Incorporating Computational Modules in Undergraduate MSE Courses

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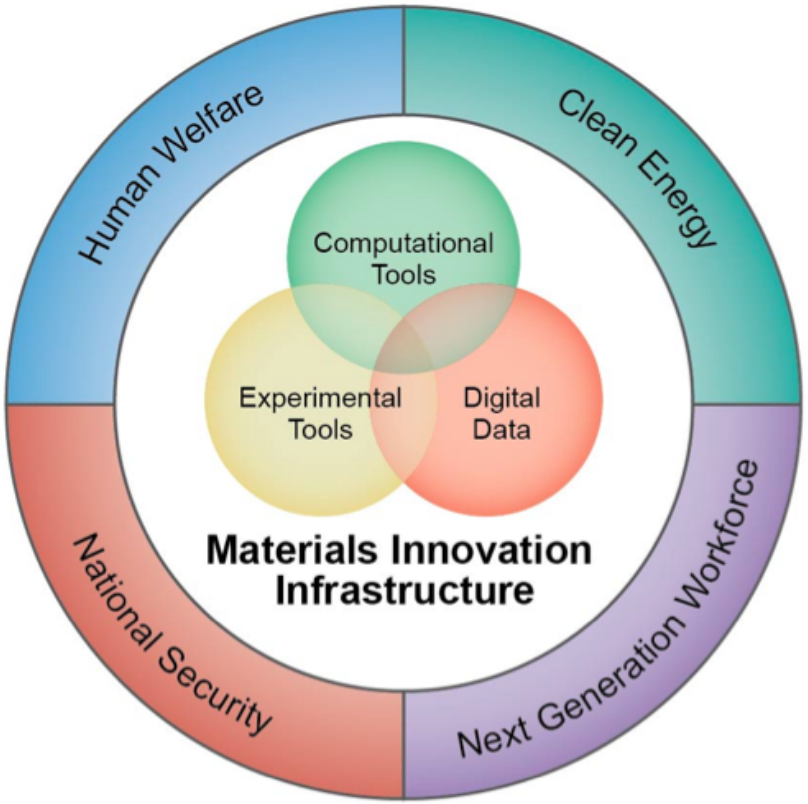
Outline

- **Motivation**
- **Implementation of CMSE in Education**
  - –General discussion
  - –Examples from UM
  - –Summer School for ICMEd
- **Summary**

Motivation: MSE is Evolving



Diving Forces:

- **Materials Genome Initiative & funding**
- **Growing computational power**
- **Wider availability of computational tools**
- **Demonstrated utility of computational approaches**

. . . This initiative offers a unique opportunity for the United States to discover, develop, manufacture, and deploy advanced materials at least twice as fast as possible today, at a fraction of the cost.

President Barack Obama, 24 June 2011
Announcing the *Materials Genome Initiative*

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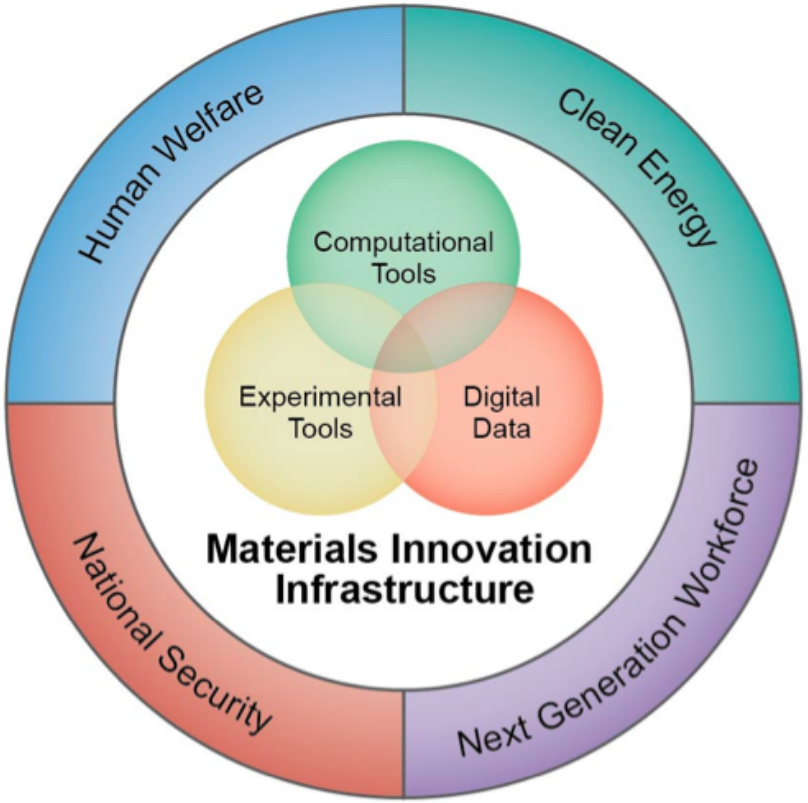

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Education and training is essential for a rapid integration of computational tools, digital data, and experiments.

Many targets, different approaches

Undergraduate Education	• Stand-alone courses • Module integration into courses (JHU)
Graduate Education	• Degree & certificate programs (NWU) • Summer schools (Texas A&M)
Continuing Education	• Short courses & workshops (TMS, PRISMS) • Online webinars/courses (TMS, ASM, ...)
Instructor Training	• Short courses/summer school (ICMEd) • Online resources (nanoHub)

Above examples are not a complete list.

Motivation: Surveys on Comp. MSE Education

INSTITUTE OF PHYSICS PUBLISHING MODELLING AND SIMULATION IN MATERIALS SCIENCE AND ENGINEERING

Modelling Simul. Mater. Sci. Eng. **13** (2005) R53–R69 doi:10.1088/0965-0393/13/2/R01

TOPICAL REVIEW

Current status and outlook of computational materials science education in the US

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In MSMSE, 2005

Feature *Materials Education*

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

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

In JOM, 2009

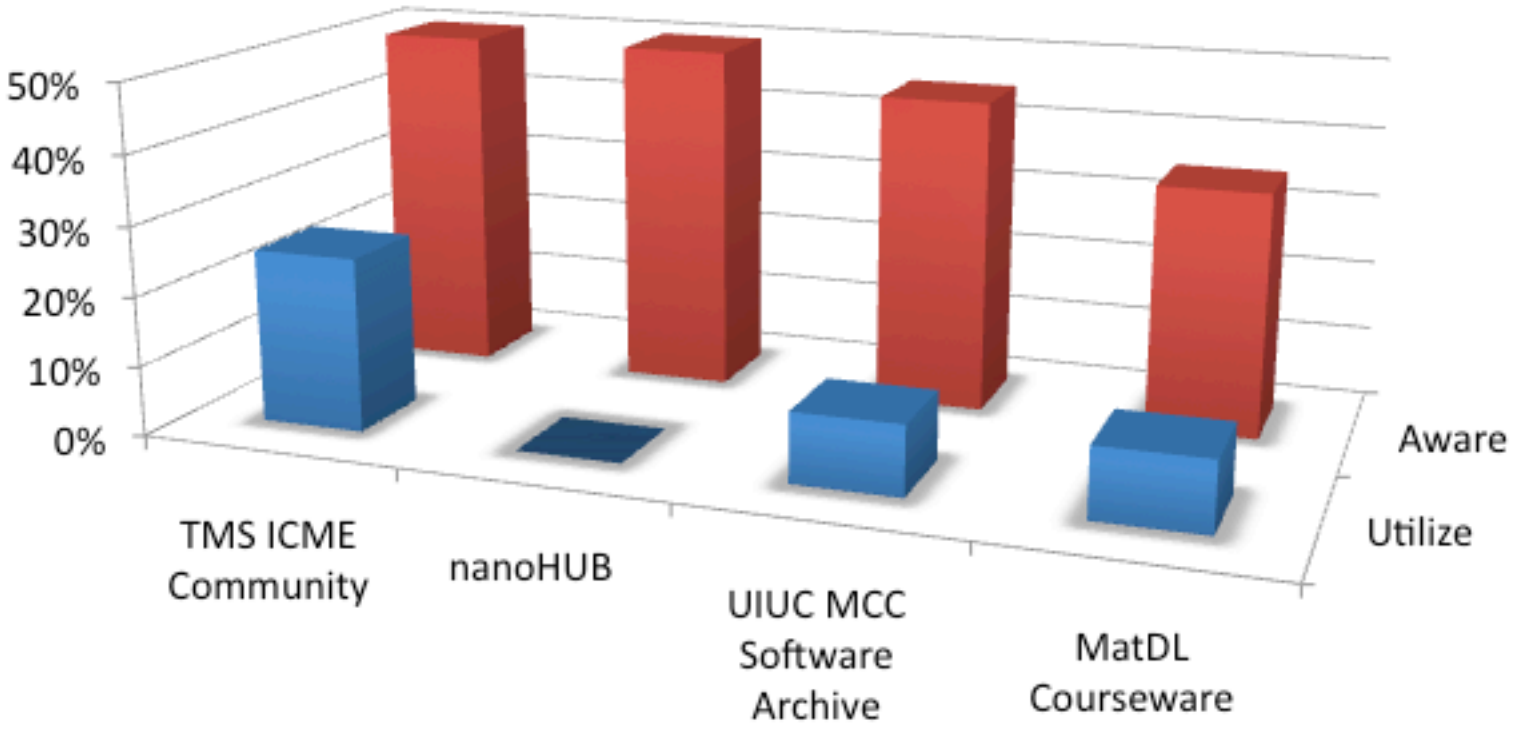
traditionally viewed as an experimental discipline, many researchers have begun to take advantage of rapidly growing computing resources and associated algorithmic and theoretical developments, and the capabilities of integrated computational approaches

gree to which such efforts are already under way, and what steps must still be taken to address these NRC recommendations remain unclear. Therefore, we have undertaken a survey of the field to assess the current status of computational materials science and engineer-

Summary of Issues Raised

- **Limited availability of faculty** in implementation of CMSE components in MSE curricula.
- Practical concerns of **reallocation of resources** to enable implementation of CMSE into education.
- Employers finding **gaps between tools taught and those commonly in use**.
- **Web-based dissemination** of educational materials for CMSE alone **may not be optimal**.

Resource Development and Dissemination (JOM Survey)



Many computational faculty are aware, but do not utilize resources on the web!

How to Integrate Computation Into MSE Curriculum

- **Stand-alone course(s) in CMSE**
  - Traditional way; can be with hands-on component
- **Modules within existing standard courses**
  - Easier to synchronize/link theory & computation
- **Integration into laboratory/design courses**
- **Seminar course focused on CMSE**
  - Could be a second course for an instructor where the course load is > 1 per term
- **Undergraduate research in CMSE**
  - Small group research enables more reach and potentially better outcome

Computational MSE Education @ UM

- **Integration of tools into individual courses**
  - Thermodynamics, mechanical behavior of materials, metallurgy
- **Coordinated experimental-computational laboratory**
  - About half of the course is computational
- **Senior-Level elective computational materials science course**
  - Overview including atomistic to continuum modeling
  - Emphasis on hands-on experience; laboratory module on most techniques
  - Seniors uses the techniques learned in the course in Senior Design

General Progression for MSE UG @ UM

All engineering students are required to take a programming course (MATLAB/C++) in the first year

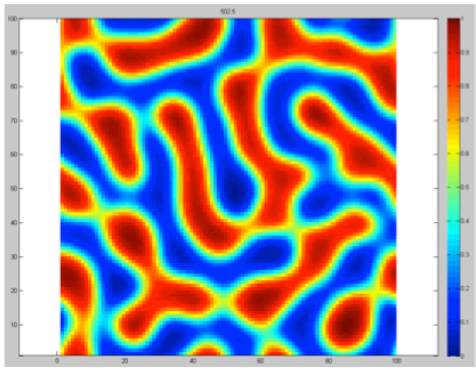
Year/Term	Courses	Notes
Junior/Fall	**Junior Lab I (Exp/Comp)**	**Required**
Junior/Winter	**Junior Lab II (Exp/Comp)**	**Required**
Senior/Fall	**Computational Approaches in MSE** Senior Design I	**Elective** Required
Senior/Winter	Senior Design II	Required

Integration into Required Courses

- **It is essential that computation is introduced in required courses**
  - Higher enrollment in elective courses on CMSE
- **A model may include shared TA (UIUC)**
  - Also, some research scientists may be interested in teaching experience
- **Another model: Lab modules**

Advantage of Introducing CMSE in Lab is the Long Duration

- **1st hour: Shock & resentment**
  - "Do we really have to do this?!!"
  - "I don't know what we are supposed to be doing."
- **2nd hour: Acceptance**
  - Most quietly work on the problems
- **3rd hour: Seeing the fruit of the labor**
  - The lab starts to be filled with excitement
- **4th hour: Joy!**
  - "I just wanted to thank you for creating the MSE365 computational kinetics lab... We have been studying spinodal decomposition in Metals class, and this lab finally got me to understand its finer details."



Instructor Training: Summer School for Integrated Computational Materials Education

- **Was supported by NSF with supplemental funding of Michigan Center for Theoretical Physics and TMS in-kind support**
- **Educate the educator (graduate students, postdocs and faculty)**
- **The two-week program includes**
  - a "crash course" on computational materials science
  - focus sessions on educational modules that can be adopted into existing core courses
- **The "Fellows" will take their knowledge & materials back to their institutions and teach computational materials science modules within existing *required* undergraduate courses**
- **Key Contributors: Mark Asta, Edwin Garcia, Larry Aagesen, John Allison, Laura Bartolo, Jon Guyer, Paul Mason, Anton Van der Ven, Greg Olson, Tershia Pinder-Grover**

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Issues Raised in Surveys

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Issues Raised in Surveys

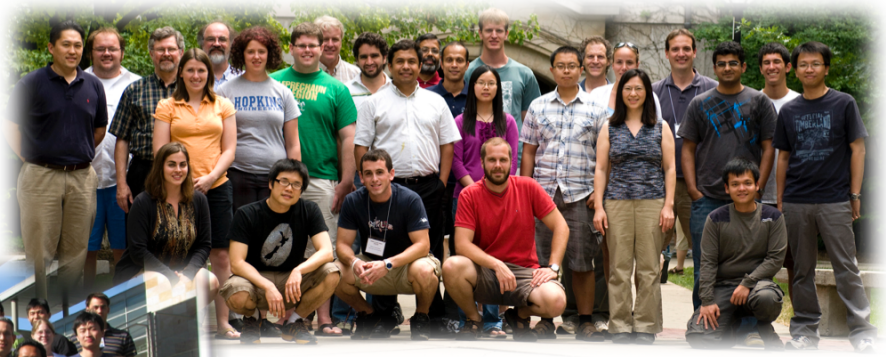
- Limited availability of faculty
- Reallocation of limited resources ($ for software & equipment, students' time)
- Employers finding gaps between tools taught & those commonly in use
- Web-based dissemination of materials not sufficient

Issues Raised in Surveys

- Limited availability of faculty
  - ✓Eliminate the need for dedicated computational faculty
- Reallocation of limited resources ($ for software & equipment, students' time)
  - ✓Will significantly reduce the burden; tutorials, problem set, solutions
- Employers finding gaps between tools taught & those commonly in use
  - ✓Balanced selection of topics
- Web-based dissemination of materials not sufficient
  - ✓Training, in addition to providing materials

Past Summer School for ICMEd

- **Thanks to the participants, the materials from the Summer School have have impacted hundreds of students!**



6th Summer School for ICMEd

- **University of Michigan, Ann Arbor, June 5 - 16, 2017**
- Application information will be available at http://icmed.engin.umich.edu
- Email icmed2017@umich.edu to get on the email list.

Future Directions: New Survey

- **The previous survey was in 2009**
  - What's the state of CMSE education?
  - What do industry use now? Have the needs changed?
- **Assessment of Summer School**
  - Where are the past participants?
  - What did they utilize?
- **New survey will be performed in fall 2017**
  - The results will be compiled thereafter and published
  - Please help us if you receive a request!

Thank you for your attention!