Computational Curriculum for MatSE Undergraduates

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Jessica A. Krogstad is an assistant professor in the Department of Material Science and Engineering at the University of Illinois, Urbana-Champaign. She received her PhD in Materials at the University of California, Santa Barbara in 2012. Between 2012 and 2014, she held a postdoctoral appointment in the Department of Mechanical Engineering at Johns Hopkins University. Her current research explores the interplay between phase or morphological evolution and material functionality in structural materials under extreme conditions.

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Robert Maass received a triple diploma in Materials Science and Engineering from the Institut National Polytechnique de Lorraine (INPL-EEIGM, France), Luleå Technical University (Sweden) and Saarland University (Germany) in 2005. In 2009, he obtained his PhD from the Materials Science Department at the École Polytechnique Fédérale de Lausanne (EPFL) in Switzerland. During his doctoral work, Robert designed and built an in-situ micro-compression set-up that he used to study small-scale plasticity with time-resolved Laue diffraction at the Swiss Light Source. From 2009-2011 he worked as a postdoctoral researcher at the Swiss Federal Institute of Technology (ETH Zurich) on plasticity of metallic glasses. Subsequently, he joined the California Institute of Technology as an Alexander von Humboldt postdoctoral scholar to continue his research on plasticity of metals. After working as a specialist management consultant for metals at McKinsey & Co., he transferred to the University of Göttingen as a junior research group leader. He joined the faculty of the University of Illinois at Urbana-Champaign as Assistant Professor of Materials Science and Engineering in 2015.

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Prof. Matthew West, University of Illinois, Urbana-Champaign

Matthew West is an Associate Professor in the Department of Mechanical Science and Engineering at the University of Illinois at Urbana-Champaign. Prior to joining Illinois he was on the faculties of the Department of Aeronautics and Astronautics at Stanford University and the Department of Mathematics at the University of California, Davis. Prof. West holds a Ph.D. in Control and Dynamical Systems from the California Institute of Technology and a B.Sc. in Pure and Applied Mathematics from the University of Western Australia. His research is in the field of scientific computing and numerical analysis, where he works on computational algorithms for simulating complex stochastic systems such as atmospheric aerosols and feedback control. Prof. West is the recipient of the NSF CAREER award and is a University of Illinois Distinguished Teacher-Scholar and College of Engineering Education Innovation Fellow.

Computational Curriculum for MatSE Undergraduates

0. Abstract

Computational materials modeling and design has emerged as a vital component of materials research and development in academic, industrial, and national lab settings. In response, US Materials Science and Engineering (MatSE) departments and the federal government recognize the need to incorporate computational training into undergraduate MatSE education. Our faculty team at the University of Illinois at Urbana-Champaign (UIUC) is addressing this growing need with a comprehensive computational component integrated into the MatSE curriculum. Throughout their coursework, undergraduates complete a series of computational modules of progressing complexity, each module modeling the principles taught in its containing course. Computational lectures accompany most modules and further illustrate how computational methods solve real-life science and engineering problems. The computational curriculum is supported by a dedicated teaching assistant who helps with module development, delivers computational lectures, and offers additional office hours. Now, three years since initial implementation, multiple student cohorts have experienced the computational curriculum at all course levels. In this paper, we present new results on the efficacy of the computational curriculum and share more information about our continued efforts to improve the computational modules, lectures, and their integration within the broader MatSE curriculum.

1. Introduction and Background

The rise of materials modeling has generated a nationally recognized need for materials scientists and engineers with computational training[18;23;24]. In industry and academic settings alike, computational materials science skills are in high demand as researchers seek to accelerate materials design with computational tools[24]. Yet, a 2009 survey revealed that, on average, employers desire for 50% of new hires to have computational training, while only 37% of recent graduates actually have such training[24]. These trends mandate that materials science and engineering departments around the country must better serve their students, industry, and the nation by providing more instruction in computational thinking at the undergraduate level.

However, undergraduate programs in materials science and engineering typically saturate student schedules with traditional content, leaving little margin for additional coursework focusing exclusively on development of computational skills. Instead, integrating computational instruction into traditional courses not only provides computational training, but also facilitates improved learning of the traditional content[14;15;21]. In the Department of Materials Science and Engineering (MatSE) at the University of Illinois at Urbana-Champaign (UIUC), a team of faculty has integrated computational curriculum into the core curriculum[15;16]. In this paper, we describe our continued improvements to this curriculum and new results on its efficacy.

2. Approach to Curricular Reform

As discussed in[15;16], the curricular reforms described in this paper were supported by the Strategic Instructional Initiatives Program (SIIP) of the College of Engineering at UIUC. Inspired by the efforts of Henderson et al.[4;9–11], SIIP catalyzes the creation of collaborative teaching environments that enable faculty to enhance instruction iteratively and sustainably, targeting large-enrollment core courses in particular[12;27;28]. A Community of Practice (CoP) forms such an environment, serving to share knowledge, experience, and resources among members and to lower the barrier to introducing, sustaining, and optimizing practices[13;25;26].

Three tenured and six tenure-track faculty in the UIUC MatSE Department assembled into a CoP to collaboratively explore, implement, and evaluate instructional and curricular innovations in developing the computational curriculum for MatSE undergraduates. Tables 1 and 2 summarize which courses and faculty were involved in the CoP orchestrating the integration of the computational curriculum. In some courses, multiple instructors collaborated across semesters to continue iterating reforms. Since most of the faculty do not specialize in computation, support from the CoP and a Computational TA was essential to successful integration of the computational curriculum.

Number	Course Name	Level	Type
201	Phases and Phase Relations	Sophomore	Required
206	Mechanics for MatSE	Sophomore	Required
304	Electronic Properties of Materials	Junior	Semi-required
401	Thermodynamics of Materials	Junior	Required
402	Kinetic Processes in Materials	Junior	Required
406	Thermal and Mechanical Behavior of Materials	Junior	Required
440	Mechanical Behavior of Materials	Junior/Senior	Semi-required
498	Computational MatSE	Senior	Elective
404	Laboratory Studies in MatSE: Computational MatSE	Senior	Elective

Table 1: Summary of courses referred to throughout this paper. Semi-required courses are required for some areas of concentration within the undergraduate MatSE program.

Course	Fall 2013	Spring 2014	Fall 2014	Spring 2015	Fall 2015	Spring 2016	Fall 2016
201	Leal	Kilian	Leal*†	Kilian*†	Leal*†	Kilian*†	Leal*†
206		Trinkle$^{\circ *}$		Krogstad*†		Trinkle$^{\circ *\dagger}$	
304		Weaver		Schleife$^{\circ *\dagger}$		Schleife$^{\circ *\dagger}$	
401	Dillon		Dillon		Dillon*†		Dillon*†
402		Averback		Averback		Bellon*†	
406	Trinkle$^{\circ}$		Trinkle$^{\circ *\dagger}$		Maass*†		Maass*†
440	Aboukhatwa		Krogstad*		Shang		Krogstad*†
498	Ferguson$^{\circ\dagger}$		Ferguson$^{\circ\dagger}$		Ferguson$^{\circ\dagger}$		
404							Ferguson$^{\circ\dagger}$

Table 2: Participating faculty by course and semester. The double line shows the inception of the MatSE CoP. Blank entries indicate that a course was not offered in the corresponding semester. † indicates that a course included computational assignments and/or lectures, * indicates that a course included other pedagogical reforms, and $^{\circ}$ indicates faculty specializing in computational MatSE.

3. Pedagogical and Curricular Reforms

The instructional reforms originally described in [15;16], including clickers, tablets, online homework, and discussion sections, were expanded to more courses. Table 3 shows in which semester each course implemented these evidence-based [5;8;17] pedagogical practices.

In addition, most courses incorporated computational lectures to accompany the computational assignments. Typically delivered by the Computational TA, these lectures provided more context to the computational modules by introducing the theory, applications, and limitations associated with the computational method being used. They also emphasized the connection between the computational assignment and the pertinent course material, improving continuity and integration of the computational component within the containing course, and in turn, improving integration of the whole computational curriculum within the undergraduate MatSE program.

Finally, MSE 498 started as an elective outside of the core curriculum. In Fall 2016, the course was redesignated as MSE 404, a fully integrated laboratory course that fulfills the senior laboratory requirement. The course was also split into two half-semester courses: one focusing on microscale behavior (MSE 404 MICRO) and the other on macroscale behavior (MSE 404 MACRO). Improved integration of the course into the core curriculum and the additional flexibility offered by the half-semester courses has made the course more accessible to students with busy schedules.

Course	Clickers	Tablets	Computational Assignments	Computational Lectures	Online Homework	Discussion Sections
201	F14	F14	F14	F14	F14	
206	S14	S14	S15	S16	S14	S14
304	S15	S15	S15		S15	
401	F13		F15			
402	S16	S16	S16	S16		S12
406	F14	F14	F14	F16	F14	F14
440		F14	F16	F16		
498/404			F13	F13		

Table 3: Pedagogical reforms instituted by course. For each course, the semester in which each reform was implemented is listed.

4. Description of Additional Computational Modules

The computational modules address four computational methods used to model materials at different time and length scales in addition to the general topic of numerical computing. A total of seven different software packages are used:

- Quantum Espresso [7] for density functional theory (DFT)
- LAMMPS [19] and GROMACS [3] for molecular dynamics (MD) and OVITO [22] for atomistic visualization

- OOF2[20] for finite element method modeling (FEM)
- Thermo-Calc[2] for calculation of phase diagrams (CALPHAD)
- MATLAB[1] for numerical computing

In improving integration of the computational component into the existing curriculum, special efforts were dedicated to developing and deploying new modules in additional courses. The modules previously described in[15;16] formed the foundation of the current computational curriculum, and they have been retained with only minor changes. Here, we describe new modules implemented after Spring 2015. Table 4 summarizes the computational methods used in the modules in each course.

Course	DFT	MD	FEM	CALPHAD	MATLAB
201	X			X	
206			X		X
304	X				
401		X*		X*	
402		X*			X*
406		X	X		
440			X*		X*
498/404	X	X	X	X	X

Table 4: Computational methods integrated by course. * indicates new modules described in this paper; the remaining modules are described in[15;16].

4.1. Molecular Dynamics

Thermodynamics of melting: Students in MSE 401 use LAMMPS and OVITO to simulate and visualize atomic motion in melting aluminum both under constant volume and constant pressure conditions. They analyze the thermodynamic data produced by the simulation in order to extract the melting temperatures, heat capacities, heat and entropy of melting, and other related thermodynamic quantities. Students also assess how their results depend on system size.

Diffusion coefficients: Students in MSE 402 use LAMMPS to simulate diffusion of particles in water. They investigate the diffusion coefficient's dependence on particle radius and temperature, comparing their results to the Stokes-Einstein and Arrhenius equations.

4.2. Finite Element Method

Thermal residual stress and microcracking: Using OOF2, students in MSE 440 model the stress distribution in two alumina microstructures with different average grain sizes after cooling at different rates. For each combination of microstructure and cooling rate, students compute the maximum grain boundary stress intensity factor to determine whether a crack would form.

4.3. Calculation of Phase Diagrams

Phase-based screening of anode materials: Students in MSE 401 use Thermo-Calc to identify and characterize binary alloys that could serve as the anode material in a magnesium battery. Students maximize gravimetric capacity while avoiding plating. For each candidate identified, students produce and analyze free energy curves, activity curves, and the voltage profile as a function of magnesium concentration in the host.

4.4. MATLAB

Chemical oscillators: Students in MSE 402 use the MATLAB ODE solver to model the chemical reactions in the Belousov-Zhabotinsky oscillator and approximate the region of initial conditions that results in chemical oscillation.

Strain-rate dependence of yield strength: Given three sample data sets from compression tests, students in MSE 440 use MATLAB to apply the analysis methods described in [6] and determine the Johnson-Cook parameters for a Ti-Al-V alloy. Using these parameters, they then predict the yield strength of the alloy for a different set of experimental conditions.

5. Impact of Curriculum Changes

Surveys administered in each course assessed students' attitudes toward and reflections on the computational curriculum. Preliminary results derived from these surveys and an evaluation of impact on exam-based performance are discussed in [15;16]. Here, we describe new results obtained from studying students' perspectives on the computational curriculum and their own computational competency as they progressed through the undergraduate program.

5.1. Students' Fulfilled Desire for Computational Instruction

Two survey questions used a 5-point Likert scale to measure students' perception of the importance of computational skills and their desire for more computational material:

- "I think computational materials science skills are important for my post-graduation career." (Strongly Agree — 1 2 3 4 5 — Strongly Disagree)
- "I would like to use computation in my MatSE classes…" (Much More — 1 2 3 4 5 — Much Less)

Figures 1 and 2 show the distribution of responses from students in two required courses, MSE 201 and MSE 406, for three semesters. MSE 201 is the first disciplinary course taken by materials science majors that includes computational material, so MSE 201 students share very similar backgrounds in all three semesters. Indeed, two-tailed t-tests demonstrate that the mean ratings for these two questions do not differ significantly for any pair of semesters ($p > 0.3$).

In contrast, MSE 406 is a junior-level course that students take after many of the other courses containing computational material. With each semester since the introduction of the computational curriculum in Fall 2014, MSE 406 students have been exposed to more and more

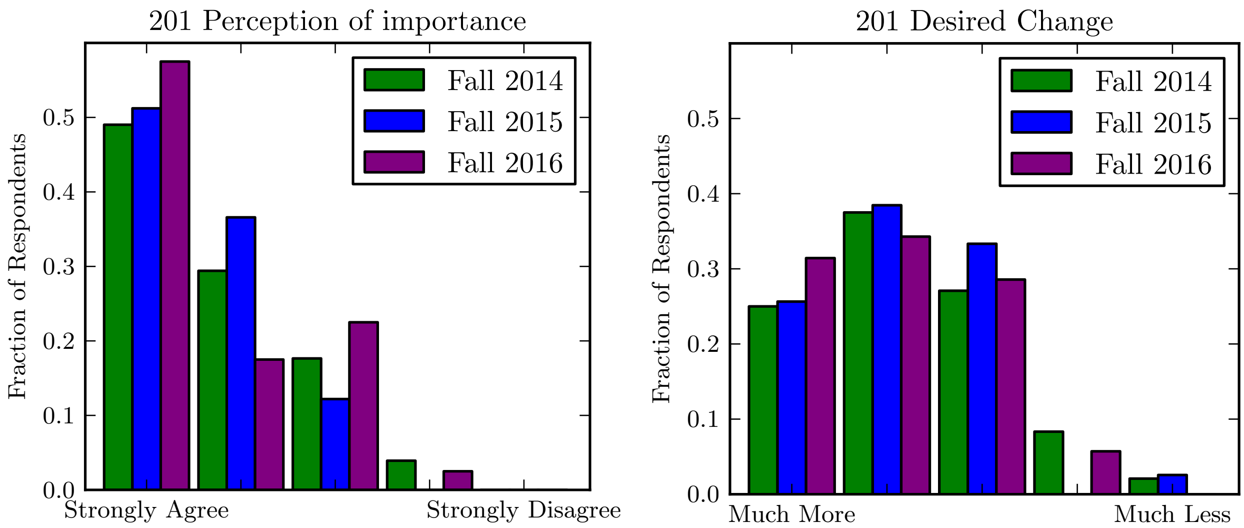

Figure 1: Distribution of MSE 201 students' perception of the importance of computational skills (left) and desire for more computation in the MatSE curriculum (right) in Fall 2014, Fall 2015, and Fall 2016. The sample sizes were 53, 43, and 46, respectively.

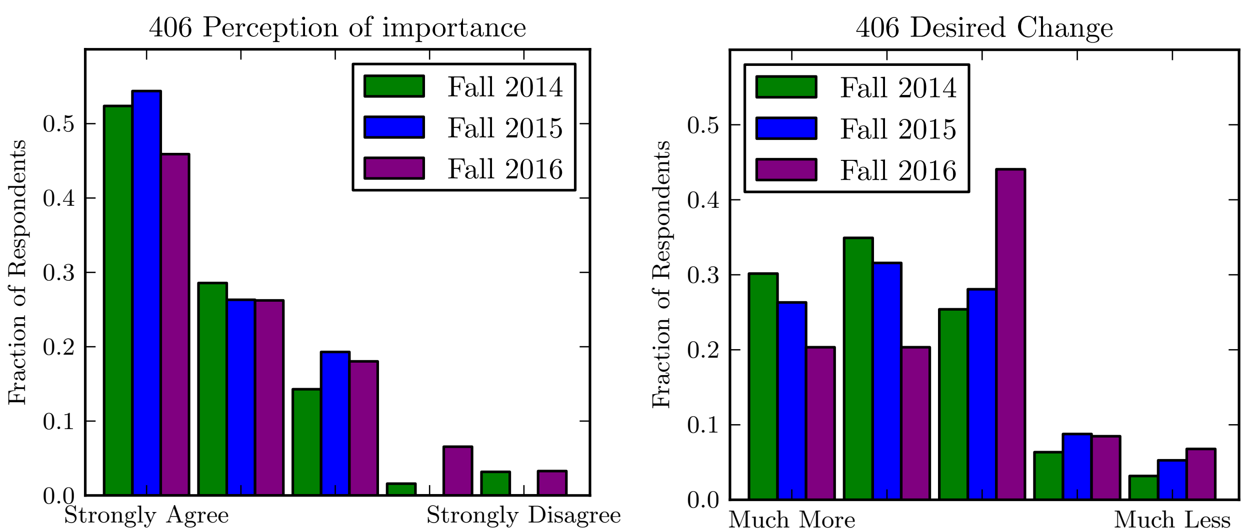

Figure 2: Distribution of MSE 406 students' perception of the importance of computational skills (left) and desire for more computation in the MatSE curriculum (right) in Fall 2014, Fall 2015, and Fall 2016. The sample sizes were 63, 68, and 70, respectively.

computation in their previous coursework. While the curricular reforms had no significant impact on students' perception of the value of computational skills ($p = 0.26$ between Fall 2014 and Fall 2016), they did start to satisfy students' desire for computational MatSE curriculum ($p = 0.02$ between Fall 2014 and Fall 2016).

5.2. Students' Progressing Perception of Computational Competence

To measure students' sense of computational proficiency, several survey items asked students to rate their level of comfort with using a variety of computational methods to perform a certain calculation related to the content of the respective course. The following questions, each rated on a 5-point Likert scale, are representative examples:

- MSE 206: If you were asked to determine the bending of a beam under loads, how comfortable would you be using the following approaches?
  (Very Comfortable — 1 2 3 4 5 — Very Uncomfortable)
- MSE 304: How comfortable would you be using the following approaches to determine the density of states of GaAs?
  (Very Comfortable — 1 2 3 4 5 — Very Uncomfortable)
- MSE 406: If you were asked to determine the stress field ahead of a crack tip, how comfortable would you be using the following approaches?
  (Very Comfortable — 1 2 3 4 5 — Very Uncomfortable)

Figure 3 illustrates the distribution of students' comfort with FEM tools at the end of the most recent iterations of courses that included at least one FEM module (MSE 206 Spring 2015, MSE 406 Fall 2016, and MSE 440 Fall 2016). Although the results from MSE 440 do not differ significantly from those of the other courses ($p > 0.10$), the small size of the class ($N = 12$) may have prevented a clear statistical trend. Nonetheless, students' sense of proficiency in FEM increases dramatically between MSE 206 and MSE 406, both large enrollment core courses, with the mean rating lowering from 4.07 ± 1.30 to 2.89 ± 1.31 ($p < 10^{-5}$).

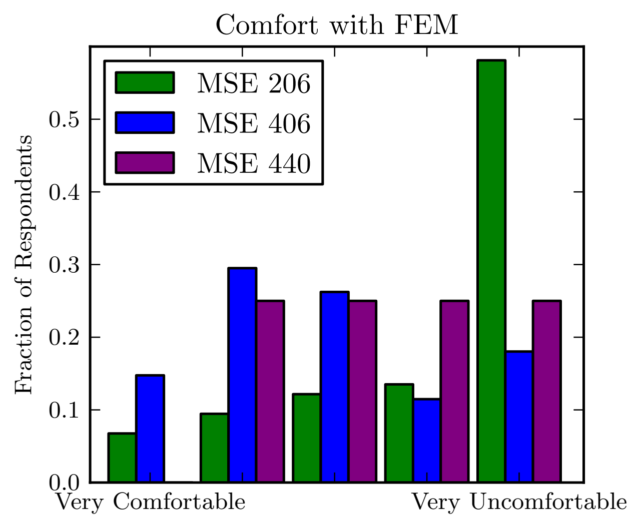

Figure 3: Students' perception of competency with FEM (OOF2). The sample sizes were 75, 70, and 12 for MSE 206 in Spring 2016, MSE 406 in Fall 2016, and MSE 440 in Fall 2016, respectively.

Flexible scheduling of the required junior-level courses (MSE 401, 402, and 406), potential selection bias in semi-required, specialized courses (MSE 304 and MSE 440), and the small size of and graduate student enrollment in more advanced courses (MSE 440 and MSE 498/404) all make it difficult to draw further comparisons of students' perception of competency with specific computational methods as they progress through the undergraduate program.

5.3. Efficacy of Capstone Computational Lab

To measure how the capstone Integrated Computational Materials Science and Engineering courses (formerly MSE 498; now MSE 404 MICRO and MSE 404 MACRO) affect students' attitudes toward computation, enrolled students were surveyed at the beginning and end of each half-semester course. Two questions, again rated on a 5-point Likert scale, queried information similar to what is discussed in the previous section:

- Entrance Survey: How confident are you in using the following computational tools? (Very Confident — 1 2 3 4 5 — Not at all confident)
- Exit Survey: How confident do you feel in your ability to go out and independently use the software packages we have worked with?
  (Very Confident — 1 2 3 4 5 — Not at all confident)

Figure 4 plots the distribution of responses in MSE 404 MICRO and MSE 404 MACRO in Fall 2016. As summarized in Table 5, two-tailed t-tests demonstrate that students' perception of competency in each computational method rises significantly after each course.

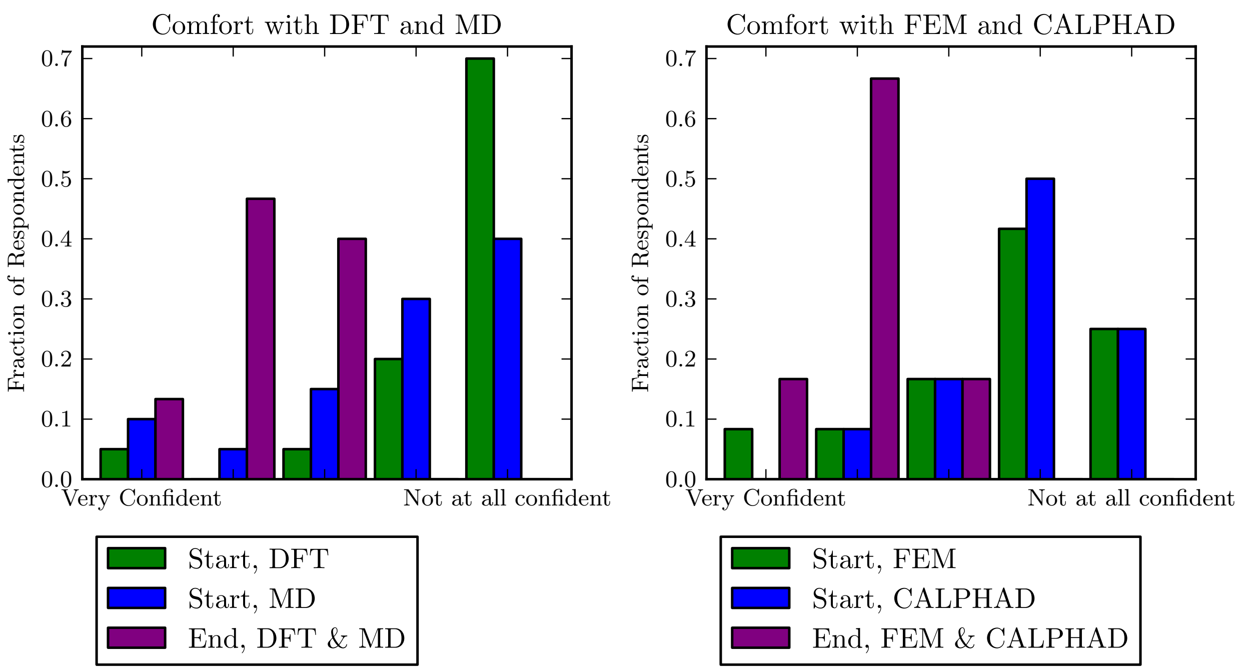

Figure 4: Students' perception of competency with density functional theory and molecular dynamics (left) and the finite element method and calculation of phase diagrams (right) upon entering and exiting MSE 404 MICRO and MACRO, respectively, in Fall 2016. The sample sizes ranged from 12 to 20.

6. Conclusions

Since the inception of the computational curriculum, students have consistently believed that computational skills are very important for their future careers. Accordingly, they have a strong

MSE 404 MICRO

	Mean Rating	p-value
End	2.27 ± 0.68	
Start, DFT	4.50 ± 0.97	$< 10^{-5}$
Start, MD	3.85 ± 1.28	5×10^{-5}

MSE 404 MACRO

	Mean Rating	p-value
End	2.00 ± 0.58	
Start, FEM	3.68 ± 1.17	3.8×10^{-4}
Start, CALPHAD	3.92 ± 0.86	$< 10^{-5}$

Table 5: Summary of Likert scale results from surveying MSE 404 students' confidence in using computational tools. The p-value listed for each entrance question is calculated relative to the corresponding exit question.

appetite for learning such computational skills early in the undergraduate program and in the absence of prior computational curriculum. As students experience more of the computational curriculum, their desire to learn computational skills lowers, demonstrating that the computational curriculum is starting to satisfy their interest in computation.

Moreover, students report a significantly higher perception of computational competency after completing two courses incorporating a particular computational method than after one. On average, students still felt “Uncomfortable” applying FEM after completing one FEM module, but felt slightly more comfortable than “Neutral” after completing three FEM modules. From this, we conclude that repetition and progressing complexity of computational material is essential to student learning and to the success of the computational curriculum.

Finally, students taking the capstone Integrated Computational Materials Science and Engineering course report increased confidence in computational ability across all methods covered in the course. Therefore, a dedicated computational laboratory course is extremely effective in providing comprehensive computational training.

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