics and materials science. Topics include elementary statistical mechanics, Monte Carlo and molecular dynamics methods, techniques for generating different ensembles and calculating free energies and transport coefficients. Application areas for research projects include soft matter, fluids and solids.

For example, this lecture shows how the effect of surface tension at liquid-vapor interfaces can be explained at the atomic level and evaluated using molecular dynamics simulations.

Syllabus: The syllabus will include chapters from the required textbook, discussion of the case studies and research articles in computational materials science. Each student will lead a project on a topic of research or computational interest. Final report should be written up in a format of a research paper and include an introduction, description of a simulation model and parameter values, analysis of simulation results with figures, and conclusions. Supplementary materials will be posted on the Angel webpage. Interaction among students is encouraged but the final report has to written individually.

Prerequisites: Undergraduate thermodynamics, some programming experience in either C or Fortran.

Grading Scheme: The course grade is based on the final project.
