ICME and the MGI at Northwestern

Lincoln J. Lauhon
Associate Chair, Director of Graduate Studies

From the 2008 NRC report on ICME:

Recommendation 8: The **University Materials Council (UMC)**, with support from materials professional societies and the National Science Foundation, should develop *a model for incorporating ICME modules into a broad spectrum of materials science and engineering courses*. The effectiveness of these additions to the undergraduate curriculum should be assessed using ABET criteria.

Northwestern Materials Science and Engineering

Chair: Michael J. Bedzyk

- **Research:** 22.5 FTE (11 non-MSE PhD)
- **Graduate Programs:** 160 PhD, 20 MS
- **Undergraduate Programs:**
    - ~70 BS in MSE (15-20 majors per year)
    - ~8 BS in Materials Science (2-3 per year)

Historical View of MGI Related Activities

Activity	Date
Computational Materials Design as capstone experience.	1989
Integrating computation and design in the undergraduate curriculum.	1994-
Graduate courses in computational materials science.	2000-
Graduate cluster program in Predictive Science and Engineering Design.	2009
MS Certificate Program in ICME	2011

Outline

- MSE Undergraduate Curriculum
- Approach to integrating computation throughout the undergraduate curriculum
- Computational Materials Design Capstone
- Graduate Level Initiatives
    - Grad Electives in Computational Materials Science
    - Cluster Program in Predictive Science and Engineering Design
    - MS Certificate Program in ICME

Characteristics of Core Undergrad Classes

- All courses have lecture components.
- Physical laboratory activities are integrated into courses (no independent lab courses).
- ***Computational activities are integrated into courses.***
- Approximately half of courses include evaluation of a final project.

MSE Undergraduate Curriculum*

Capstone design project, research experience	**390**, 396
Characterization of Materials and Processes	361, **391**
Origins of Physical Properties Mechanical, Electronic	**332**, 351
Origins of Physical Structure Thermodynamics, Kinetics, Defects, Microstructure	331 314, **315, 316**

*Partial list

http://www.matsci.northwestern.edu/courses/index.html

Examples of Computation

***Demonstrations** illustrating basic principles*

- **Thermo-Calc** phase diagrams for comparison with cooling curves measured in lab.
- **DICTRA** diffusion curves for comparison with carburization experiments.
- **MATLAB** computation of equilibrium crystal shapes based on surface energies.
- DFT (**PWSCF**) calculation of elastic constants for comparison with ultrasonic testing.

Examples of Computation

*Using tools in **analysis** and **design***

- Mechanical Behavior of Solids (MSE 332)
  - 4 week experimental project simulating industrial R&D investigation- evaluation for application
  - 4 week FEA project using **Abaqus**- model structures
- Process Design (MSE 391)
  - Student-initiated group projects apply principles of statistical process design.
  - Minitab used to lay out experimental design and to perform statistical analysis, e.g., optimization of processing parameters.

Approach to Integration

- Tools should help establish a fundamental understanding of scientific principles.
- Introduce some tools that can handle real (i.e. multi-component) systems and interface with databases (Materials Genome).
- Emphasize model-based prediction.
- Projects initiated and tools acquired can be incorporated into capstone MSE 390 experience.

Outline

- MSE Undergraduate Curriculum
- Approach to integrating computation throughout the undergraduate curriculum.
- Computational Materials Design Capstone
- Graduate Level Initiatives
  - Grad Electives in Computational Materials Science
  - Cluster Program in Predictive Science and Engineering Design
  - MS Certificate Program in ICME

MSE 390: Materials Design (Capstone)

- Analysis and control of microstructures.
- Quantitative process-structure-property-performance relations with case studies.
- Computer lab for modeling multicomponent thermodynamics and transformation kinetics.

MSE 390 Computational Labs

Lab 1. CES Ashby Materials Selection Software: Formulating Design Objectives

Lab 2. TCW: Basic CALPHAD Calculations

Lab 3. CMD1: TCC-based Design Modeling

Lab 4. CMD2: Model Integration in Parametric Design

Lab 5. DICTRA/PrecipiCalc: Dynamics Simulation

Spring 2012 Projects

I. **Civil Shield (EDC)**
Client: ONR, DHS, Trinity R
Advisor: Dr. Zack Feinberg
Team: Ma, Maethasith, Richardson, Schwenker, Zhao

II. **Earthquake Steel**
Client: ArcelorMittal
Advisor: George Fraley
Team: Cool, Gross, Rawlings, Tran

III. **FSW Joinable Aluminum**
Client: Boeing, Ford
Advisor: Ricardo Komai
Team: Brodnik, McGinnis, Pai, Ricks

IV. **HP Magnesium**
Client: ARO, GM, DOE
Advisor: Dr. Dennis Zhang
Team: Han, Na, Park

V. **TRIP Titanium**
Client: ONR
Advisor: Jiayi Yan
Team: Savoie, Wengrenovich

VI. **HP Shape Memory Alloy (EDC)**
Client: Medtronic, GM
Advisor: Dana Frankel
Team: Jin, Kadleck, Poupard, Yoo

Observations

- Integration of research and education is a hallmark of the program.
- The curriculum design is top-down, but computational tool introduction bottom up.
- Capstone design course serves many roles and constituencies.

Outline

- MSE Undergraduate Curriculum
- Approach to integrating computation throughout the undergraduate curriculum.
- Computational Materials Design Capstone
- Graduate Level Initiatives
  - Grad Electives in Computational Materials Science
  - Cluster Program in Predictive Science and Engineering Design
  - MS Certificate Program in ICME

Graduate Computational MatSci: Principles

- Courses provide a scientific foundation for computational tools to train future developers.
- Courses introduce widely used methods to train future users.
- The curriculum is comprehensive, from atomistic to continuum calculations.

Grad-Level Computational MatSci

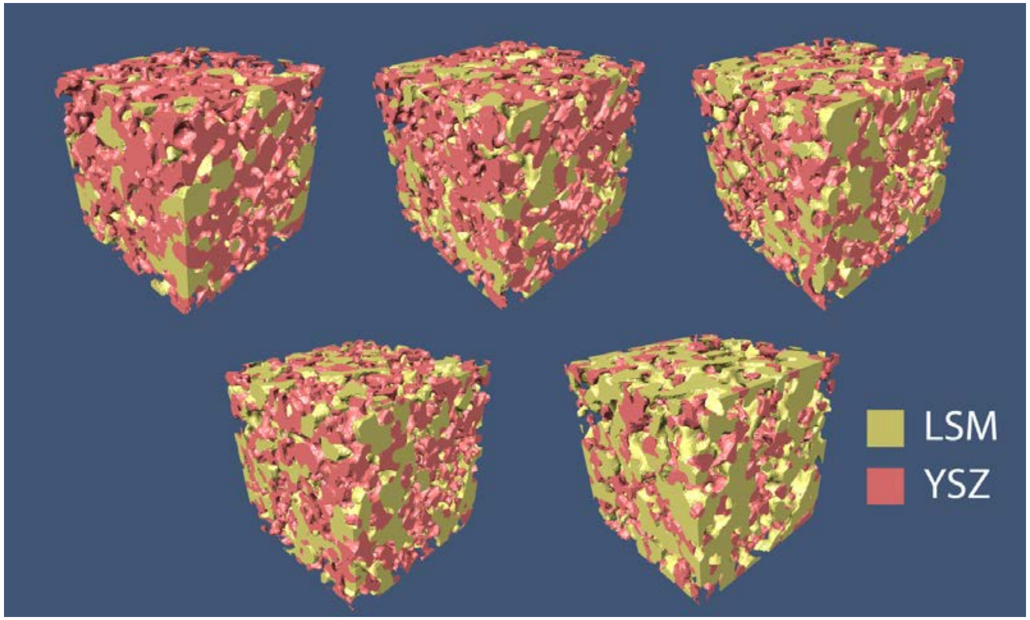
Course	Title	Content	Developer
458	Atomic-Scale Computational Materials Science	Density Functional Theory (PWSCF) , Monte Carlo, Molecular Dynamics (LAMMPS)	Chris Wolverton
411	Computational Materials Science at the Mesoscale	Multi-Component Diffusion, Phase Field, Multi-Particle Models	Peter Voorhees
495	Modeling of Soft Materials (w/ESAM)	Monte Carlo and Molecular Dynamics, mathematical methods underlying modeling	Erik Luijten

451: Quantum Mechanics

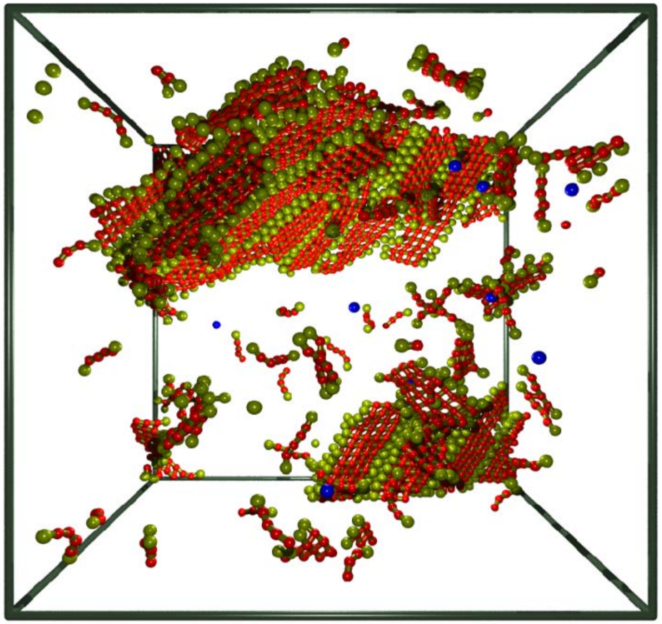
495: Statistical Mechanics

Computational Projects in 458*

3-D Reconstruction of Solid Oxide Fuel Cells with Monte Carlo Simulation



Molecular Simulation of Self-Assembling Organogelators



*Students are given time on cluster.

Outline

- MSE Undergraduate Curriculum
- Approach to integrating computation throughout the undergraduate curriculum.
- Computational Materials Design Capstone
- Graduate Level Initiatives
  - Grad Electives in Computational Materials Science
  - Cluster Program in Predictive Science and Engineering Design
  - MS Certificate Program in ICME

Predictive Science & Engineering Design (PS&ED)

Graduate Interdisciplinary Cluster Program founded in 2009
Directors: Wei Chen, Greg Olson & Wing Kam Liu

- Discover, develop, and teach the common principles and techniques underlying PSED
- Engage faculty in collaborative, interdisciplinary research to pursue new funding opportunities
- Provide an alternative intellectual community with “dual citizenship”
- Enhance the technical depth of design initiatives

http://psed.mccormick.northwestern.edu/

PSED Curriculum Structure

- **Core Area 1:** PSED Seminar
  - Introduces common principles and techniques underlying PSED.
  - Initiate interdisciplinary projects related to the current design focus of PS&ED.
- **Core Area 2:** Modeling, Simulation, and High Performance Computing
- **Core Area 3:** Computational Design Methods

http://psed.mccormick.northwestern.edu/

ICME MS Certificate Program

	F	W	S
Required Core	MSc 401 Analytical & Statistical Thermodynamics PSED 510-1 (0.5) ICME Seminar	MSc 408 Phase Transformations in Materials MSc 458 Computational Materials	MSc 390 Materials Design PSED 510-2 (0.5) ICME Seminar
Recommended Electives	MSc 391 Process Design CEE327/ME 365 Introduction to FEM ME 341 Computational Methods for Engineering Design (or ME 441 Engineering Optimization for Product Design & Manufacturing)	MSc/ESAM 495 Introduction to Statistical Mechanics ME/CEE 426-1 Computational Mechanics I ME 366 Finite Elements for Design & Optimization	MSc 406 Mechanical Properties of Materials ME/CEE 426-2 Computational Mechanics II Phys 450 Advanced Computational Condensed Matter Physics

Required for Certificate

Additional Tools

http://www.matsci.northwestern.edu/docs/ICME_Brochure%205-27-11.pdf

ICME Education: Dimensions of Integration

- **Design-Enabling Multidisciplinary Science**

  -Materials Science, Applied Mechanics, Quantum Physics
- **Research & Education**

  -Grad/Undergrad Hierarchical Coaching Infrastructure
- **Science-Based Engineering**

  -Contextual Science within Systems Framework; V&V/UQ
- **Techmanities Education**

  -Contextual Analysis & Creative Synthesis
- **Accelerated Qualification & Implementation**

  -Probabilistic, materials-aware component simulation
- **Concurrent Design of Materials/Devices**

Historical View of MGI Related Activities

Activity	Date
Computational Materials Design as capstone experience.	1989
Integrating computation and design in the undergraduate curriculum.	1994-
Graduate courses in computational materials science.	2000-
Graduate cluster program in Predictive Science and Engineering Design.	2009
MS Certificate Program in ICME	2011

Observations on Integration @ NU

- Integration of research and education is a hallmark of the program.
- Computational resources have been introduced in a bottom-up fashion.
- Content and tools are important, but human infrastructure is the most important element in teaching the materials **design** process.

Challenges & Opportunities

- Hiring outstanding academic researchers who are qualified to mentor students in engineering
- Supporting the infrastructure
  - Cadre of PhD students who can mentor new students in academic research and ICME practices.
  - Selecting and paying for the tools needed to practice ICME.
- Classroom to CO-OP continuum.

For Further Info

- Prof. Lincoln Lauhon, Assoc. Chair
  - lauhon@northwestern.edu
- Dr. Kathleen Stair, Asst. Chair: laboratories and undergraduate curriculum.
- Prof. Greg Olson: ICME, design in engineering curriculum