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Successes and Lessons Learned in an Undergraduate Computational Lab Sequence for Materials Science and Engineering

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Abstract

In 2012, with a switch from quarters to semesters of instruction during the academic calendar year, the Materials Science & Engineering Department at The Ohio State University added a series of computational labs to the required undergraduate curriculum. Over the course of the next 4 academic years, the achievement of student outcomes and student feedback on the courses were monitored while minor changes were made to the curriculum. While student outcomes were generally achieved, student dissatisfaction with the course structure was high. In the 2016- 2017 academic year, several substantial changes were made to the sophomore and junior lab courses in response to this data. Curricular changes included an increased emphasis on pseudo-code development, routine reflection on assumptions and limitations of models used in lab meetings, and a move of the lectures and discussions to after the in-depth lab assignments. In addition, short modules on data analysis, elementary statistics, and linear algebra were included. Interestingly, student feedback revealed that a number of "problems" with the lab sequence stem from the perception that either computational thinking is not a relevant skill for a materials engineer, or that students were not in fact learning more than how to use a specific software package. To combat these factors and increase students' self-efficacy, a "marketing campaign" was implemented for these courses. The results of these five years of aggressively including computational modeling into the undergraduate materials science curriculum, including student perceptions and achievement before and after these changes, can provide valuable insight for any department interested in making similar changes.

Keywords

Materials Science, Modeling, Computation, Curriculum

Introduction

Simulations and "big data" are increasingly critical components of research and engineering, and engineers must be trained in basic competencies of these methods. While most (if not all) MSE departments recognize this, the challenges inherent in meeting this demand by employers is often complicated. First, the subject lacks a well-defined structure or sense of baseline equivalencies. Faculty expertise with computational methods is also varied, and few textbooks devoted to the topic exist. In their review of the status of computational materials science education in 2003, Thornton and Asta noted that even among the minority of programs offering computational undergraduate Materials Science & Engineering (MSE) courses, those courses had been added since the year 2000 (Thornton and Asta, 2005).

The Ohio State University switched from a quarter-based curriculum year with 3 quarters on instruction to one based on 2 semesters starting in the 2012 – 2013 academic year. This change required major revisions to parts of the MSE curriculum. As part of these changes, 3 required computational labs were added as required courses for all undergraduate MSE majors. Many disciplines require computational tools and methods be taught in introductory engineering courses during students' first year, or that students take additional courses on tools later during their tenure. This is the method implemented in other engineering disciplines at OSU. In 2012, several other institutions were incorporating computational assignments and/or courses into the required *MSE* curriculum, but not to the extent of 3 semester-long required lab courses. By developing new courses specifically designed to tie computational assignments to concurrent and preceding courses in the undergraduate curriculum, OSU made use of significant faculty expertise in modeling and simulation to develop and teach this curriculum. By operating these courses as weekly labs with significant instructor and TA oversight during extended hands-on course sections, the courses focused on the need for students to learn to use computational tools by doing.

This paper introduces the curriculum of this 3-semester computational laboratory sequence, discusses the largely qualitative analyses done to measure its efficacy via different metrics, and proposes reasons for some of the successes and failures.

Curriculum

The "Modeling and Simulation in Materials Science" sequence of courses included three labs administered in the 4^{th}, 6^{th}, and 7^{th} semesters of a "standard" 8-semester undergraduate curriculum in MSE. While there are always deviations from a standard course map for individual students, the course offerings at OSU are such that most students did take this sequence of courses in that order (which is required) and in those particular semesters. The general outline and descriptions of the courses are outlined in Table 1.

Table 1: Overview of Curriculum for 3 the 3-Semester Sequence of Computational MSE Labs

	Lab 1 (Semester 4)	***Lab 2 (Semester 6)***	***Lab 3 (Semester 7)***
Computational Tools Used	MATLAB (8 weeks) CES EduPack (3 – 4 weeks) Crystal Maker (3 – 4 weeks)	MATLAB	MATLAB LAMMPS ABAQUS CES EduPack
Courses aligned with assigned computational problems	Intro to Materials Science (previous semester) Thermodynamics (concurrent) Cyrstallography and Characterization (concurrent)	Phase Transformations and Processing (previous semester) Kinetics and Diffusion (previous semester) Mechanical Behavior of Materials (concurrent)	Mechanical Behavior of Materials (previous semester) Senior Design (concurrent or subsequent semester) Materials Selection (concurrent)

MATLAB was selected as the primary computational tool because it was already introduced to all MSE students in the first year engineering sequence and was the most frequently used tool (other than Microsoft Excel) for data analysis and graphing at the university. CES was already used extensively in a required course on Materials Selection taught in the senior year. Crystal Maker was already being used in elective and graduate level crystallography courses, and it was felt that including it in the undergraduate curriculum would help students learn and visualize more complicated crystal structures. To facilitate weekly labs, a significant departmental infrastructure investment was made to equip one of the computer labs with additional lecture equipment and to arrange workstations to be conducive to working in small groups of 3-6 students.

Each course is separated into 3 units, and each unit was taught by one professor and 3 or 4 instructional assistants. This allowed the topics to be taught by faculty with expertise in the content and computational methods being used and for the students to have significant one-on-one help from both the professor and IAs during the class meetings. Each course consists of a 1-hour long weekly lecture in addition to the labs. In the first year, these lab sessions occurred once weekly for students for 2.25 hours, thus maintaining a ratio of instructor-to-student of at least 1:8. In the second and third courses, labs met twice weekly for 1.5 hours each and the ratio was closer to 1:13.

The curriculum and assignments were developed by professors at OSU, and reading and support material was assigned from various texts available as eBooks on the university's library system. The typical workflow for students included initial reading and video watching done individually out of class, followed by a reading quiz and pen-and-pencil activity during lecture. In labs, students are given short warm-up activities introducing them to the use of a new program function or computational method. The rest of the lab period was devoted to in-class exercises that covered a computational application or concept similar to the homework assigned for the week. In this way, most of the deep learning occurred in the presence of peers and with the support of frequent help the instructors. In completing assignments that required writing scripts from scratch, students are encouraged to write out pseudo-code or "map" their programming plan.

As with any new course, minor modifications to pedagogy, structure, and assignments were made in each iteration and assessments were frequently shared between instructors of the courses. Student evaluations conducted mid- and post- semester influenced these relatively minor modifications. This was a significant change to the curriculum, however, and a cohort of students who had taken all 3 lab courses would not graduate until the 2014 – 2015 academic year. Therefore, it was decided that no major curricular revisions would be made for at least 3 years. Generalized results of these first 4 years indicate a number of successes as well as several unanticipated difficulties.

Assessment and Discussion

In evaluating the success of this laboratory sequence, three questions were asked:

1. Are the learning objectives for each course being met?
2. Are students incorporating the use of these tools in other courses more frequently or with better results?
3. What is the general attitude of students to the modeling & simulation course sequence and its effects on their preparation for future success?

Direct assessment methods are implemented for many undergraduate courses in the MSE curriculum, including the modeling & simulation labs. Additionally, the depth of interaction between the IAs and students allowed for the use of formal and informal assessment of students' skills and attitude. These assessments indicate that the majority of students are at the "meets expectations" or "exceeds expectations" level of achievement for most objectives in all three computational labs from 2013 through 2016.

One expected outcome of introducing the first lab at the start of the MSE curricular sequence was that students would begin to use these tools in their courses. Discussions with other instructors recorded the exclusive use of Microsoft Excel for graphing, laboratory reports, and data analysis. While MS Excel is more widely used in industry than MATLAB, it is also true that proficiency with MATLAB could translate to Excel more easily than the reverse. The assumption was that students would use more reliable sources and effective tools if they were exposed to them and taught to build competency in these tools. While some students began to use MATLAB and CES for course projects and laboratory reports after their 4^{th} semester, this was nowhere near as widespread as anticipated despite frequent reminders and incentives from instructors. This was still the case in the 2015 – 2016 academic year, in which less than 15% of laboratory reports submitted during the Junior year lab sequence included data analysis done in MATLAB or materials data reported from CES Edupack. Thus, the goal of building familiarity and confidence with more robust computational tools did not extend to their use outside of assignments for which it was required.

Student perception of the importance of computational tools and their preparation increased as a result of taking the courses. In Spring 2016, graduating seniors and students in the junior class (anticipated graduation date of Spring or Autumn 2017) took a survey asking them a number of questions about their perceptions of the importance of various aspects of the MSE curriculum to their career and their current preparation. Four questions in particular relate directly to their perceived value and quality of preparation:

- How important to your career is the ability to use the techniques, skills, and modern engineering tools necessary for engineering practice (ABET student learning outcome (k))?
- What is your current preparation in the ability to use the techniques, skills, and modern engineering tools necessary for engineering practice?
- How important to your career is the application of computational methods to solve materials problems?
- What is your current preparation in the application of computational methods to solve materials problems?

As shown in Table 2, students on average acknowledge the importance of computational methods as an engineering tool and feel that their education is preparing them to use these tools.

Table 2: Selected results from surveys administered to Juniors and Seniors in Spring 2016.

		Number of Students Responding					
	Survey Question	**1** Not Prepared or Not Important	**2** Somewhat Prepared or Somewhat Important	**3** Prepared or Important	**4** Very Prepared or Very Important	**5** Extremely Prepared or Extremely Important	Average
Graduating Seniors Spring 2016 (35 responses)	**Importance** of Using Engineering Tools (ABET (k))	1	1	5	11	17	4.20
	Preparation for Using Engineering Tools (ABET (k))	2	4	7	13	9	3.66
	Importance of the application of computational methods	2	3	12	7	11	3.63
	Preparation for the application of computational methods	3	4	14	8	6	3.29
Juniors Spring 2016 (53 responses)	**Importance** of Using Engineering Tools (ABET (k))	0	0	7	20	16	4.36
	Preparation for Using Engineering Tools (ABET (k))	1	3	22	22	6	3.57
	Importance of the application of computational methods	0	1	7	25	20	4.21
	Preparation for the application of computational methods	0	1	21	18	3	3.25

However, students have often expressed frustration with the computational lab courses since their inception. Initially, student comments indicated this dissatisfaction could be attributed to aspects of the course organization and communication and the difficulty of the assignments. Also, the first two cohorts of students to graduate after 2012 did not experience the courses until later in the curriculum and did not benefit from the full 3-course sequence. However, the improvements made in the first three years did not significantly increase student satisfaction with the courses. In the survey administered to graduating seniors and juniors administered in spring 2016, students were also asked to indicate the course or series of courses most and least valuable to their education and why. A startling number of students indicated that the computational lab sequence was the least valuable, as shown in Table 3.

Table 3: Student perceptions of the value of the computational labs as recorded by a survey administered to graduating seniors and junior students in spring 2016.

	*What course in the MSE curriculum has been the **MOST** valuable to you, and why?*	*What course in the MSE curriculum has been the **LEAST** valuable to you, and why?*
*Number of **graduating seniors** in spring 2016 who selected the modeling & simulation laboratory sequence (n = 35)*	2 (6%)	13 (37 %)
*Number of **juniors** in spring 2016 who selected the modeling & simulation laboratory sequence (n = 53)*	2 (4 %)	8 (19 %)

While these survey results are from a single year, there is a clear disconnect between their perception of the value and preparation related to computational tools resulting from their education and the perception that the computational labs are not valuable. Analysis of students' reasons indicate two broad themes:

The courses are too difficult. Students often felt that previous coursework and preparatory materials did not provide sufficient preparation. Assignments early in a semester might ask a student to analyze, comment, or debug a script in MATLAB but they were not able to make the transition to developing their own pseudo-code or writing a script "from scratch". Students had less difficulty with software packages that included a strongly graphical user interface such as CES Edupack and Crystal Maker.

The computational lab material is not valuable for career preparation. Many students expressed opinions that can be summed up by one interviewee's comment: "I will never need to program or use computational tools *like that*". Specifically, the use of MATLAB was frustrating for a number of students because they believed that the work they would do as an engineer would never require the use of "programming". A number of students indicated that only Excel was used in their internship experiences, but did not realize that the logic and pseudo-code used in MATLAB assignments translates to techniques that would be used to analyze similarly complex problems in Excel (or a number of other computational tools). In short, students were often not clearly differentiating the tasks and lower level skills necessary to use MATLAB from the overarching concepts about modeling being taught.

The computational labs are not directly related to materials science. This opinion was frankly perplexing to the instructors. All activities using CES and CrystalMaker were clearly related to materials science topics. While some of the in-lab activities used to introduce a technique, series of commands, or toolbox in MATLAB were discipline agnostic, the homework assignments that followed these were directly related to materials science topics. Future surveys and interviews will probe this question further.

Conclusions

The inclusion of a set of 3 semester-long computational labs to the required MSE undergraduate curriculum has successfully improved the skills of students to use a variety of computational tools. Various direct assessments including lab-based practical skills tests conducted in each class confirm that course learning objectives are largely being met. However, widespread use of the tools has not extended to other courses. More importantly, the perception of a significant minority of students is that computational tools as taught in these courses is not valuable. Several students have complained that the courses are far too difficult and previous exposure to MATLAB in the first-year engineering courses was insufficient. To address this, modifications are being made to introduce and reinforce very basic MATLAB skills at the start of the semester in the first computational materials lab course. Content from the computational labs is also being integrated with concurrent courses to a greater degree.

At the risk of overgeneralization, the successes and difficulties outlined in this analysis indicate that perception and culture may be just as important as curriculum in preparing undergraduates to be computationally proficient engineers. It is possible to dramatically improve students' skills at using computational methods by adding courses and/or exercises to the curriculum. Additionally, students increasingly identify computational skills in particular as being important for their career success. However, the link between the curriculum and the more nebulous concept of "computational thinking" required for all engineers is often inscrutable for students. For broader success, it seems that instructors must guide the students in the metacognitive aspects of developing computational skills that are broader than simple syntax and tool-specific tasks and *very explicitly* and *frequently* reinforce the concepts of computational thinking being taught. Future modifications to this course sequence will focus on unifying the 3 courses as a full sequence and addressing these perception issues. Further research studies are also being developed to investigate additional barriers to student success.

References

1 Thornton, K., and Mark Asta. "Current status and outlook of computational materials science education in the US." *Modelling and Simulation in Materials Science and Engineering* 13.2 (2005): R53.