Computational Materials Science and Engineering in University Education

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Computational Materials Science and Engineering Education: Trends and Needs

Why Should We Care?

- Every field, including MSE, can take advantage of the increasing computational resources to accelerate advances.
- Engineers: Trained personnel can help implement new approaches to engineering (e.g., ICME).
- Scientists: Widespread use of computational tools makes their scientific work more relevant to technology.
- Students: Common concepts in computational approaches – allows them to learn/use tools outside of MSE.
- Educators: Provides opportunities for "active learning" and virtual experiments of scientific concepts.

Integrated Computational Materials Education Summer School, June 11-22, 2012

Introduction and Philosophy

To address the challenges in integrating computational techniques into the undergraduate MSE curricula, the "Summer School for Integrated Computational Materials Education" was held at the University of Michigan in Ann Arbor, Michigan in 2011 and 2012. This Summer School is a two-week program that includes a "crash course" on computational materials science and engineering (CMSE) and focus sessions on educational modules that can be adopted into existing core courses. Specifically, we have targeted the introduction of computational tools into undergraduate-level thermodynamics, kinetics, mechanics, and physics of materials courses. We anticipate offering the Summer School again starting in 2014.

The application to participate is open to faculty, postgraduate researchers, and graduate students from MSE departments and programs in the U.S. Our approach is to "educate the educator." The Summer School participants (Fellows) learn both the theory and practical application of computational approaches in materials science and engineering, and then return to their home institutions to help integrate these techniques into the undergraduate curriculum. Each year approximately 20 Fellows from universities across the country have participated .

Approach and Schedule

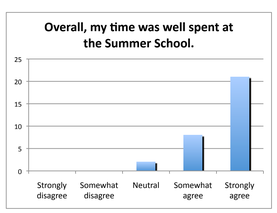
During the first week of the program, participants attend lectures about the theory behind the computational techniques by leading subject matter experts, as well as lectures on effective teaching techniques and success stories. They also gain hands-on experience during four instructor-led modules that introduce them to several popular computational materials science tools. During the second week, the format becomes participant-led, as the Fellows work through the modules again independently, then have the opportunity to practice teaching the modules themselves.

Schedule of Events

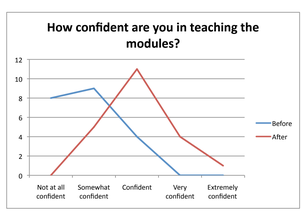
Date	Day	AM (Course Work)	PM (Computational Lab)
6/11	Monday	Program Orientation and Introduction Overview of CMSE (Katsuyo Thornton) Density Functional Theory (Mark Asta)	Welcome Luncheon at Noon Molecular Dynamics (Mark Asta) Monte Carlo & Kinetic Monte Carlo (Anton Van der Ven)
6/12	Tuesday	Computational Kinetics/Phase-Field Modeling (Jon Guyer) Computational Mechanics/FEM (Edwin Garcia)	Computational Orientation (Katsuyo Thornton/Larry Aagesen) Software Installation, Basics (Larry Aagesen/Katsuyo Thornton)
6/13	Wednesday	Computational Materials Design in Education (Greg Olson) Computational Thermodynamics (Paul Mason)	Module 1 (directed) Computational Thermodynamics (Paul Mason/Katsuyo Thornton/Larry Aagesen)
6/14	Thursday	Module 3 (directed) Computational Mechanics (Edwin Garcia/ Katsuyo Thornton/Larry Aagesen)	Module 2 (directed) Kinetics (Jon Guyer/Katsuyo Thornton/Larry Aagesen)
6/15	Friday	High Performance Computing Resources: Introduction (Katsuyo Thornton) Effective Teaching (Tershia Pinder-Grover)	Module 4 (directed) Density Functional Theory (Katsuyo Thornton/Larry Aagesen)
6/16	Saturday	(Students are expected to review materials over weekend)	Canoe Trip (optional) Argo Canoe Livery
6/17	Sunday	Scripting Workshop (Laura Bartolo)	(Students are expected to review materials over weekend)
6/18	Monday	Module 1 (self-directed) Computational Thermodynamics (Katsuyo Thornton/Mark Asta/Larry Aagesen)	Module 2 (self-directed) Kinetics (Katsuyo Thornton/Mark Asta/Larry Aagesen)
6/19	Tuesday	Module 3 (self-directed) Computational Mechanics (Katsuyo Thornton/Mark Asta/Larry Aagesen)	Module 4 (self-directed) Density Functional Theory (Katsuyo Thornton/Mark Asta/Larry Aagesen)
6/20	Wednesday	ICME (John Allison) Review/preparation time for Practice Teaching Sessions (Students)	Practice Teaching Sessions (Students, ETCs) Additional time to finish modules
6/21	Thursday	Practice Teaching Sessions (Students)	Practice Teaching Sessions (Students, ETCs) Research Presentations
6/22	Friday	Research Presentations & Research Q&A	Research Q&A/Departure

Surveys of Participants' Level of Confidence and Satisfaction 2011-2012

To provide a metric for the success of the Summer School, surveys were conducted of the participants' confidence in using the computational tools, confidence in teaching the material (for students and postdocs), and overall level of satisfaction with the Summer School. The surveys generally found significant increases in levels of confidence. In some cases the Modules were revised based on feedback from the surveys, which resulted in improved levels of confidence in that Module for the following year. 94% of participants reported they agreed or strongly agreed that their time had been well-spent at the Summer School.



2011-2012 Combined



2011-2012 Combined (students and postdocs)

Summer School Module Content

Each of the four modules emphasize concepts taught in the undergraduate Materials Science and Engineering curriculum. Below the basic goals each of module are described, followed by a detailed description of Module 1.

Module 1: . This module emphasizes basic concepts in thermodynamics at the undergraduate level, using the commercial software package Thermo-Calc, from Thermo-Calc Software Inc. Using basic thermodynamic principles coupled with free energy databases, it can calculate phase stability and composition. Several exercises walk participants through how to use the software to solve real-world engineering problems.

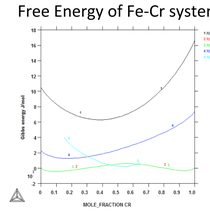
Module 2: The focus of the module is teaching the students to solve the diffusion equation numerically. This module emphasizes concepts usually encountered in an undergraduate kinetics of materials course. This module uses FiPy, an open-source partial differential equation solver, developed at the Center for Computational Materials Science at the National Institute for Standards and Technology (NIST).

Module 3: This module is aimed at teaching concepts encountered in mechanics of materials courses. The finite element method is used to solve mechanics problems numerically using OOF2 software developed at at the Center for Theoretical and Computational Materials Science and the Information Technology Laboratory at NIST.

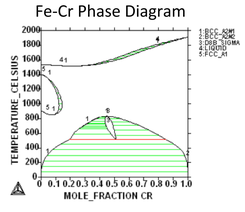
Module 4: The final module introduces students to density functional theory (DFT) and how it can be applied to solve problems typically found in an advanced undergraduate-level physics of materials course. It uses Quantum Espresso software for the DFT calculations, running on the nanoHUB, a web-based interface for educational software in science and engineering.

Module 1 Detail: Computational Thermodynamics

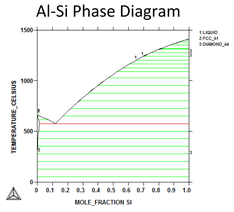
Free Energy of Fe-Cr system



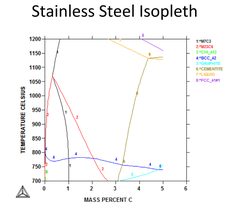
Fe-Cr Phase Diagram



Al-Si Phase Diagram



Stainless Steel Isopleth



Module 1 begins with an instructor-led walk-through of how to use Thermo-Calc to plot Gibbs free energy versus composition for the Fe-Cr system, calculate the Fe-Cr phase diagram, and an isopleth for a multi-component system. Following the walk-through, participants are given a set of exercises to complete independently, with instructor assistance available. Exercises include:

1. Plotting Gibbs free energy versus composition for the Cu-Ni system, and using the plot to determine the stable phases. This is used to reinforce conceptual understanding of the criteria for phase stability.
2. Calculating phase boundaries at important points for the Al-Si eutectic system, and plotting these points on a phase diagram. This exercise helps understand how phase diagrams are constructed. Plotting an isopleth for addition of Mg teaches how to use Thermo-Calc to determine phase stability.
3. The final exercise is based on a real-world engineering problem using Thermo-Calc to optimize the properties of a martensitic stainless steel. Fellows use phase stability calculations to determine how carburization can increase hardness at the surface, while understanding why corrosion resistance is simultaneously reduced. Participants need to optimize concentration to balance these properties. (Exercise is based on T. Turpin, J. Dulcy, M. Gantois, *Met. Trans. A*, 36A, 2751 (2005).)

Integrated Computational Materials Education at the University of Michigan

Integrated Computational-Experimental Laboratory (2nd Semester of Junior Year)

At the University of Michigan, all undergraduate students have been introduced to computational tools and techniques through an innovative laboratory course that combines computation and experiments. The laboratory setting, which allows four consecutive hours during which students familiarize themselves with new concepts and apply them to examine complex materials science problems, was found to be ideal for introducing computational approaches. The materials used are in part based on the Summer School described above. The examples of laboratory modules are described below.

Experimental Verification of Thermo-Calc (Microstructure analysis and phase equilibrium): Students obtained micrographs of Al-Si alloys with different compositions and processing conditions, and observed the changes of microstructure and phase fractions. Quantitative analysis of the phase fraction was performed via a software, Image-J. The students also performed Thermo-Calc calculations of phase equilibria of these alloys. They analyzed the results and developed insights into cast Al alloys. Then, the experimental data and computational predictions were compared, and agreements and disagreements were discussed.

Nucleation and Growth Modeling using MATLAB (Phase field modeling): In this module, the students were given a refresher on MATLAB programming and an introduction to finite difference methods in the first week. In the second week, they were asked to write a simulation code based on the phase field model, which is a combination of thermodynamics and kinetics of materials. While this module posed a significant challenge to students, and nearly all of them had no experience in developing a simulation code, all of them were able to complete the code while in the lab. The module also contained questions based on simulation results that illustrates the concept of nucleation and growth as well as spinodal decomposition.

Computational Approaches in Materials Science & Engineering (Senior Year)

This is a stand-alone course that covers the concepts and application of computational MSE approaches in much more depth. While this is not a required course, many students select this course after being introduced to computational MSE in the Junior Laboratory, described above. The course is designed to offer a balance between breadth and depth, between fundamentals and tools, and the needs of those entering industry or continuing in academia. The students gain expertise in computational MSE tools while developing further understanding of materials science. The final project provides the "sandbox" in which they can apply a method to a problem of interest.

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