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WORK IN PROGRESS: Computational Modules for the MatSE Undergraduate Curriculum

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Computational Modules for the MatSE Undergraduate Curriculum

1. Introduction and Background

As the use of simulations, big data, and numerical methods increases, the engineers of the future will increasingly be expected to possess computational competencies not only to perform well on the job, but even to understand the complex systems that govern the problems in their disciplines[1-3]. Computational competencies such as programming and the use of modeling and simulation tools are becoming core forms of literacy for most engineers on par with mathematics and the engineering sciences. The 2011 White House Materials Genome Initiative has created a particular imperative for computational competencies in Materials Science and Engineering, creating a demand for students who can engage in the computer-aided design of materials[4].

Meeting this new demand for computational competencies is not straightforward, as simply adding new subject matter independent of the traditional content is not viable in already packed curricula. To add these new competencies, we must either teach a smaller technical core to create space for computational competencies or find ways to synergize the instruction of computational competencies with the traditional content so that learning computational competencies accelerates learning of traditional content and vice versa.

Fortunately, early research into the use of modeling and simulation tools suggests that integrating these tools into instruction can foster deeper understanding of complex engineering concepts and problems[5-7]. In particular, these types of representations are particularly useful for helping students understand microscopic or abstract phenomena.

The Department of Materials Science and Engineering (MatSE) at the University of Illinois at Urbana-Champaign is synthesizing computational tools and skills across the curriculum. Over two years, using a collaborative course-development approach, a team of six faculty (one tenured professor and five assistant professors) have integrated training in computational competencies across five courses (MSE 201 – Phases and Phase Relations, MSE 206 – Mechanics for MatSE, MSE 304 – Electronic Properties of Materials, MSE 406 – Thermal and Mechanical Behavior of Materials, MSE 498AF – Computational MatSE). In this paper, we first describe the process for creating this curriculum revision and then describe the teaching methods and assignments of the revised courses. We conclude by presenting evidence for the effectiveness of this reform effort through the analysis of examination scores over multiple years.

2. Approach to course and curriculum reform

The College of Engineering's Strategic Instructional Initiatives Program (SIIP)[8] was created to transform and revitalize core engineering courses. Over the past three years, the program has catalyzed innovation in most departments and large-enrollment, core courses in the college[9,10]. Inspired by the work of Henderson et al., SIIP was designed to focus on creating collaborative teaching environments that enabled faculty to iteratively and sustainably innovate instruction. This environment was created by organizing faculty into Communities of Practice (CoPs) that would choose what innovations to pursue and evaluate their efforts to create those innovations. A

CoP is an organizational structure that effectively spreads knowledge, decreases the learning curve for novices, minimizes reenactments of failures, and promotes creativity[11,12].

The MatSE CoP is composed of one tenured and five tenure-track faculty who meet on a weekly basis to discuss course administration, data collection, and future plans. The goal of these meetings is to develop a common set of resources, policies, teaching methods, and learning objectives across the courses to facilitate students' computational competencies and technical content knowledge across the targeted course sequence.

The revisions to the MatSE undergraduate curriculum were guided by two curriculum and course reform aims: (1) integrating computational materials modeling in sophomore and junior-level core courses and (2) developing a capstone senior materials modeling elective. The integration of computational materials with technical content took place in MSE 201, MSE 206, MSE 304, and MSE 406, each of which has 100+ students enrolled each semester. Together, these courses span three broad areas of materials science: mechanics, thermodynamics, and electronic properties. The longitudinal integration of computational modules across the sophomore and junior years was intended to reinforce student awareness of computation, build confidence in using computational tools, and cement the idea of computation as the third pillar of science alongside experiment and theory. Accordingly, we expected that this integration would (a) make abstract theoretical concepts more accessible, (b) promote active learning and hands-on engagement, and (c) develop student competency in computational materials science software tools.

The second aim of this effort was to develop a new senior-year computational materials science elective MSE 498AF. The course has been dramatically reconceived to serve as an integrated computational materials science and engineering capstone design course to tie together students' experiences in the other courses. In this course, students solve a materials engineering design problem at multiple length and time scales using a diversity of software packages and computational tools, gaining broad experience and confidence in industrially relevant MatSE software packages, and a first-hand appreciation for the power and limitations of computational methods.

Team members have committed to recording and hosting all computational modules, lectures, and course forums online to facilitate access and dissemination of these materials.

3. Pedagogical reforms in courses

Aside from integrating computation across the curriculum, course reforms also focused on integrating evidence-based instructional practices into the courses[13-15]. Pedagogical reforms focused on integrating classroom responses systems (i>clickers), tablets for presenting content, online homework for rapid feedback, and discussion to promote deeper thinking and learning. In all cases, final annotated slides were posted for student access, as well as full lecture capture: video of projected slides and lecture audio.

4. Description of Computational Tools and Modules

The computational modules we have developed target four prime areas of computational materials science at different length scales using popular software packages: (i) density functional theory (DFT) with Quantum Espresso[16], (ii) molecular dynamics (MD) with LAMMPS[17] and Gromacs[18], (iii) finite element method (FEM) modeling with OOF2[19], and (iv) thermodynamic calculation of phase diagrams (CALPHAD) using Thermo-Calc[20]. By longitudinal integration of the modules into the core undergraduate curriculum, students will be repeatedly exposed to computational content over their academic trajectory at increasing levels of difficulty and complexity, ultimately preparing them for a capstone senior integrated computational materials engineering experience.

Each class has 2-3 computational modules associated with it. The current basic structure of a module is as follows: First, the subject, background, and tools of the module are introduced during a class lecture. Then, the module is given as a homework assignment, which students are expected to complete over the course of 1-2 weeks, with the aid of a dedicated computational TA, who holds 2-4 sessions of office hours in a computer lab that is accessible 24/7, in which the required software has been installed.

In Table 1 and the sections below, we briefly describe the particular modules developed, and their deployment in the target courses.

	DFT	MD	FEM	CALPHAD	Matlab
MSE 201	X			X	
MSE 206			X		X
MSE 304	X				
MSE 406		X	X		
MSE 498	X	X	X	X	X

Table 1. Deployment of computational modules into targeted courses.

Density Functional Theory (DFT)

Si crystal. Using the Quantum Espresso software with a GUI provided by nanohub.org[21], students in MSE 201 were asked to compute the equilibrium lattice constants of silicon for three different crystal structures using plane wave self-consistent field (PWSCF) calculations. Building on this module, students in MSE 304 and MSE 498 were asked to calculate the bulk modulus of silicon from pressure perturbations to the lattice constant and to calculate and visualize the band structure of silicon and compare the computed band gap property with experiment. As another extension, students in MSE 498 were asked to perform geometry relaxation and energy convergence with respect to the plane wave cutoff and k-point sampling, and explore the effect of different exchange correlation functionals and bound electron pseudopotentials.

Molecular Dynamics (MD)

Properties of Al. Students in MSE 406 used the LAMMPS software package to investigate the movement of a dislocation through a solid block of aluminum. They used the stress-strain curve to predict the Peierls stress of a dislocation, and the Ovito software package to visualize the movement and the change in stress-strain over the course of the simulation. As an extension, students in MSE 498 also predicted the Young's Modulus, and used both pieces of information to parameterize a finite element simulation, demonstrating the construction of an Integrated

Computational Materials and Engineering (ICME) bridge from one level of simulation to the next.

Nonequilibrium Folding. Students in MSE 498 used the Gromacs software package to perform a nonequilibrium pulling simulation of the unfolding of a ß-hairpin protein and to estimate the work required for the unfolding to occur.

Finite Element Method (FEM)

Temperature effects on strain. Students in MSE 206 used the OOF2 software package on nanohub.org to investigate the effects of geometry on a system of steel pins holding a dogbone-shaped aluminum sample. Students solved the coupled heat flux and force balance equations over a finite element mesh to compute the temperature and stress fields over the strip and predict its deflection. They then compared the stress patterns in systems with differently-shaped pins. As an extension, students in MSE 498 used Matlab to develop their own implementation of finite element software to solve the one-dimensional heat equation.

Nanocomposites. Students in MSE 406 used the OOF2 software package to explore the effects of fibers on strain and bulk modulus in a composite. They solved the force balance equations over a finite element mesh, in which applied strains were perpendicular and parallel to the direction of fibers along a composite. They investigated the effects of changing the Young's modulus of the fibers and of the matrix and visualized the resulting stress distribution.

Stress Field of a Crack. Students in MSE 406 used the OOF2 software package to explore the stress distribution around a crack tip. They solved the force balance equations over a finite element mesh for systems of a narrow and blunt crack and visualized the results. As a first extension, students in MSE 406 compared the results of the OOF2 simulation with the results obtained from performing a LAMMPS molecular dynamics simulation of crack propagation in aluminum and visualizing the dynamic stress distribution using Ovito. This module demonstrated the strengths and weaknesses of the two different software packages to the students. As a second extension, students in MSE 498 used the stress field at the tip of the crack to determine whether or not crack propagation would occur.

Matlab

Beam Design. Students in MSE 206 used Matlab to numerically determine the bending moment of differently-shaped beams in order to predict the most appropriate geometry with the goal of minimizing the stress a beam experienced under load.

Calculation of Phase Diagrams (CALPHAD)

Ag-Sn-Cu phase diagram. Students in MSE 201 used the Thermo-Calc software package to compute the $T - x$ phase diagram for each of the binary alloys and then computed the ternary phase diagram qualitatively by hand, as a demonstration of the design of an alloy for soldering applications.

Steel phase diagram and design. Students in MSE 498 used the Thermo-Calc software package to compute the $T - x$ phase diagram for a Fe-C carbon steel, and used this diagram to design an equilibrium microstructure with desired materials properties, computed the maximum operating temperature of their steel as a function of composition, and predicted the equilibrium fractions of pearlite and pro-eutectoid α-ferrite / cementite for eutectoid, hypoeutectoid, and hypereutectoid steels. Secondly, students in MSE 498 computed the ternary phase diagram for a Fe-C-Cr martensitic stainless steel, and determined an appropriate level of case hardening by surface carburization to trade-off competing constraints of hardness, toughness, and melting point to design a case hardened steel optimized for a particular application.

5. Student performance on examinations

In this section, we present data on the impact of the curriculum changes on students' exam scores. We focus only on MSE 201 and 206 because these two courses were the only ones taught by at least two different members of the CoP that also had similar enough exams between semesters to facilitate valid comparisons of student performance across semesters.

For MSE 206, final examination data was collected from the Spring 2014 and Spring 2015 semesters. Both examinations had 45 multiple-choice items (questions), of which 31 items (68%) were identical between semesters except for changes in the numbers used for calculations (i.e., the same figures and calculations could be used to solve the problem). Of these 31 items, 25 items (56%) were perfectly identical between semesters. For this analysis, all items were scored dichotomously (assigned a 0 for wrong, 1 for correct) so that a maximum score was 45 points.

Descriptive statistics for both examinations are presented in Table 2. 118 students took the final examination during Spring 2014, and 102 students took the final examination during Spring 2015. For all comparisons of performance between semesters, we used a 2-tailed t-test with a p-value of 0.05 as the threshold for significance and rejecting the null hypothesis. If a difference between course offerings is described as significant, it should be interpreted as $p < 0.05$.

Using all examination items, we found that students performed significantly better in Spring 2015 than in Spring 2014.

	N	μ	σ
SP14	118	32.3	6.9
SP15	102	35.3	6.3

Table 2. Statistics for all examination items for MSE 206.

To make sure that the difference in performance was not an artifact of differences in performance on the non-identical items, we repeated the above analysis on only the 25 perfectly identical items between semesters. Descriptive statistics of this subtest are presented in Table 3. Using only the perfectly identical examination items, we found that students still performed significantly better in Spring 2015 than in Spring 2014.

	N	μ	σ
SP14	118	18.3	4.0
SP15	102	20.3	3.7

Table 3. Statistics for identical items for MSE 206.

For MSE 201, final examination data was collected from the Fall 2013 and Fall 2014 semesters. Both examinations had 17 items (questions), of which 14 items were written to test the same concepts. For this analysis, all items were scored with a minimum score of 0 and maximum score of 1. We present only an analysis of those items that were intended to test the same conceptual content, so a maximum score is 14 points.

Descriptive statistics for both examinations are presented in Table 4. 48 students took the final examination during Fall 2013, and 57 students took the final examination during Fall 2014.

	N	μ	σ
FA13	48	12.07	1.5
FA14	57	12.95	1.7

Table 4. Statistics for all items for MSE 201.

We found that students performed significantly better in Fall 2014 than in Fall 2013.

Student performance on computationally related questions

Because a core goal of the evaluation was to determine whether adding computational modules improved students' understanding of core content, we repeat the above analysis examining only those items that assess students' knowledge of content covered by the computational modules in each of the courses.

In MSE 206, five items pertained directly to the content covered by the computational modules. Descriptive statistics of this subtest are presented in Table 5.

Using only the items that covered content related to the computational modules, we found that students performed significantly better in Spring 2015 than in Spring 2014.

	N	μ	σ
SP14	118	3.6	1.2
SP15	102	3.9	1.1

Table 5. Statistics for computational items for MSE 206.

In MSE 201, three items pertained directly to the content covered by the computational modules. Descriptive statistics of this subtest are presented in Table 6.
Using only the items that covered content related to the computation modules, we found no significant difference in performance between semesters.

	N	μ	σ
SP14	48	2.7	0.4
SP15	57	2.8	0.3

Table 6. Statistics for computational items for MSE 201.

6. Discussion of Student Learning Outcomes

Results from MSE 201 and 206 suggest that the combination of pedagogical changes and the addition of computational modules has improved students' learning outcomes in MSE 201 and

206. The reform efforts revealed significant improvements in exam scores. These improvements are robust across courses, minimizing the likelihood that the changes are dependent on changes in instructors. The improvements in student performance cannot be explained by students' access to previous exam questions either as the improvements in students' learning is robust across identical and non-identical exam items.

It is not clear from the data whether the improvements in students' learning was caused primarily by the pedagogical changes or the addition of computational modules. The subtests of computation questions had insufficiently large samples to draw strong conclusions. The data suggests that the computation modules may play a role in improving student learning, but the results are not robust across courses. At minimum, though, the addition of the computation modules did not undermine or hinder students' learning of the core disciplinary content. Critically, then, students were able to learn additional computational content important for success in industry and post-graduate academic work without compromising their ability to learn the original content of the classes.

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