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

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Outline

• MSE Undergraduate Curriculum
• Approach to integrating computation throughout the undergraduate curriculum
• Computational Materials Design Capstone
• Graduate Level Initiatives
  o Grad Electives in Computational Materials Science
  o Cluster Program in Predictive Science and Engineering Design
  o 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 332, 351
Mechanical, Electronic

Origins of Physical Structure 331
Thermodynamics, Kinetics, Defects, Microstructure 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.
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MSE 390: Materials Design (Capstone)

- Analysis and control of microstructures.
- 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.
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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

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

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.
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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

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

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**
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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
  o Cadre of PhD students who can mentor new students in academic research and ICME practices.
  o Selecting and paying for the tools needed to practice ICME.

• Classroom to CO-OP continuum.
For Further Info

• Prof. Lincoln Lauhon, Assoc. Chair
  o lauhon@northwestern.edu

• Dr. Kathleen Stair, Asst. Chair: laboratories and undergraduate curriculum.

• Prof. Greg Olson: ICME, design in engineering curriculum