Course Meets: TR 4:30 – 5:45 P.M. Felgar 334

Instructor: Takumi Hawa, Assistant Professor
Office hours: TR noon – 1:30 P.M.
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Course Description: Intro to Kinetics
Intro to Statistical Mechanics and Thermodynamics
Molecular Dynamics Simulations
Monte-Carlo Simulations
Intro to MPI programming


Pre-requisites by Topic: Thermodynamics (AME 2213), Fluid Dynamics (AME 3153), and Programming (Fortran, C, C++, Matlab)

Course Objectives: To provide a solid background for senior undergraduates or graduate students in atomistic simulation methods.

To relate the theory and numerical methods to diverse nanoscience and nanotechnology applications.

To write a molecular dynamics and a monte-carlo simulation codes.
Grading Criteria:  
Homework 80%  Approx. final grade: 90 - 100 %  A  
  
Final Presentation 10%  80 - 89 %  B  
Final Report 10%  70 - 79 %  C  
  
60 - 69 %  D

Computer Usage:  
Require use of computer in homework assignments and the final project.

Remarks:  
1. The homework assignments, a computer project and a final presentation which you submit are expected to consist of your own work although discussions with your classmates and/or instructor are encouraged (Please use office hours).  
2. Homework and projects will be graded from 0 to 10.  
3. Homework will be available on the course webpage (www.ou.edu/mms/courses_f13g2.html).  
4. Travel plans should take into account that the last day of the class end at 6:30 PM on Tuesday, December 10, 2013.  
5. A computer project and a final report are due on Tuesday, December 10, 2013.