Computational Materials Science and Engineering
MSE 6140; MonWed 2:00-3:15pm, Room 299 Love

Instructors: Prof. Rampi Ramprasad (Love 366; ramprasad@gatech.edu)
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Objectives: This course aims to provide a broad understanding of a spectrum of modern state-of-the-art computational methods used in materials science and engineering. Lectures, case studies, demonstrations and hands-on lab exercises are planned to provide theoretical depth and a practical perspective on the role of modern computational methods in revealing process-structure-property relationships and in aiding the design/discovery of new materials.

Suggested Textbooks: (1) Ellad B. Tadmor and Ronald E. Miller: Modeling Materials: Continuum, Atomistic and Multiscale Techniques; (2) Richard Lesar: Introduction to Computational Materials Science; (3) Alexander Forrester, Andras Sobester, Andy Keane: Engineering Design via Surrogate Modelling: A Practical Guide

Grade: 3 Midterm Exams and + 2 Assignments (20% each)

Midterm Exam Dates: 9/11 (Ramprasad), 10/16 (Jang), 11/6 (Ramprasad)
Assignment Submission Due Dates: 10/16 (Jang), 12/6 (Deo)
Ramprasad Lectures: 8/19, 8/21, 8/26, 8/28, 9/4, 9/9, **9/11-Exam (7)**, 10/23, 10/28, 10/30, 11/4, **11/6-Exam (5)**,
Jang Lectures: 9/16, 9/18, 9/23, 9/25, 9/30, 10/2, 10/7, 10/9, 10/16, **10/21 -Exam (10)**
Deo Lectures: 11/11, 11/13, 11/18, 11/20, 11/25 **(5)**

No Classes: 9/2 Labor Day; 10/14-10/15 Fall Break; 11/27 Student Recess; 11/28,11/29 Thanksgiving Break;
Note: 12/2-12/3 Final Instructional Class Days; 12/4 Reading Day; 12/5-12/12 Final Exams

Syllabus

Part I: Atomistic Methods – Density Functional Theory — **Ramprasad**
1. Why Materials Modeling?
2. Quantum Mechanics & Density Functional Theory (DFT)
3. DFT in practice

Part II: Interatomic Interactions: Force Fields — **Jang**
1. Force Fields: Bonded Interactions
2. Force Fields: Non-Bonded Interactions

Part III: Modeling and Simulation Methods — **Jang**
1. Full-Atomistic Molecular Dynamics Simulation Methods
2. Coarse Grained Modeling and Simulation Methods

Part IV: Data-driven Methods: Informatics & Machine Learning — **Ramprasad**
1. What is machine learning?
2. Machine learning components: data, fingerprinting, learning
3. Machine Learning in materials science
4. Other advanced methods and materials design

Part V: Meso-scale & Macro-scale Methods — **Deo**
1. Intro to calphad and computational thermodynamics
2. Examples of thermocalc
3. Introduction to phase field method
4. Examples from MEMPHIS – phase field code of Sandia-CINT