Survey on Computational Materials in University Education

Results of a Recent Study

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Introduction

- Over 10 years of experience in computational materials science
- Two papers on survey results and overview of computational materials science education
- A strong supporter of ICME
- Inaugural Chair of the TMS ICME Committee
- Currently leading a proposal on Summer School on Integrated Computational Materials Science Education

Outline

- **Motivation**
- **Summary of the 2003-2004 Survey**
- **Recent Survey**
  - Support for CMSE education at the undergraduate level
  - What should be taught and how to implement
  - Employers’ perspective
  - Discussions
- **Ongoing Efforts: Summer School**

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Why Should We Care?

- Every field, including MSE, can take advantage of the increasing computational resources to accelerate advances.
- Engineers: Trained personnel can help implement new approaches to engineering (e.g., ICME).
- Scientists: Wide spread use of computational tools makes their scientific work more relevant to technology.
- Students: Common concepts in computational approaches – allows them to learn/use tools outside of MSE.
- Educators: Provides opportunities for “active learning” and virtual experiments of scientific concepts.

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Previous Survey


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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Previous Survey: Description

- **Survey Sent to Faculty from Top Materials Programs (14 responses received)**
  - Solicited information on number and types of courses offered
  - Solicited input on course content
- **Perspectives Solicited from National Labs**
  - Input from J. Warren (NIST), E. A. Holm (Sandia), M. Baskes (LANL)
- **Perspectives Solicited from Industry**
  - Input from J. Allison (Ford), C. Bampton (Boeing) and C. Kuehmann (QuesTek)
- **Anecdotal Information – Limited Statistics**

Implementation Approaches

- **Few offered CMSE education at the undergraduate level**
- **Majority of universities offered at least one CMSE course at the graduate level**
- **Survey Courses**
  - Example: Undergraduate and Graduate Courses at MIT
- **Courses on "Core" Materials Topics**
  - Models, Simulation Methods within Context of Courses on "Core" MSE Undergrad and Grad Curricula
- **Courses focused on a CMSE topic/method**
- **Course Series**
  - Example: Northwestern Graduate Course Sequence in Molecular Modeling and Nano/Micro Mechanics

Perspectives from Employers

National Labs (Small Sample)

- **Need for Interdisciplinary Education**
  - Importance of topics typically outside MSE curriculum (numerical analysis, stat. mech., condensed matter physics)
- **Need for Awareness of Variety of Methods and When Applicable**
  - Applicability of ab initio vs. atomistic vs. meso-scale vs. continuum
  - Familiarity w/ methods desired also for experimentalists
- **Need to Emphasize Critical Analysis and Validation**
  - Connection between idealized models and real materials
  - How to establish precision and accuracy

Perspectives from Employers

Industry (Small Sample)

- **Need for Model Building Ability**
  - Ability to understand necessary ingredients and physical assumptions required to build a valid model
- **Need for Abilities in Numerical Methods and Coding**
  - Knowledge of optimal numerical methods to design efficient and robust simulation codes
- **Need for Emphasis on Validation**
  - How to establish applicability of model assumptions
  - How establish accuracy of numerical implementations
  - How to establish sensitivity of results to input parameters

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Recent Survey

- **K. Thornton, S. Nola, R.E. Garcia, M.A. Asta, and G.B. Olson, JOM, 61, 12 (2009).**

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

Enhanced for the Web

*This article appears on the JOM web site (**www.tms.org/jom.html**) in html format and includes links to additional on-line resources.*

Results from a recent reassessment of the state of computational materials science and engineering (CMSE) education are reported. Surveys were distributed to the chairs and heads of materials programs, faculty members engaged in computational research, and employers of materials scientists

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 are increasingly being utilized to accelerate materials design and development. Recent National Research Council (NRC) reports[1,2] indicate that successful integration of computational tools has also begun to be demonstrated in industrial settings, comparing its potential impact to that of bioinfomatics.

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 engineering (CMSE) education. A summary is presented below, which serves as an update to a previously published report[3] based on similar surveys performed in 2003–2004. See the sidebars on page 13 for a survey description and the list of respondents.

Recent Survey: Overview

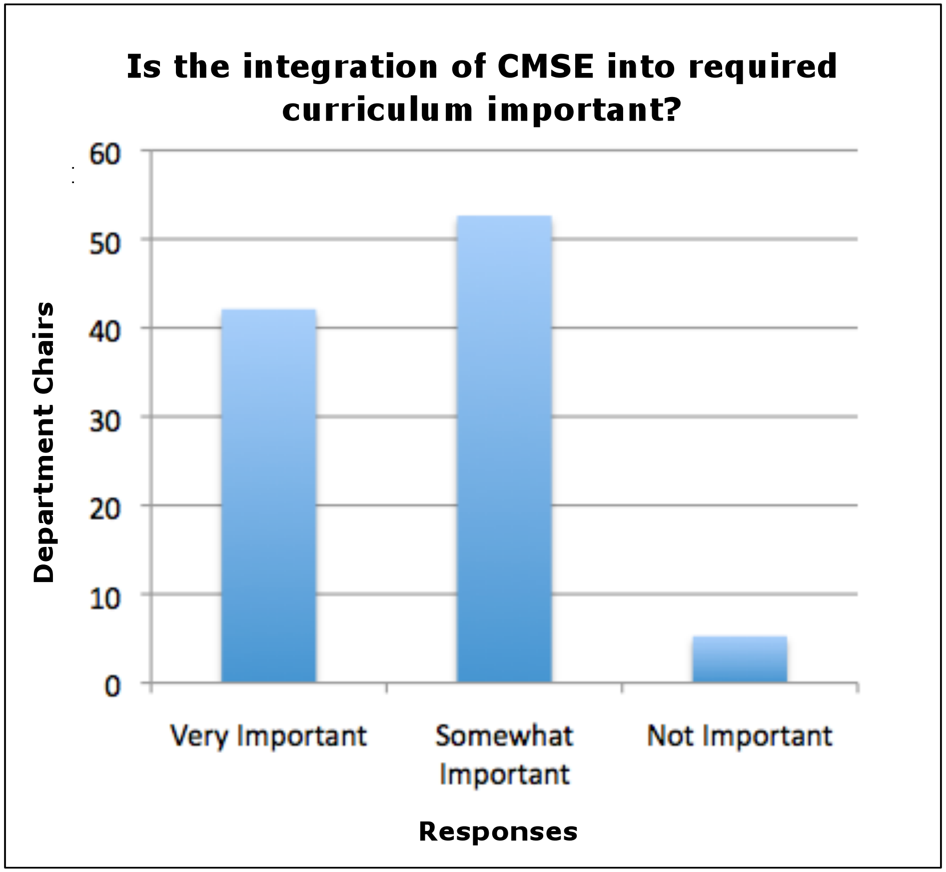
- Survey Sent to Department Chairs
  - 5 questions related to need and support of CMSE undergraduate education
  - Responses from 19 Chairs
- Survey Sent to Computational Materials Faculty
  - Questions related to course offerings, teaching approaches, resources
  - Responses from 23 faculty
- Perspectives Solicited from Employers
  - Questions related to role of CMS in organization, and recommendations related to CMSE in curriculum
  - Responses from 12 employers

Recent Survey: Goals

- **Assess the current climate for implementation of CMSE into undergraduate and graduate curriculum**
- **Determine the preferences of what should be taught and how it should be implemented into curriculum**
- **Collect the information on what tools are being taught**
- **Collect information on software used in industry and employer's needs**
- **Evaluate web-based dissemination of CMSE education materials**
- **Data reflect faculty & researchers opinions – not the only approach, but should be considered & is a good place to start**

Support for CMSE Education

Majority of chairs view integration of CMSE into curriculum important

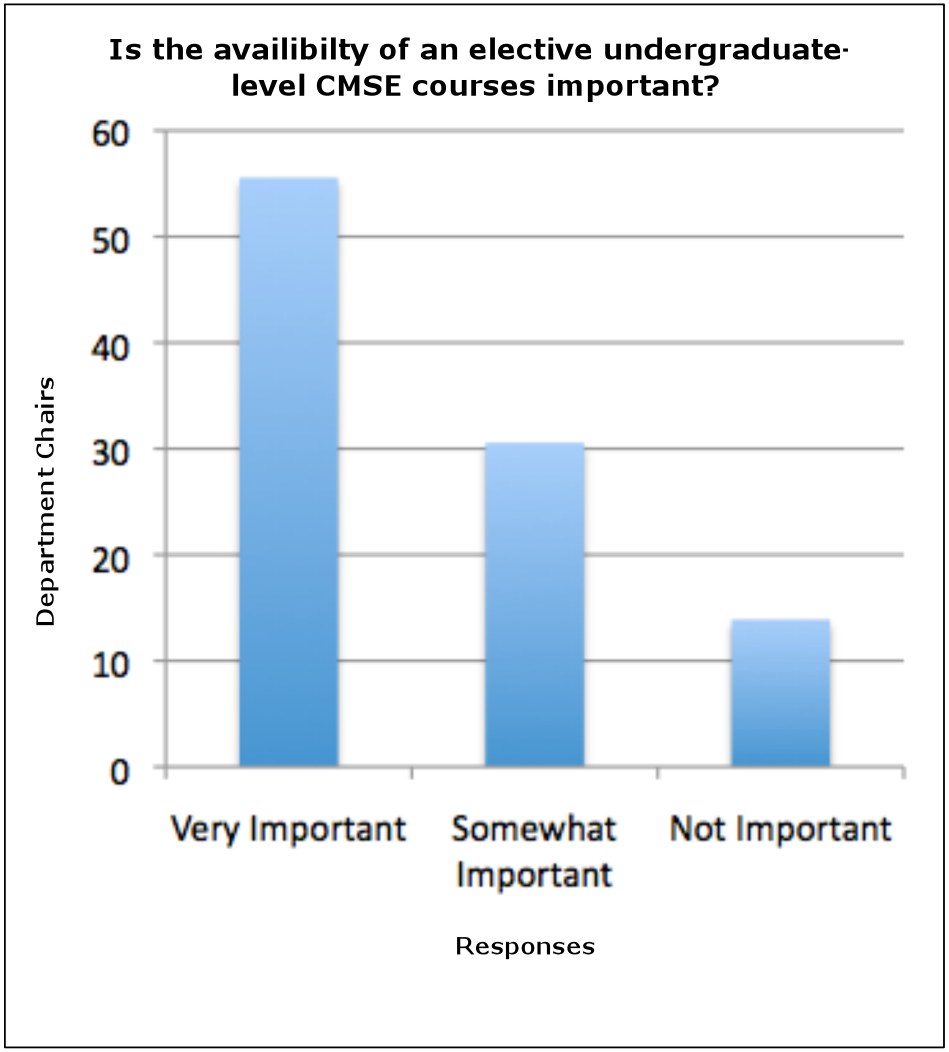


Comments from Chairs

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

Support for CMSE Education

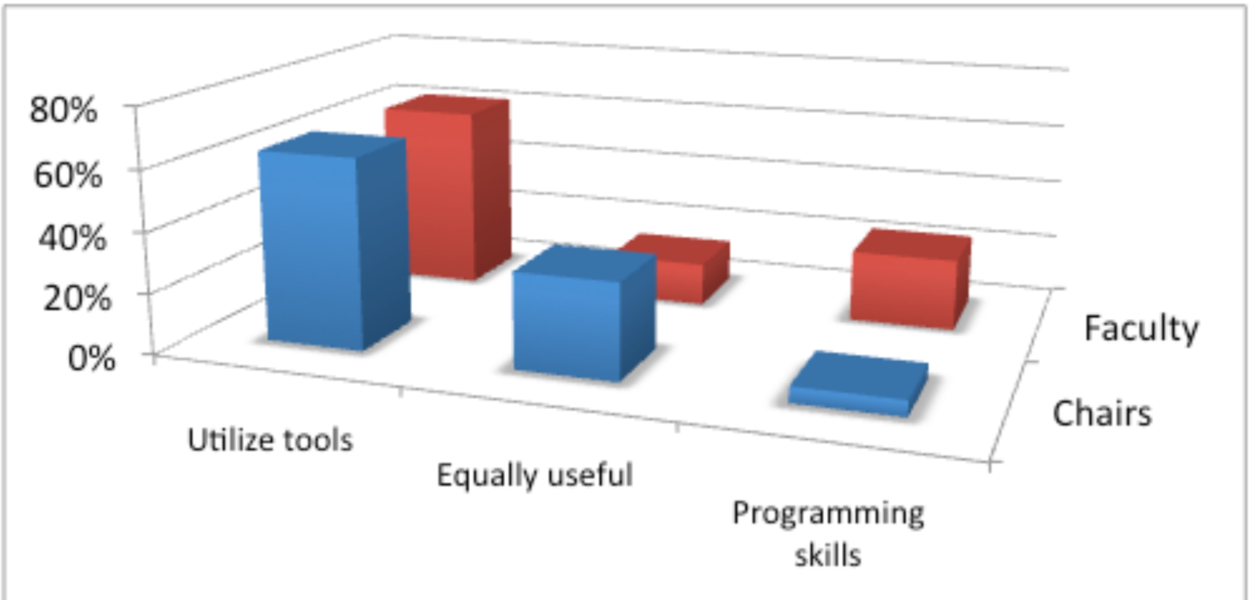
Majority of chairs view availability of elective CMSE course important



Comments from Chairs

- 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."

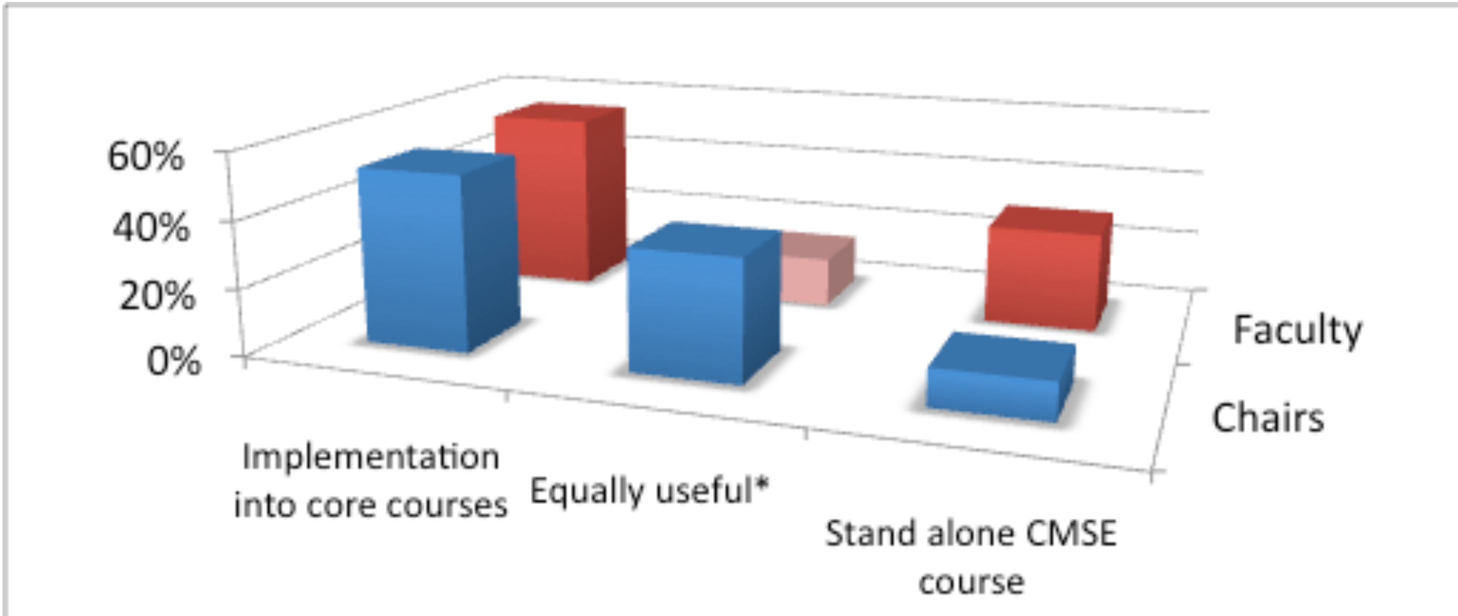
What Should be Taught?



Comments from Chairs

- "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?



Comments from Chairs

- "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."

Employers' Perspective

Regarding the computational education of recently hired graduates, what changes in materials science education would you like to see?

BS/MS

- More **applied modeling** background, understanding basic parameters and range of **software capability**
- Understand the **physics** that are to be modeled
- **Quantitative focus**
- Familiarity with types of modeling tools that exist…relative maturity and applications…a better sense that **modeling should be integral to all aspects of engineering**
- Know that computational **modeling and simulation existed** and maybe [exposure] to **very simple examples**
- More **numerical methods**; emphasis on **integration of tools** to solve problems

PhD

- More first principles modeling background
- Independent **selection** of appropriate modeling tools, material law, and adaption to the applied case
- More **quantitative focus**; broad understanding of quantitative processing-structure-property relationships. **Integration skills**. **IT and Software skills**
- Ideal training is all of **physics and**… **materials science**…strong focus in thermodynamics and mechanics…strong additional bank of knowledge in statistical mechanics, quantum…computer science and software development
- Much better view of **real-world engineering**
- Understanding its place, alongside experiments, in materials design

Employers' Perspective

What do you view as aspects of CMSE education that require improvement?

- For me it is very important to teach methods that can be applied to **engineering problems** (components) and not only on idealistic structures
- Integration of multiple tools, Computer science and IT skills
- Understanding of **model accuracy**, need for sensitivity analysis, **validation** procedures. Basically an understanding that you don't just blindly trust what comes out of the models
- **Fundamentals**, fundamentals, fundamentals...and a little more math
- More first principles modeling, understanding basic mechanisms and fundamental physics, thermodynamics and kinetics of complex materials systems
- **Thermo courses should incorporate computation tools.** Phase transformation courses should require students to use thermo codes to answer **phase transformation** problems. Fracture **mechanics** should incorporate simulation tools and then relate that to real world problems. Students should also be given instruction in general numerical methods techniques
- It appears that in most cases US students go in to Materials Science because they perceive that math and computer skills are less emphasized than in EE, ME, or physics. And with current curricula, they are often right…would like to see undergraduate and graduate curricula that gave students **a strong foundation in the math and computer skills** they would need to be comfortable taking on a Computational Materials project

Software used in Undergraduate Teaching

Table A. Examples of Reported Packages used in Undergraduate Materials Education

Software Categories	Example Packages	Reference
CAD	Solid Works[c]	*www.solidworks.com/*
Computational Thermodynamics	Thermo-Calc[c]	*www.thermocalc.com/*
Crystallography	CaRIne[c]	*http://pagespro-orange.fr/carine .crystallography/*
Density Functional Theory	ABINIT[f]	*www.abinit.org/*
	PWSCF[f]	*www.pwscf.org/home.htm*
	VASP[c]	*http://cms.mpi.univie.ac.at/vasp/*
High-Level Programming Language	MatLab[c]	*www.mathworks.com/*
Materials Properties	CES Materials Selector[c]	*www.grantadesign.com/products/ces/*
Molecular Dynamics	LAMMPS[f]	*http://lammps.sandia.gov/*
	NAMD[c]	*www.ks.uiuc.edu/Research/namd/*
Spread Sheet	Excel[c]	*http://office.microsoft.com/excel*
Symbolic Mathematics	Mathematica[c]	*www.wolfram.com/*
Visualization	Minitab[c]	*www.minitab.com/*

[c] Denotes commercial code; [f] denotes free software

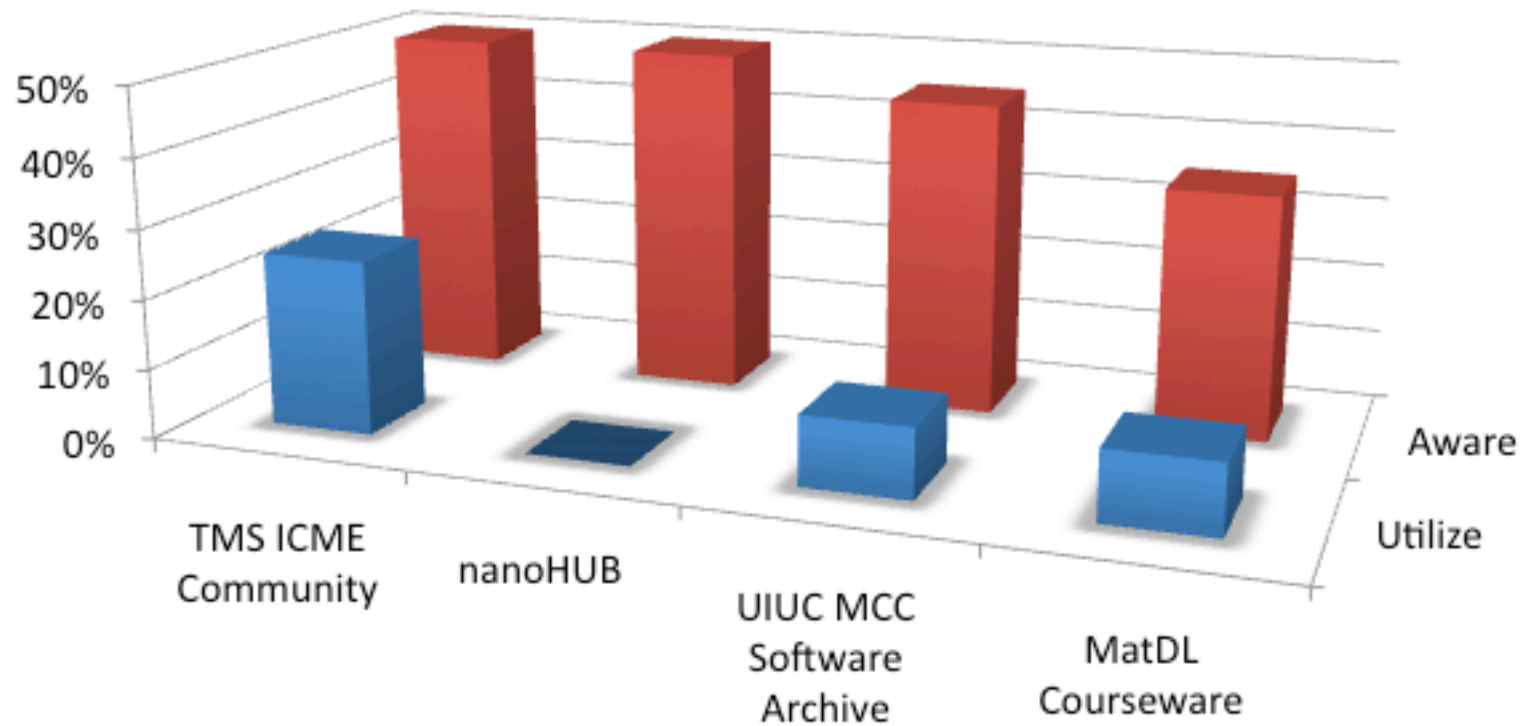
Software used in Industry

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.

Resource Development and Dissemination



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

Issues Raised

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

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Ongoing Effort: Summer School for Computational Materials Education

- **Proposed to NSF (Daryl Hess, DMR-CMMT)**
- **Educate the educator (graduate students, postdocs and faculty)**
- **A three-week program includes**
  - a "crash course" on computational materials science
  - focus sessions on educational modules that can be adopted into existing core courses

  (a pilot program will be shorter)
- **The "Fellows" will take their knowledge back to their institutions and teach two computational materials science modules within existing *required* undergraduate courses**
- **Key Participants: Mark Asta, Edwin Garcia, John Allison, Laura Bartolo, Jon Guyer, Paul Mason, Anton Van der Ven**
- **TMS in-kind support**

Issues Addressed by Summer School

- ✓ Limited availability and challenges in implementation of CMSE components in MSE curricula. **– A goal**
- ✓ Employers finding gaps between tools taught and those commonly in use. **– Will balance**
- ✓ Practical concerns of reallocation of resources to enable implementation of CMSE into education. **– Will significantly reduce the burden**
- ✓ Web-based dissemination of educational materials for CMSE alone may not be optimal. **– Training, in addition to providing materials**

Not the only answer, but we believe it's a worthy effort as a first step!

Next Steps

- **Develop forums for active discussions on education in computational materials science and engineering**
  - First World Congress on ICME will include a session on education
  - TMS, MRS, MS&T, …
- **Collection of case studies from existing efforts**
- **Feedback on Summer School**
- **Coordination of efforts: MRS, TMS, …**

Thank you for your attention!

Please direct your feedback to:
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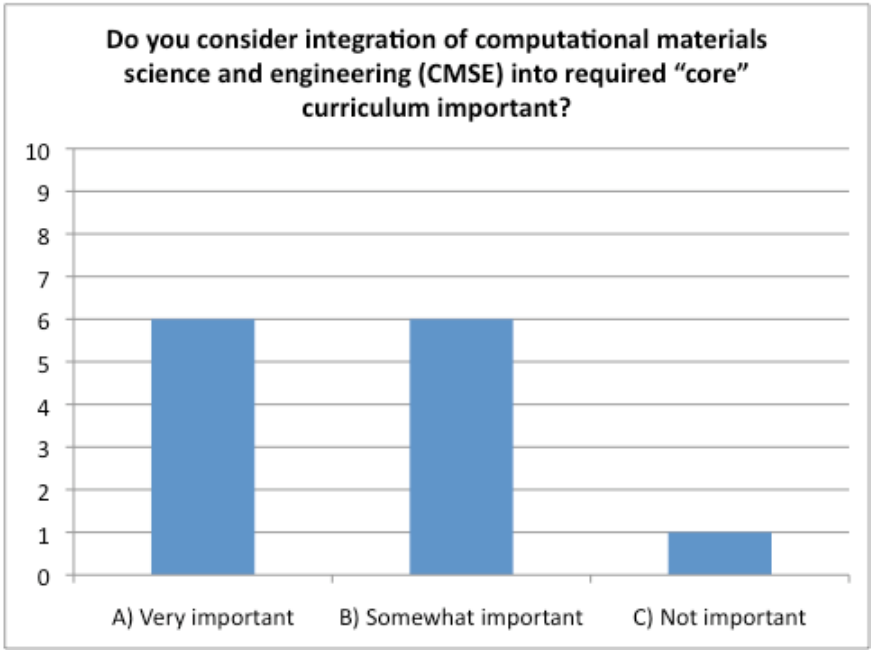
Computational Faculty Survey

Majority agree important to integrate CMSE into core curriculum

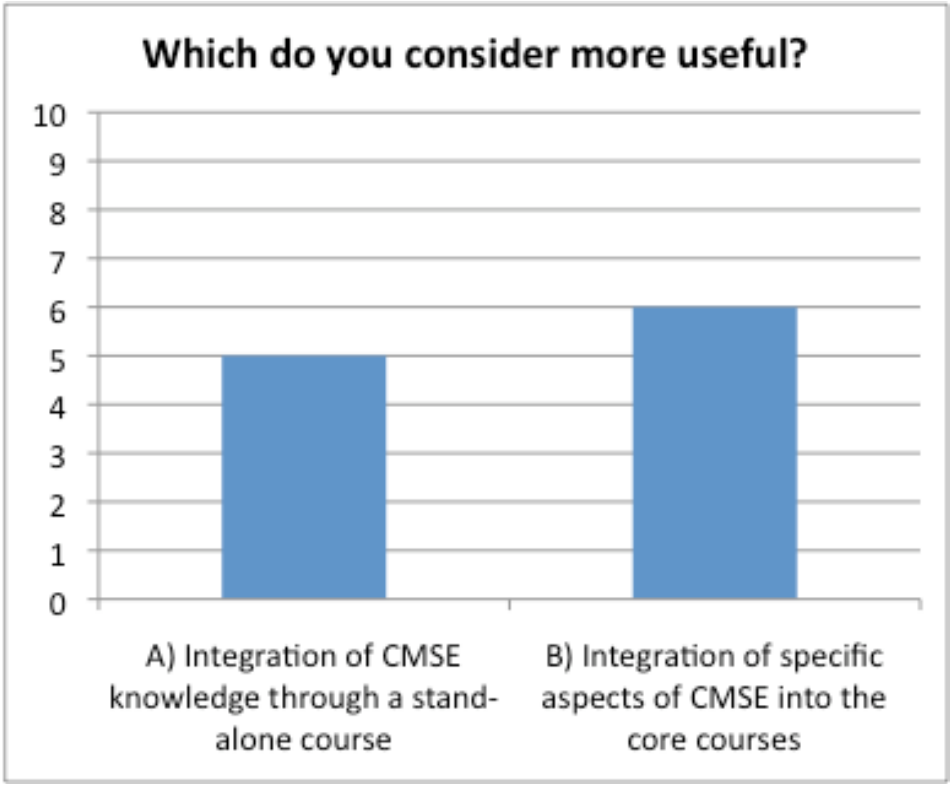


Comments

- Our industrial advisory board has recommended more of the "soft skills" rather than abstract, theoretical work
- We are pursuing exactly this in a new certificate program for MSE at Umass
- Integration is the best method to teach computational (or math or other) skills, but it is harder to achieve as each instructor places a different value on this and each has a different comfort level in teaching it.
- It is important for even experimental students to be comfortable in understanding the process and results of simulations to the same degree as CMS students are (or should be) comfortable in thinking about experimental results. It is not necessary that they learn to use CMS tools themselves; indeed, using such tools without really understanding can be very misleading.

Computational Faculty Survey

Stand-alone vs integration w/ existing courses: nearly equally split

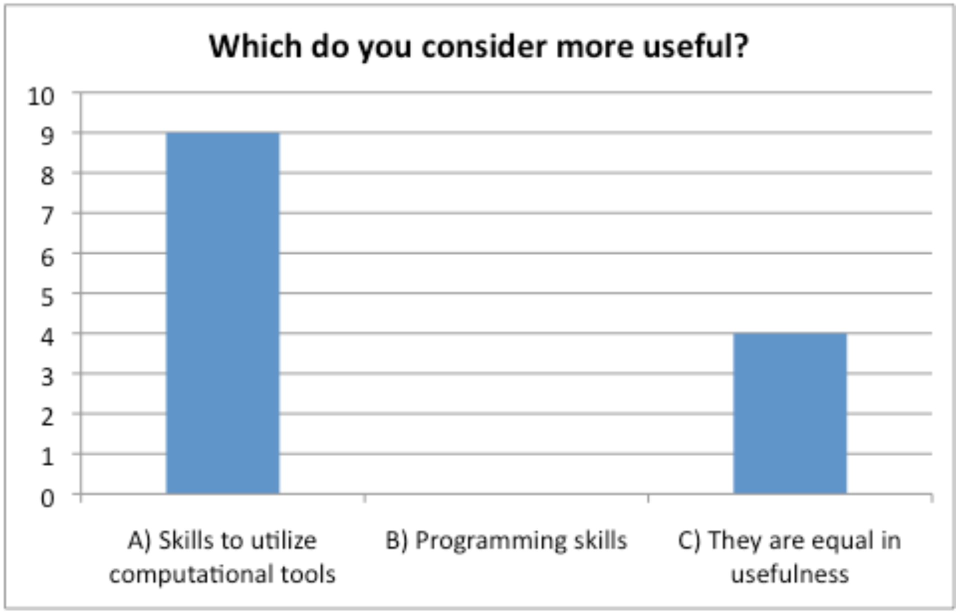


Comments

- Specific aspects, particularly at the level of understanding simulations results, should be integrated. However stand-alone courses are also essential for the future practitioners
- This is a classic chicken-and-egg problem. Integration of CMSE requires a high level of background knowledge that may not be available without a specific prerequisite course. On the other hand, a general course in CMSE that precedes the specific courses on the physics would be very difficult to do well
- Both quite important; if the integration is only in "stand-alone" courses..experimental students will likely have no exposure to computational methods. On the other hand, if it is solely integrated into the core, then students specializing in computation will not receive enough in-depth instruction

Computational Faculty Survey

Majority chose skills to utilize tools over programming skills

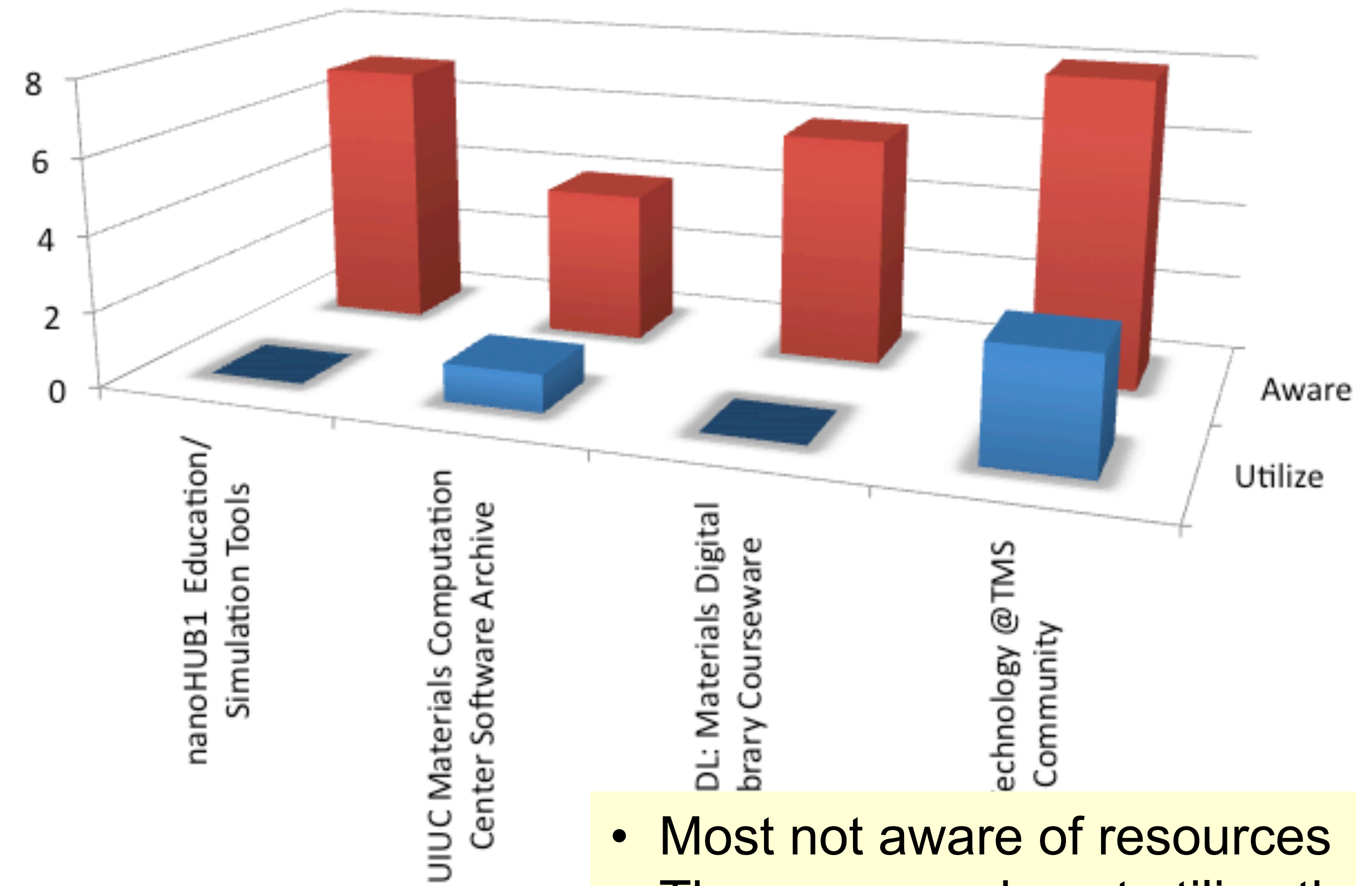


Comments

- Programming skills for all but the highest end computational tasks can be learned on the job relatively easily. The scientific skills needed to intelligently design, use and analyze results from scientific software are harder to acquire and require greater intellectual development.
- Without programming, a computer is a toolbox. With programming, a computer is a machine shop.
- For students with interest in experimental work..the ability to utilize computational tools is more important. For…students who…see computational materials science as their future field of research, good programming skills are important. Both groups should be able to do simple “programming” using some software like Matlab – to analyze mathematical functions and solve simple equations.

Computational Faculty Survey

Resource Utilization



- Most not aware of resources
- Those aware do not utilize them
- Why? What to do?