# UMC Workshop on Computational Materials Education

held 23-24 June 2010 Northwestern University

# goal of workshop

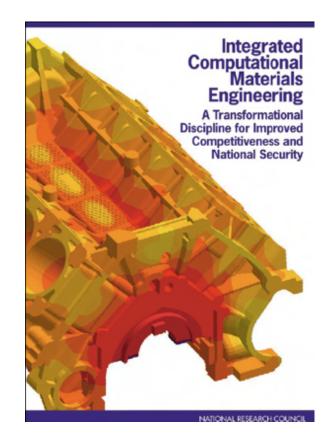
# to respond to:

- National Academy study on Integrated Computational Engineering
- apparent need for increased focus on computational materials science and engineering in the curriculum

# Integrated Computational Materials Engineering

### U. S. National Academies

study sponsored by DoD, DOE/NNSA, DOE/EERE



#### Recommendations

#### 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.

#### Recommendation 9:

Professional Materials Societies should

- Foster the development of ICME standards (including a taxonomy) and collaborative networks,
- Support ICME-focused programming and publications, and
- Provide continuing education in ICME.

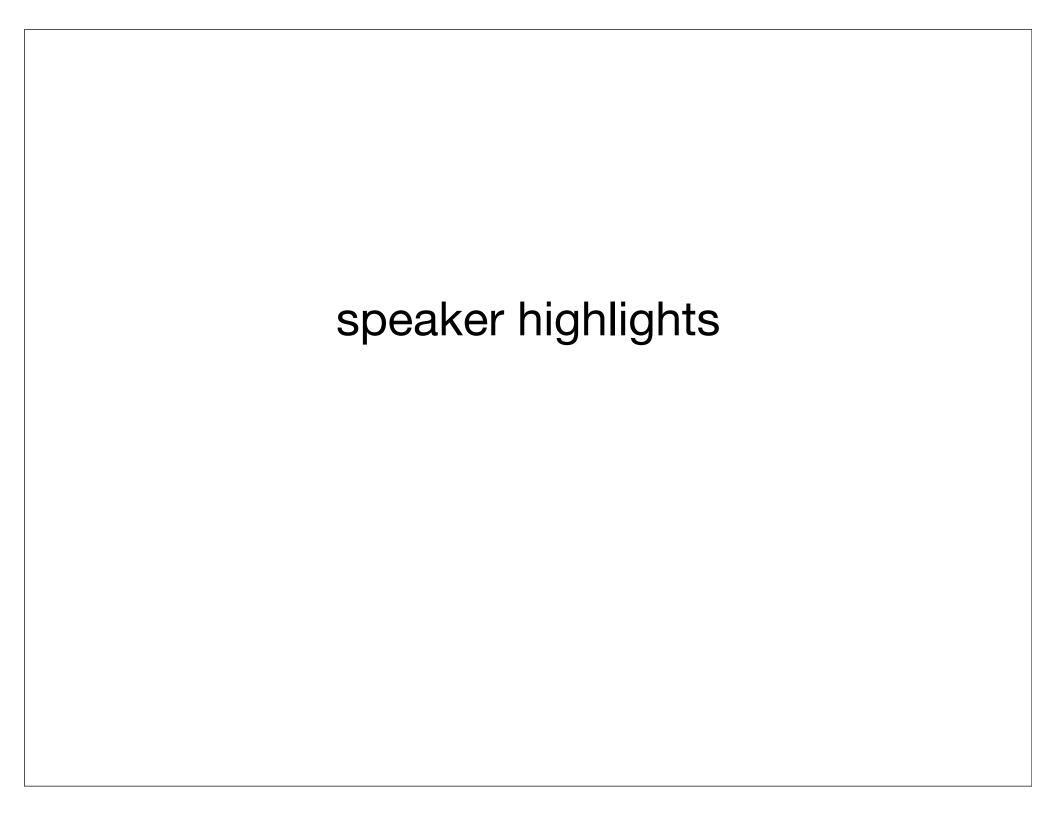
08:00	Continental Breakfast
08:30	Introduction - Peter Davies, President of the University Materials Council
08:40	Integrated Computational Materials Engineering: the National Academy Study - Richard LeSar, Iowa State University
09:10	Survey on Computational Materials in University Education - Katsuyo Thornton, University of Michigan
09:40	Industrial Perspectives on ICME: John Allison, Ford Motor Company
10:10	Break
10:30	ICME in Education: General Suggestions - George Spanos, TMS
11:00	Educational Resources - Michele Manual, University of Florida
11:30	Computational Resources - Alejandro Strachan, Purdue University
12:00	Lunch
1:30	Vignette - Greg Olson, Northwestern University

2:00	Vignette - Mark Lundstro, Purdue University
2:30	Vignette - Laura Bartolo, Kent State University
3:00	Break
3:15	Discussion: What role should computational materials engineering play in our undergraduate and graduate materials curriculum? How should computational materials engineering be integrated into the curriculum?
5:00	Adjourn

08:00	Continental Breakfast
08:30	Discussion: Can we develop curriculum aids (instructional materials, code packages, etc.) that could be widely disseminated in the community?
09:00	Discussion: How can we begin to ally ourselves with our industrial partners to enhance computational materials engineering education?
09:30	Break
09:45	Discussion: Identification of follow up issues and assignment of teams. Conclusion of workshop.
11:00	<ul> <li>UMC Business Meeting - Peter Davies, University of Pennsylvania</li> <li>Consideration of "Memorandum of Understanding" with MRS.</li> <li>UMC survey</li> <li>Election of UMC officers for 2010/11</li> </ul>
12:00	Adjourn

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# Survey on Computational Materials in University Education

Results of a Recent Study

Katsuyo Thornton and Samanthule Nora, University of Michigan

R. Edwin Garcia, Purdue University

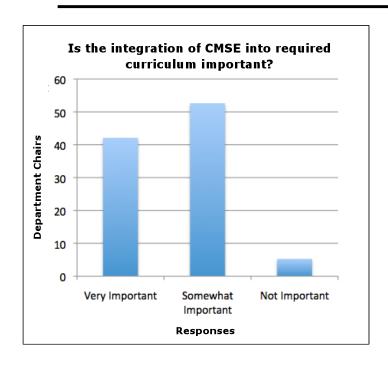
Mark Asta, University of California Berkley

G. B. Olson, Northwestern University

Work Supported by US National Science Foundation: DMR-0502737 and DMR-0746424

### **Support for CMSE Education**

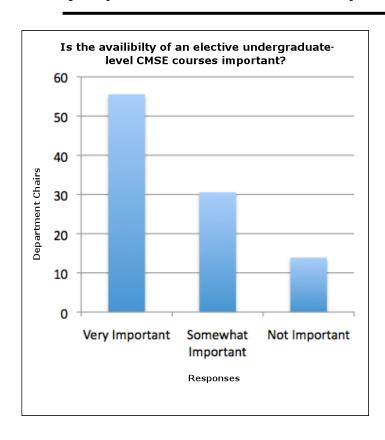
Majority of chairs view integration of CMSE into curriculum important



- · Few written comments
- · "Is there room?"
- "Somewhat important at undergrad level, very important at grad level"

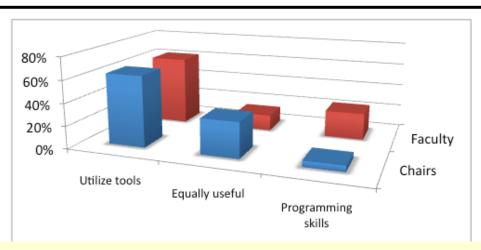
### **Support for CMSE Education**

Majority of chairs view availability of elective CMSE course important



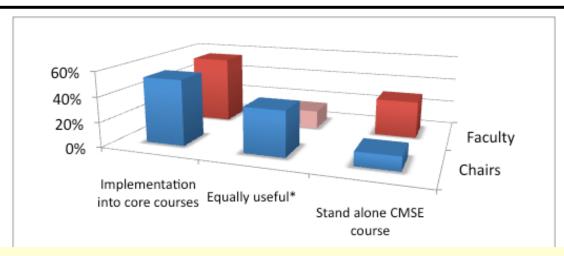
- Written comments were very negative
- "Most students seek electives in business or statistics, very few would sign up for computational materials science course."
- "I am not aware of any demand for such a course – certainly none of the many students I have advised have asked for one. Also, very few of our students take a non-required CS course as a technical elective."
- "They will not be sufficiently populated to justify their existence."

### What Should be Taught?



- "For UGs computation is a tool and should be handled as such in undergraduate education."
- "Most of our graduates will not become programmers most will use computer applications. ... They do need to understand what an algorithm is etc. ... this is covered in the required CS course."
- "The world is full of programmers who are highly skilled. MSE people should learn to take advantage of this rich resource."

# **How to Implement?**



- "Just as we integrate lifelong learning, contemporary topics, communication skills, etc."
- "Integration through existing classes is the best approach. Requires no additional funds or approval."
- "There is so little room in the UG curriculum."

# Integrated Computational Materials Engineering (ICME): An Industrial Perspective

John Allison
June 23, 2010
UMC Workshop on
(Integrated?) Computational Materials
Engineering



#### The VAC Business Case

- Targets
   IMPROVE TIMING: Reduce product and process development time 15-25%
- IMPROVE QUALITY:
  - Improve launch quality /reduce scrap
  - Eliminate failures during product development
  - Ensure high mileage durability
- IMPROVE PERFORMANCE:
  - Enable high performance heads & blocks
  - Reduce weight of components
- REDUCE COST:
  - Reduce costs by \$10-20M per year



#### **GLOBAL ENGINEERING USERS**

- North American Powertrain Operations
- (Volvo, Jaguar, Land Rover)
- Mazda
- European Powertrain Ops
- Ford of Australia



# Ford Virtual Aluminum Castings Estimated Resources and ROI

#### Resources

- \$15M over 5 years (over 50% experimental work)
- Approximately 25 people involved (15 internal + research at 7 universities)

#### **Return on Investment:**

- Over \$100M in cost avoidance or cost save (7/1 ROI)
- 15-25% reduction in product development time
- Capability for upgrading and extending at significantly lower cost

# Integrating ICME into MSE Curricula

- Develop awareness that ICME is possible and valuable
- Use ICME tools as a means to enhance the learning experience within the current curricula (but they're not available yet...)
- Curated knowledge repositories
  - Use in research and education
  - Culture of sharing
- Focus on:
  - ICME as an Engineering tool
  - Quantitative & predictive understanding
  - Computational methods
  - <u>Linkages</u> between specialty areas
  - <u>Linkages</u> between science and engineering

# other things from talks

- Purdue's nanohub as resource
- MatForge repository (Bartolo at Kent State)
- few have a systematic approach to integration within curriculum
- no consensus on modeling platforms, codes, strategies
- interesting opportunity at Ohio State as it must revamp its curriculum as it moves to semesters

# summary of current practice

- no common approach
- some programs include modeling within existing classes, some have speciality classes, and some do both
- few have a systematic approach to integration within curriculum
- no consensus on modeling platforms (MATLAB vs ...), codes, etc.
- should it be CMS, CME, CMSE, ICME, ...?

# however, ...

 there was a strong interest in developing better strategies to include more modeling/simulation, at both the undergraduate and graduate level, as it is clear that *industry* is beginning to recognize its value

## status

we set up a series of working groups to examine various issues and to make recommendations:

- development of common resources
- proposals for curricula
- these reports are not yet available

# next

will summarize the meeting and the working groups in a final report to be available in the spring