

# Integrated Computational Materials Engineering in the Materials Science and Engineering Curriculum

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Special thanks to Katsuyo Thornton, University of Michigan

The logo for the University Materials Council features a horizontal bar with a colorful, abstract background of blue, green, and purple. The text "University Materials Council" is written in a bold, white, sans-serif font across the center of the bar.

**University Materials Council**

# Outline

- 1. What is (and who are) the UMC?**
2. ICME charge to the UMC
3. The workshop, findings, and recommendations.
4. Plans for the future.

# What is the University Materials Council (UMC)

The University Materials Council is composed of Department Heads, Chairpersons, Directors, and group leaders from academic programs in the materials field in U.S. and Canadian universities. (The UMC consists of approximately 100 departments and programs )

The Goals of the UMC are to:

- To help define and influence new directions for the field
- To promote the field
- To strengthen the educational component of the field
- To foster improvements in the number and quality of students in MSE

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**University Materials Council**

# What does the UMC do?

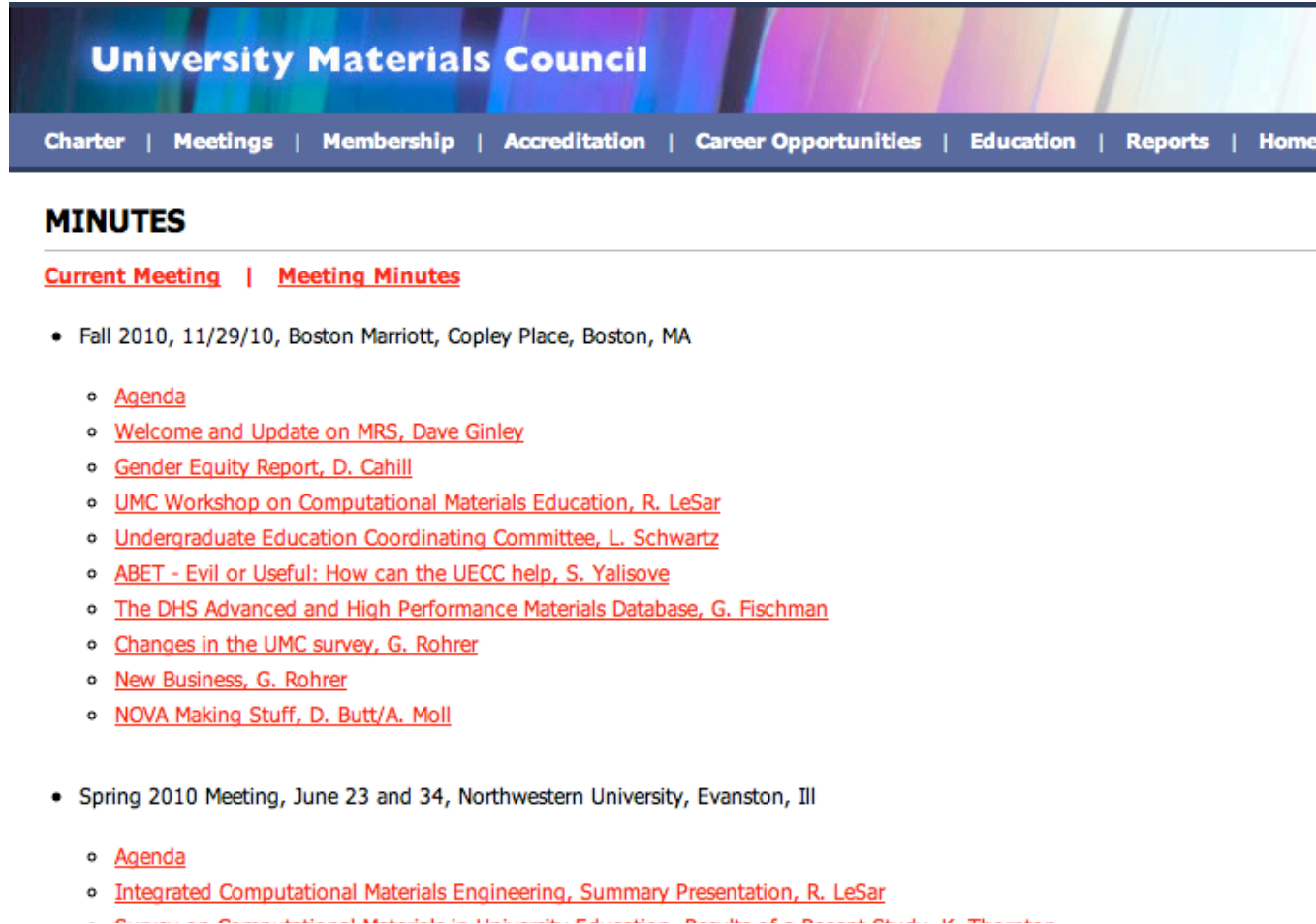
**We meet twice annually**

**UMC meetings are a forum for department heads/chairs/directors of materials programs to share best practices in areas such as:**

- **student recruitment**
- **ABET accreditation**
- **emerging research areas**
- **ideas for curricular implications of the latest materials studies,**
- **special topical workshops**
- **research funding for MSE**
- **other issues of interest to the academic community.**

# The meeting minutes are available to all on our website

<http://www.umatcon.org/files/minutes.shtml>



The screenshot shows the website for the University Materials Council. At the top, there is a navigation bar with the following links: Charter | Meetings | Membership | Accreditation | Career Opportunities | Education | Reports | Home. Below the navigation bar, the page is titled "MINUTES". Underneath, there are two sub-sections: "Current Meeting" and "Meeting Minutes". The "Current Meeting" section lists two meetings: a Fall 2010 meeting on 11/29/10 in Boston, MA, and a Spring 2010 meeting on June 23 and 24 at Northwestern University in Evanston, Ill. Each meeting has a list of agenda items, including "Agenda", "Welcome and Update on MRS, Dave Ginley", "Gender Equity Report, D. Cahill", "UMC Workshop on Computational Materials Education, R. LeSar", "Undergraduate Education Coordinating Committee, L. Schwartz", "ABET - Evil or Useful: How can the UECC help, S. Yalisove", "The DHS Advanced and High Performance Materials Database, G. Fischman", "Changes in the UMC survey, G. Rohrer", "New Business, G. Rohrer", and "NOVA Making Stuff, D. Butt/A. Moll".

**University Materials Council**

Charter | Meetings | Membership | Accreditation | Career Opportunities | Education | Reports | Home

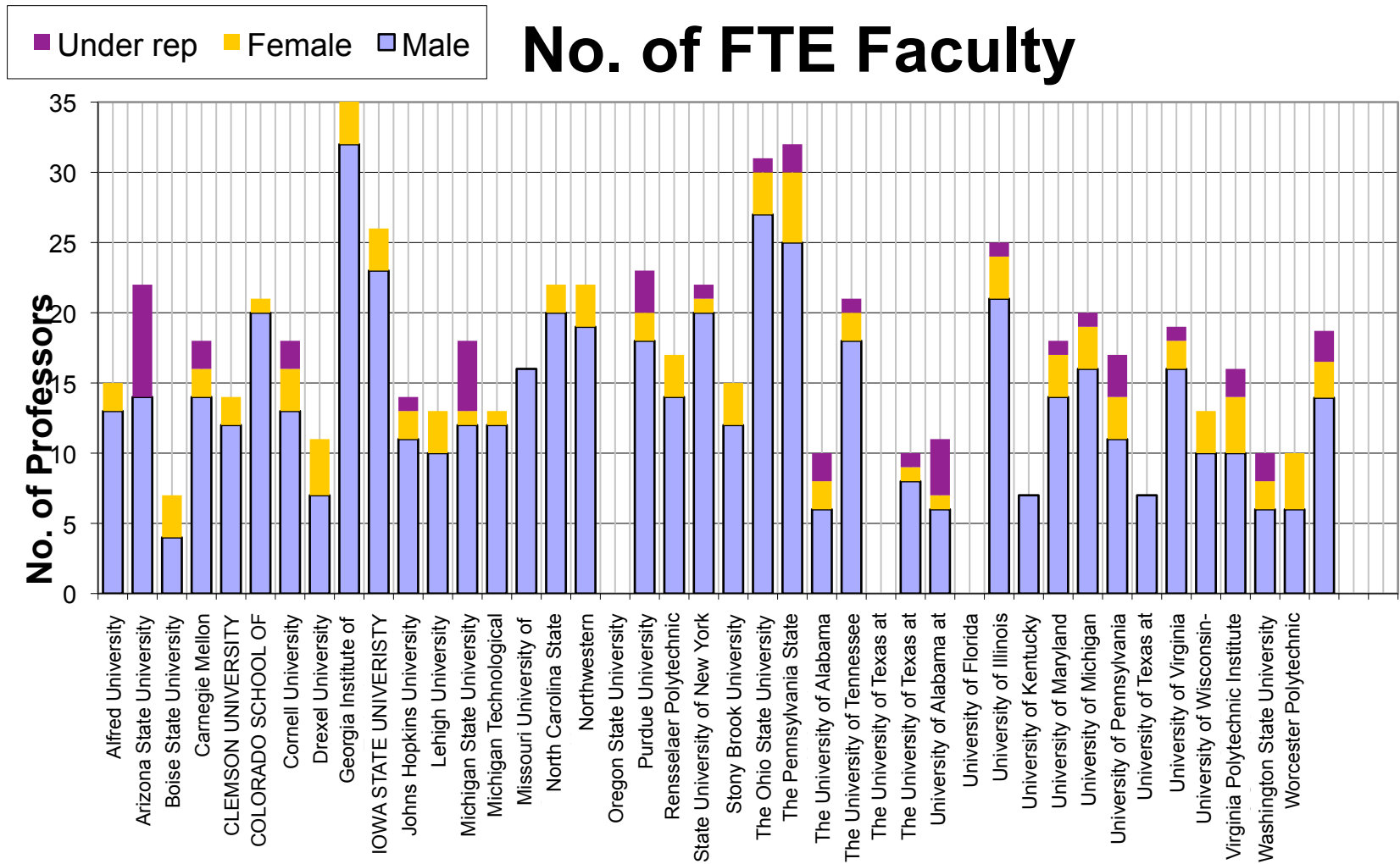
## MINUTES

[Current Meeting](#) | [Meeting Minutes](#)

- Fall 2010, 11/29/10, Boston Marriott, Copley Place, Boston, MA
  - [Agenda](#)
  - [Welcome and Update on MRS, Dave Ginley](#)
  - [Gender Equity Report, D. Cahill](#)
  - [UMC Workshop on Computational Materials Education, R. LeSar](#)
  - [Undergraduate Education Coordinating Committee, L. Schwartz](#)
  - [ABET - Evil or Useful: How can the UECC help, S. Yalisove](#)
  - [The DHS Advanced and High Performance Materials Database, G. Fischman](#)
  - [Changes in the UMC survey, G. Rohrer](#)
  - [New Business, G. Rohrer](#)
  - [NOVA Making Stuff, D. Butt/A. Moll](#)
- Spring 2010 Meeting, June 23 and 34, Northwestern University, Evanston, Ill
  - [Agenda](#)
  - [Integrated Computational Materials Engineering, Summary Presentation, R. LeSar](#)
  - [Summary Computational Materials University Education Results of Recent Studies, M. Thornton](#)

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# The UMC also collects and distributes statistical data about MSE departments



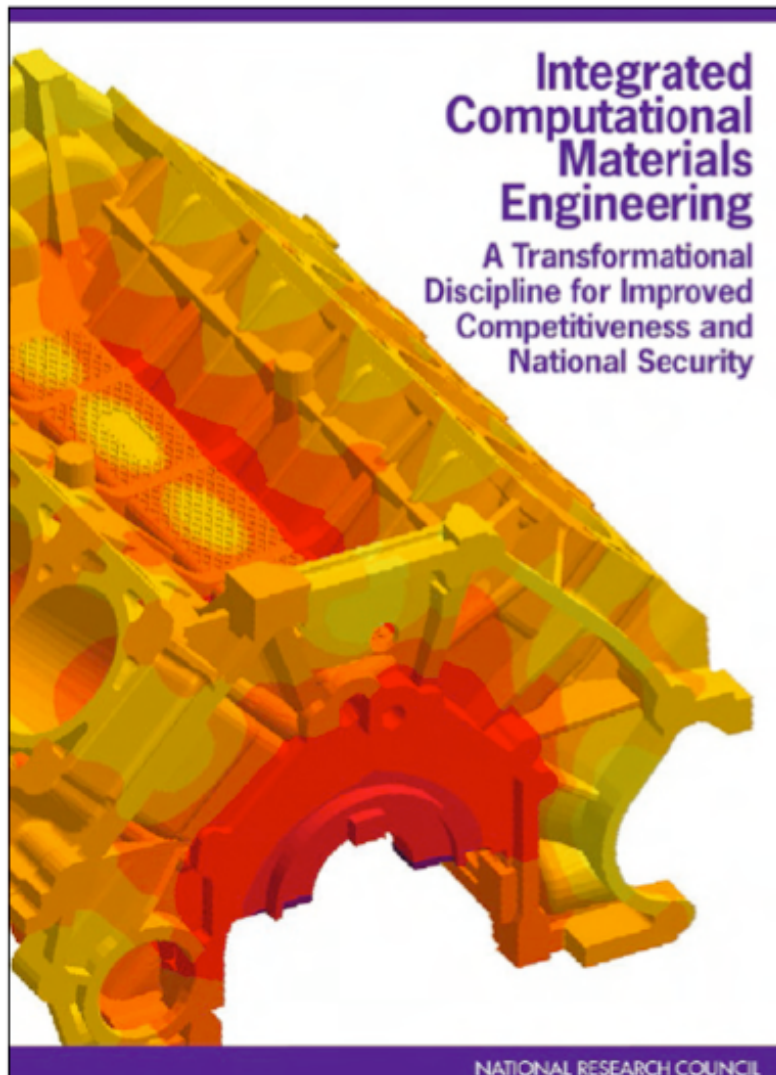
# Some Recent Activities of the UMC

- **Gender equity workshop**
- **ICME workshop**
- **Discussion of Materials Genome Initiative with OSTP**
- **Memoranda of Understanding with MRS and TMS provides resources and staff assistance for UMC activities and a framework for collaboration**

# Outline

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# ICME Study: 2008



## Selected conclusions:

- For ICME to succeed, it must be embraced as a discipline by the materials science and engineering community
- Industrial acceptance of ICME is hindered by the scarcity of materials engineers trained to use them.

# Charge to the UMC

**“The committee considers that the UMC is in a unique position to influence curricula and change the culture of MSE academic institutions and that it could take an active role in promoting ICME and the curricular changes that support improvements in the computational ability of the students who graduate from their departments.”**

**Response so far:**

**At the June 2009 UMC meeting in Arlington, VA, we voted to sponsor a workshop - how best to teach computational materials within the undergraduate and graduate curricula**

- **Richard LeSar was asked to chair that meeting**
- **The organizing committee was made up of Peter Voorhees, Northwestern University, Susan Sinnott, University of Florida, Alejandro Strachan, Purdue University**

# Status of Computational MSE Education

Feature Computational Materials Education

## Computational Materials Science and Engineering Education: A Survey of Trends and Needs

K. Thornton, Samantha Nola, R. Edwin Garcia, Mark Asta, and G.B. Olson

Thornton K, Nola S, Garcia RE, Asta, M, Olson, GB, "Computational Materials Science and Engineering Education: A Survey of Trends and Needs," JOM 61 (2009) 12-17.

Table I. Tools Cited by Employers, Categorized and Ranked by the (Normalized) Frequency of Cites, along with Corresponding Results from the Computational Faculty Survey

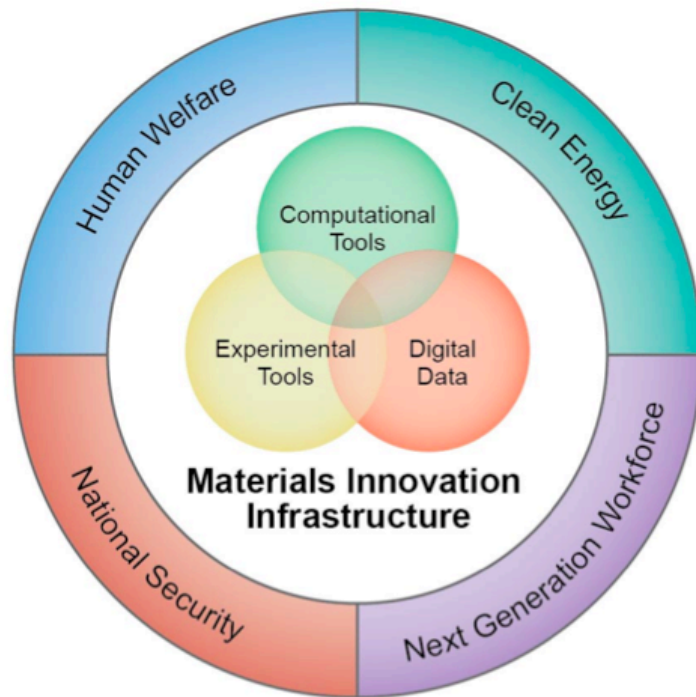
Category	Example	Employer	Faculty*
Mechanics (mostly FEA)	DEFORM, ABAQUS	80%	14%
Thermodynamics (CALPHAD)	ThermoCalc, Pandat	53%	7%
Density Functional Theory	VASP, ABNIT	47%	21%
Programming Language/Integration	Matlab, Fortran, iSight	40%	43%
Casting	ProCAST, MAGMAsoft	40%	—
Molecular Dynamics/ Monte Carlo	LAMMPS	27%	14%
Fluid Flow/ Heat Transfer	COMSOL, Fluent	20%	7%
Diffusion/ Microstructural Evolution	DICTRA, PrecipiCalc, JMatPro	20%	—
Statistics	Informatics	13%	7%
Materials Modeling Suite	Materials Studio	13%	—
General Visualization	Mathematica, Tecplot	7%	29%
General Data Processing	Spreadsheet	7%	21%
Special Purpose	K-Flow, WARP 3D	7%	—
Materials Selection	CES Materials Selector	—	36%
Crystallography	CaRIne	—	7%

\*Some of the responses did not provide specific software/categories, and therefore we expect some degree of undercounting in this data.

**This study suggested that the views of educators are out of step with industry.**

**In addition, faculty are generally aware of resources, but do not use them and this indicates a barrier.**

# Materials Genome Initiative



## 3. Equipping the Next--Generation Materials Workforce

Success of this initiative cannot be measured by the tools alone, but rather by the pervasiveness of their use and the outcomes they enable. **Equipping our next- generation workforce with the tools and approaches necessary to achieve our national goals will require stakeholders in government, academia, and industry to embrace the scope and contents of the materials innovation infrastructure. This will be achieved with a focus on education, workforce development, and a generational shift toward a new, more integrated approach to materials development.**

**University Materials Council**

# Outline

1. What is (and who are) the UMC?
2. ICME charge to the UMC
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4. Plans for the future.

# Goals of the UMC Workshop

- **to discuss need for increased focus on computational materials science and engineering in the MSE curriculum**
- **to develop suggestions for a computational materials curriculum in undergraduate and graduate education**
- **to identify resources that could be shared between departments**

# UMC Workshop on ICME Education

23-24 June 2010, Northwestern University, 28 participants

<b>Carnegie Mellon University</b>	<b>Purdue University</b>	
<b>Case Western University</b>	<b>Rensselaer Polytechnic Institute</b>	
<b>Clemson University</b>	<b>Stony Brook</b>	
<b>Cornell University</b>	<b>University of Michigan</b>	
<b>Drexel University</b>	<b>University Alabama, Birmingham</b>	
<b>Illinois Institute of Technology</b>	<b>University of Delaware</b>	
<b>Iowa State University</b>	<b>University of Cincinnati</b>	
<b>Johns Hopkins University</b>	<b>University of Florida</b>	
<b>Kent State University</b>	<b>University of Illinois</b>	
<b>Lehigh University</b>	<b>University of Kentucky</b>	
<b>North Carolina State University</b>	<b>University of Maryland</b>	
<b>Northwestern University</b>	<b>University of Pennsylvania</b>	
<b>Ohio State University</b>	<b>University of Toronto</b>	
<b>Princeton University</b>	<b>Virginia Tech</b>	

**University Materials Council**

# Agenda of the UMC Workshop

- discussion of ICME - LeSar (ISU) and Allison (Michigan)
- results of recent survey of CMSE in MSE curricula - Thornton (Michigan)
- educational and computational resources - Manual (Florida) and Strachan (Purdue)
- vignettes - Olson (Northwestern), Lundstro (Purdue), and Bartolo (Kent State)

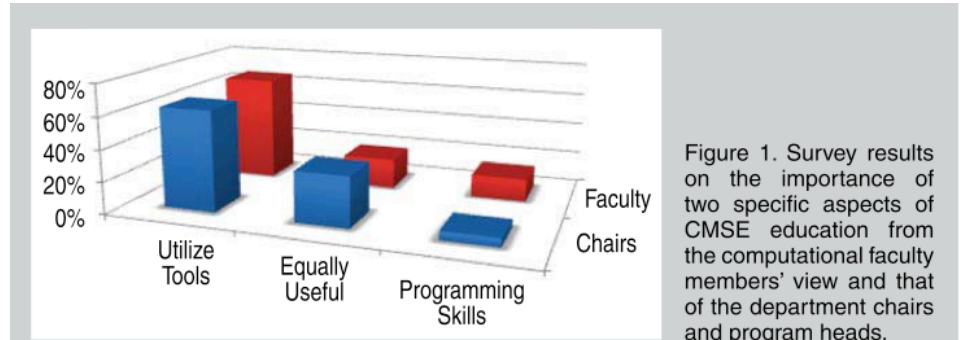
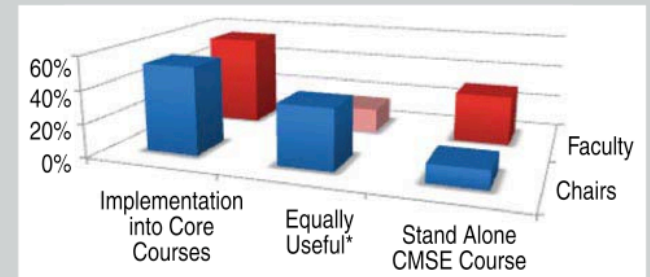


Figure 1. Survey results on the importance of two specific aspects of CMSE education from the computational faculty members' view and that of the department chairs and program heads.

Figure 2. Survey responses on how CMSE should be implemented into undergraduate MSE education, obtained from the same two groups. \*"Equally useful" option was omitted for the computational faculty survey, but some respondents wrote in this option (shown in light red).



Thornton K, Nola S, Garcia RE, Asta, M, Olson, GB, "Computational Materials Science and Engineering Education: A Survey of Trends and Needs," JOM 61 (2009) 12-17.

## Findings (1)

**There was a uniform consensus that MSE Departments need to include more computational materials science and engineering in both undergraduate and graduate curricula.**

**There is no common approach.**

**Some programs include modeling within existing classes, some have specialty classes, and some do both.**

**Most departments have had recent or ongoing efforts to evaluate and reform curriculum to be consistent with ICME**

## Findings (2)

there is no consensus on modeling platforms (e.g., MATLAB, Mathematica, ...), codes, strategies, etc.

there was some discussion on whether it should be CMS, CME, CMSE, ICME, but the group is content with ICME

# Challenges

- **There is little uniformity in current practice**
- **Many different opinions on the best way to include computation in the curriculum**
- **Many departments may not have local expertise to teach the material**
- **We need a central warehouse of computational resources to avoid duplication of efforts and to ensure some uniformity**

# Still to come

## Written report based on findings from working groups

Two working groups were identified to make concrete recommendations about:

- how to use computation to enhance the materials curriculum
- development and sharing of common computational resources, e.g.,

# Preliminary Recommendations & Example Actions

## **Coordinating Resources and Efforts in Developing Cyberinfrastructure for Education**

- TMS Working Group under the ICME Committee is developing specific plans.
- Survey: a list of resources is being collected and specific examples of resources that can be easily used to teach computation in MSE.
- NanoHUB, MatDL/MatForge

## **Supporting the Education of Educators to Increase Resource Utilization**

- “Summer School for Integrated Computational Materials Education,” University of Michigan in Ann Arbor, Michigan, July 18-29, 2011, led by Katsuyo Thornton, 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. (See Thornton’s poster for details.)
- Conference-based tutorials: One of the modules will be presented in a tutorial form at TMS.

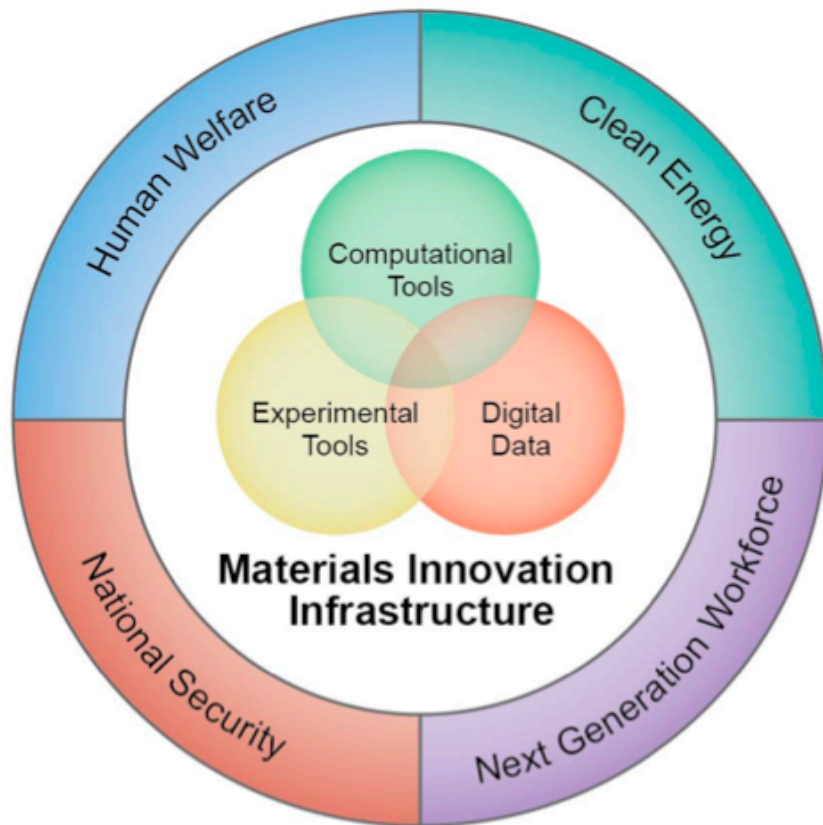
## **Coordinating and Facilitating Forums for Continuing Discussion**

- Laura Bartolo and Jim McGuffin-Cawley (Chair of MSE at Case Western Reserve University) are co-chairing the half-day symposium on ICME & Education at TMS 2012.

# Outline

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# Plans for the future are framed by the Materials Genome Initiative



### 3. Equipping the Next--Generation Materials Workforce

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**Equipping our next- generation workforce with the tools and approaches necessary to achieve our national goals will require stakeholders in government, academia, and industry to embrace the scope and contents of the materials innovation infrastructure. This will be achieved with a focus on education, workforce development, and a generational shift toward a new, more integrated approach to materials development.**

# Challenges

- 1. There is a need to change the way engineers are educated. Materials engineers rarely think about the components that materials are used in. Applied engineers (Mechanical, Electrical, Chemical) consider materials in components as having static, uniform, qualified properties. Synthesis of materials development and component design will require different educational practices.**
- 2. The necessary tools must be accessible to institutions and students.**
- 3. Knowledge of available materials must be archived and widely available.**
- 4. The topic of innovation must be included in the curriculum.**

# Goals for UMC

- 1. Engage engineering education administration and other academic units in this new approach to innovation. We must take responsibility for transforming the educational program.**
- 2. The next generation of leaders and innovators will have to understand the challenges and payoffs of ICME. We will incorporate modules throughout the curriculum and especially in capstone design classes to achieve this goal.**
- 3. The UMC will invest its resources, with the professional societies, in promoting ICME education. Interactions with TMS links us to traditional industries and interactions with MRS links us to emerging industries.**

# Goals for UMC

4. Many UMC members are from industry and many departments have industrial advisory boards. We will use these links to engage industry.
5. We will work with TMS to populate the ICME educational repository.
6. Seek NSF funding for a major initiative to transform Engineering education is a way consistent with ICME
7. Support the summer school in ICME Education

# Summary and Conclusions

**Materials Education in North America is carried out by the member departments of UMC**

**The group as a whole, and individual departments, are actively engaged in incorporating ICME principles into MSE education**

**This is currently being done within MSE departments using a combination of individual courses and units throughout the curriculum**

**There is need for MSE departments to transform education across engineering colleges by working closely with other departments, particularly in courses related to design.**

**Promoting the incorporation of ICME principles into engineering education will be the principal, multi-year goal of the UMC.**

# An Opportunity

**The Department of Materials Science & Engineering in the Carnegie Institute of Technology of Carnegie Mellon University seeks to appoint a faculty member in the area of Computational Materials Science and Engineering.** Initial appointments are anticipated to be made at the rank of Assistant Professor, but appointments at the ranks of Associate Professor or Full Professor may be available for candidates having commensurate experience.

Applicants should submit a cover letter, curriculum vitae, contact information for at least three professional references, and a statement (limited to three pages) that describes research and educational interests. All application materials should be sent to:

[msearch@andrew.cmu.edu](mailto:msearch@andrew.cmu.edu)

Applications will be reviewed as they are received until the position is filled. Women and members of traditionally underrepresented minority groups are particularly encouraged to apply. Carnegie Mellon University is an Affirmative Action/Equal Opportunity Employer.

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