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: Homework (20%), 3 Midterm Exams (20% each), Final Project (20%)
Midterm Exam Dates: 9/19 (R), 10/26 (J), 11/21 (R), 12/5 (D)
Final Project Presentations: 12/14 at 2:40 PM-5:30 PM

9/5 Labor Day
10/17-10/18 Fall Break
11/23 Student Recess
11/24 Thanksgiving Break
12/8-12/15 Final Exam

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: Atomistic Methods – Classical Approaches **Jang**

4. Classical Interatomic Potentials
5. Molecular Dynamics & Monte Carlo Simulations
6. The United Atom Method and Coarse Graining

Part III: Data-driven Methods: Informatics & Machine Learning **Ramprasad**

7. What is machine learning?
8. Machine learning components: data, fingerprinting, learning
9. Machine Learning in materials science
10. Other advanced methods and materials design

Part IV: Meso-scale & Macro-scale Methods **Deo**

11. Phase field modeling
12. Computational Thermodynamics
    Intro to calphad and computational thermodynamics
    Examples of thermocalc
    Introduction to phase field method
    Examples from MEMPHIS – phase field code of Sandia-CINT