

## **Impact of Computational Curricular Reform on Non-participating Undergraduate Courses: Student and Faculty Perspective**

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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. His work has been recognized by the NSF Career award, the Young Leaders Award from The Minerals, Metals, and Materials Society, the Emmy Noether award by the German Research Foundation, and the Young Talent Award and the Masing Memorial Medal from the German Materials Society. He is a member of the international Alexander von Humboldt network.

**Dr. Pascal Bellon, University of Illinois, Urbana-Champaign**

After earning a PhD in Materials Science from University of Paris 6, France, Pascal Bellon worked during 7 years at CEA-Saclay, France, before joining the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign as a tenure-track Assistant Professor in 1996, where he was promoted to the ranks of Associate Professor in 2002 and Full Professor in 2009. He received an NSF career award in 1998 and awards from the Academy for Excellence in Engineering Education from the University of Illinois in 1998, 1999 and 2000. He received the Don Burnett teaching award in 2000, the Accenture Engineering council award for Excellence in Advising in 2007 and the Stanley Pierce award in 2009. In 2012 Pascal Bellon was named a Racheff faculty scholar, and in 2016 he was inducted as the Donald W. Hamer Professor in Materials Science and Engineering.

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Dr. Shang received his Ph.D. from the University of California at Berkeley in 1989 and has been on the faculty of the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign since 1990. His research interests include advanced materials for environmental control, interconnect materials for microelectronics, and composite materials for structural applications.

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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.

**Prof. Timothy Bretl, University of Illinois, Urbana-Champaign**

Timothy Bretl is an Associate Professor of Aerospace Engineering at the University of Illinois at Urbana-Champaign. He received his B.S. in Engineering and B.A. in Mathematics from Swarthmore College in 1999, and his M.S. in 2000 and Ph.D. in 2005 both in Aeronautics and Astronautics from Stanford University. Subsequently, he was a Postdoctoral Fellow in the Department of Computer Science, also at

Stanford University. He has been with the Department of Aerospace Engineering at Illinois since 2006, where he now serves as Associate Head for Undergraduate Programs. He holds an affiliate appointment in the Coordinated Science Laboratory, where he leads a research group that works on a diverse set of projects (<http://bretl.csl.illinois.edu/>). Dr. Bretl received the National Science Foundation Early Career Development Award in 2010. He has also received numerous awards for undergraduate teaching in the area of dynamics and control, including all three teaching awards given by the College of Engineering at Illinois (the Rose Award for Teaching Excellence, the Everitt Award for Teaching Excellence, and the Collins Award for Innovative Teaching).

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Dr. Geoffrey L. Herman is a teaching assistant professor with the Department of Computer Science at the University of Illinois at Urbana-Champaign. He also has a courtesy appointment as a research assistant professor with the Department of Curriculum & Instruction. He earned his Ph.D. in Electrical and Computer Engineering from the University of Illinois at Urbana-Champaign as a Mavis Future Faculty Fellow and conducted postdoctoral research with Ruth Strevler in the School of Engineering Education at Purdue University. His research interests include creating systems for sustainable improvement in engineering education, conceptual change and development in engineering students, and change in faculty beliefs about teaching and learning. He serves as the Publications Chair for the ASEE Educational Research and Methods Division.

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# **Impact of Computational Curricular Reform on Non-participating Undergraduate Courses: Student and Faculty perspective**

## **1 Abstract**

A computational approach has become an indispensable tool in materials science research and related industry. At the University of Illinois, Urbana-Champaign, our team at the Department of Materials Science and Engineering (MSE), as part of a Strategic Instructional Initiatives Program (SIIP), has integrated computation into multiple MSE undergraduate courses over the last years. This has established a stable environment for computational education in MSE undergraduate courses through the duration of the program. To date, all MSE students are expected to have multiple experiences of solving practical problems using computational modules before graduation. In addition, computer-based techniques have been integrated into course instruction through iClicker, lecture recording, and online homework and testing. In this paper, we seek to identify the impact of these changes beyond courses participating in the original SIIP project. We continue to keep track of students' perception of the computational curriculum within participating courses. Furthermore, we investigate the influence of the computational exposure on students' perspective in research and during job search. Finally, we collect and analyze feedback from department faculty regarding their experience with teaching techniques involving computation.

## **2 Introduction**

A computational approach has become an indispensable tool in materials science research and related industry. In addition to the research interest, the 2009 survey by Thornton *et al.* [1] and the followup 2018 survey by Enrique *et al.* [2] showed that employers of MSE students, such as industry and national labs, clearly value computational materials science education. Both surveys found that employers expect MSE graduates to have knowledge of available computational techniques in their area of expertise as well as their applicability. These surveys also highlighted the gap between what is typically taught in courses (e.g. atomistic methods) and what is commonly used in industry (e.g. continuum models). These findings originally called for the curricular reform in our MSE program.

In response to this, our faculty team started an initiative project, under a Strategic Instructional Initiatives Program (SIIP) of the College of Engineering, which aims to establish a collaborative

teaching environment to enhance instruction and to incorporate computational modules into core classes with large enrollment. The collaborative environment is inspired by Henderson *et al.* [3, 4, 5, 6], in order to support faculty members throughout different stages of adopting innovative teaching techniques. This is done by forming a Community of Practice environment, in which knowledge is efficiently spread and learning curves of new adopters are reduced. More details can be found in our earlier publications [7, 8, 9].

Our previous studies demonstrate the effectiveness of computational curriculum reforms. Mansbach *et al.* showed that students' performance, measure by the average grade, increases after the reform [9]. Kononov *et al.* showed that while students initially expressed a desire for more usage of computational modules in the curriculum, this desire was largely satisfied once the reform extended over all course levels. Previous work also showed that students gained confidence in using computational tools after taking the reformed courses [7, 10]. However, we also noticed that the surveys in these studies are limited to students taking the SIIP courses and lacked information about the broader impacts of the reform.

In this paper, we study the effectiveness of the computational modules by tracking students' confidence in using computational tools to solve course-specific problems. We find results consistent with our early studies, showing that the students' confidence increases at the end of the courses. To address the limitation mentioned above, we devise two new surveys: One targeting MSE graduating senior students, who in principle experienced all the required courses, and another survey targeting MSE course instructors. The survey for senior students aims to identify the influence of the SIIP program on their general learning experience and their research and job hunting experience. The survey for instructors aims to solicit feedback about their experience with computer-based teaching techniques and to identify possible influence on non-SIIP courses.

The remainder of the paper is structured as follows: In Section 3, we briefly describe the computational modules used in the SIIP courses. In Section 4, we continue to track the effectiveness of the computational modules. Specifically, we look at students' confidence in using computational modules before and after taking the reformed courses. The influence of computational modules on graduating seniors students' learning, research and job hunting experience is summarized in Section 5. Lastly, we present what we find from the survey targeting department instructors in Section 6 and summarize the paper in Section 7.

### **3 Curriculum and Computational Modules**

Since 2017, the curricular reform within SIIP courses has reached a stable state and only small tuning was done afterwards. The details of the reform can be found in earlier studies in the literature [7, 8, 9]. The SIIP courses include all the required undergraduate courses and some of the semi-required and elective courses (see Table 1).

Each course has two to three computational modules, which cover topics that are directly related to the course content (see Table 2 for details). The specific tools used in computational modules include:

- Quantum Espresso [11] for density functional theory (DFT)

- LAMMPS [12] for molecular dynamics (MD)
- OVITO [13] for atomic visualization
- OOF2 [14] for finite element method (FEM)
- Thermo-Calc [15] (CALPHAD) for phase diagrams
- MATLAB [16] for numerical computing

Table 1: MSE courses involved in this paper, organized by their types and levels. SIIP courses are marked by † and courses that are not involved in our instructor survey are marked by \*.

Number	Name	Level	Type
201†	Phase and Phase Relations	Sophomore	Required
206†	Mechanics for MSE	Sophomore	Required
401†	Thermodynamics of Materials	Junior	Required
402†	Kinetic Processes in Materials	Junior	Required
406†	Thermal and Mechanical Behavior of Materials	Junior	Required
395	Materials Design	Senior	Required
304†	Electronic Properties of Materials	Junior	Semi-required
405	Microstructure Determination	Junior	Semi-required
404-BS	Laboratory Studies in MSE: Biomaterials Synthesis	Senior	Semi-required
404-BA	Laboratory Studies in MSE: Biomaterials Application	Senior	Semi-required
404-PC	Laboratory Studies in MSE: Polymer Characterization	Senior	Semi-required
404-PS	Laboratory Studies in MSE: Polymer Synthesis	Senior	Semi-required
403	Synthesis of Materials	Junior/Senior	Elective
422	Electrical Ceramics	Junior/Senior	Elective
440†*	Mechanical Behaviors of Materials	Junior/Senior	Elective
487	Materials for Nanotechnology	Junior/Senior	Elective

Table 2: Computational methods integrated in SIIP classes. The module development for each listed course has reached stable state since 2017. Course number of 404 is a general course number for lab studies and here refers to "Computation in MSE". † CALPHAD was not used for MSE 401 in 2017 and 2018.

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
404	X	X	X	X	X

#### 4 Continuous trend of improving confidence in computational tools

Our previous studies [7, 10] show that incorporating computational modules in SIIP courses improves students' confidence in using specific computational tools. In this section, we analyze survey data collected from two SIIP courses that have results for both entry and final surveys, MSE 201 (Fall 2018) and MSE 206 (Spring 2018). In order to determine whether our SIIP program is at stable state and continues to improve students' confidence in using specific computational tools, we asked the following questions.

In MSE 201, students were asked,

- If you were asked to determine the stable crystal structure and lattice parameters, how comfortable would you be? (Very comfortable — 1 2 3 4 5 — Very uncomfortable)

and in MSE 206, students were asked,

- If you were asked to determine the bending of a beam under loads, how comfortable would you be using MatLab/Finite Element (e.g. OOF2)? (Very comfortable — 1 2 3 4 5 — Very uncomfortable)

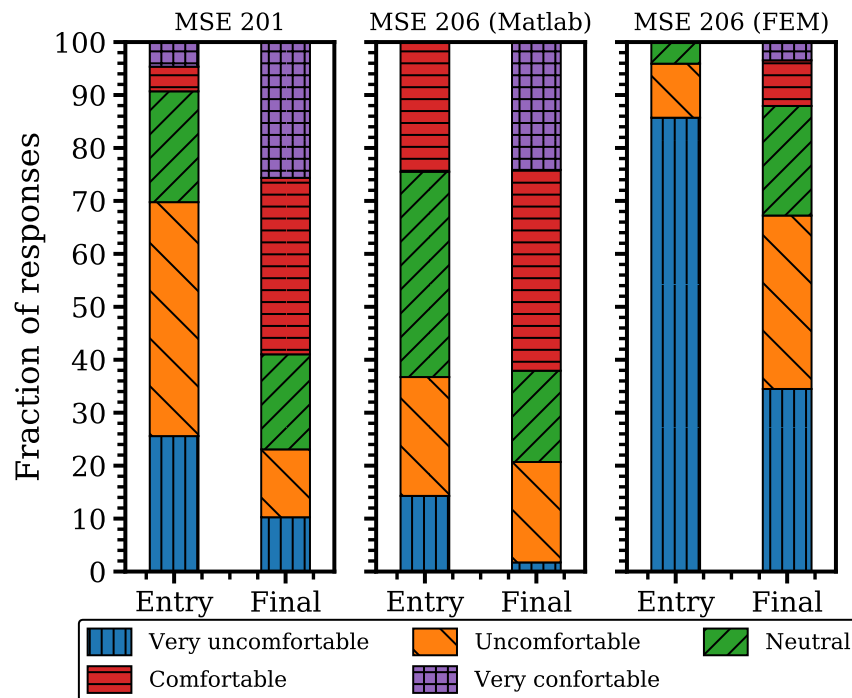


Figure 1: Students' confidence in using computational tools to solve course specific problems at entry and final surveys for MSE201 and MSE206.

Figure 1 shows consistent results with our earlier studies [7, 10]: Students become comfortable with using computational tools to solve materials science problems after taking the courses. For MSE 201, the combined fraction of students that are either comfortable (scale 2) or very comfortable (scale 1) increases from 9 % to 59 %. This is in agreement with the change in the

mean value of confidence from  $3.81 \pm 1.03$  to  $2.49 \pm 1.30$ , with 43 and 39 responses, respectively. Similarly for MSE 206, we find that the fraction of students that are either comfortable or very comfortable increases from 24 % to 62 % for MATLAB and from 0 % to 12 % for FEM. The mean value of confidence changes from  $3.27 \pm 1.00$  to  $2.36 \pm 1.10$  for MATLAB and from  $4.82 \pm 0.49$  to  $3.86 \pm 1.10$  for FEM, with 49 and 58 responses for entry and final survey, respectively. The consistent trend with previous results confirms that the computational curricular reform is at a stable state and is effective within the SIIP courses.

## 5 Graduating senior students' perception

To understand the impact of the SIIP program beyond the directly affected courses, we designed a survey targeting graduating senior students. These senior students have experienced all the computational modules throughout their curriculum and, therefore, best represent the students affected by the SIIP project. This survey was distributed in the Materials Design course (MSE 395), which is a required course for all senior MSE students. The survey focuses on three major parts: (1) Computational learning experience; (2) Research and job hunting experience; and (3) Attitude towards computational tools. We received 32 responses out of a class of 103 students.

### 5.1 Computational learning experience

To understand the influence of computational modules on student learning throughout the curriculum, we asked the following three questions:

- Q1: Do you think computational modules are helpful for you to understand the related course materials?  
(Very helpful — 1 2 3 4 5 — Not helpful at all)
- Q2: Among all the content in your curriculum, you can understand that with computational modules better?  
(Strongly agree — 1 2 3 4 5 — Strongly disagree)
- Q3: You can memorize the course materials that are connected to computational modules better?  
(Strongly agree — 1 2 3 4 5 — Strongly disagree)

Figure 2 shows that more than 50 % of senior students think the computational modules in the curriculum help them understand the course content, while less than 20 % of the students find it not helpful. However, when comparing effectiveness of computational modules to the traditional pen and paper approach, students think they are equal: About one third of the students indicate they can learn the content with computational modules better, while one third of the students disagrees. When it comes to memorizing the course content, more than 50 % of the students find it harder to memorize content connected to computational modules, while only 22 % of students find it slightly easier. This seems to suggest that computational modules are useful teaching tools but are not superior to traditional pen-and-paper approaches. However, students' responses to Q2



and Q3 could also result from the additional work load of learning computational skills while perceiving the modules as not connected closely enough to the course content. Further investigations are needed to draw a solid conclusion and we plan to ask questions regarding the connection between computational modules and course content in future surveys.

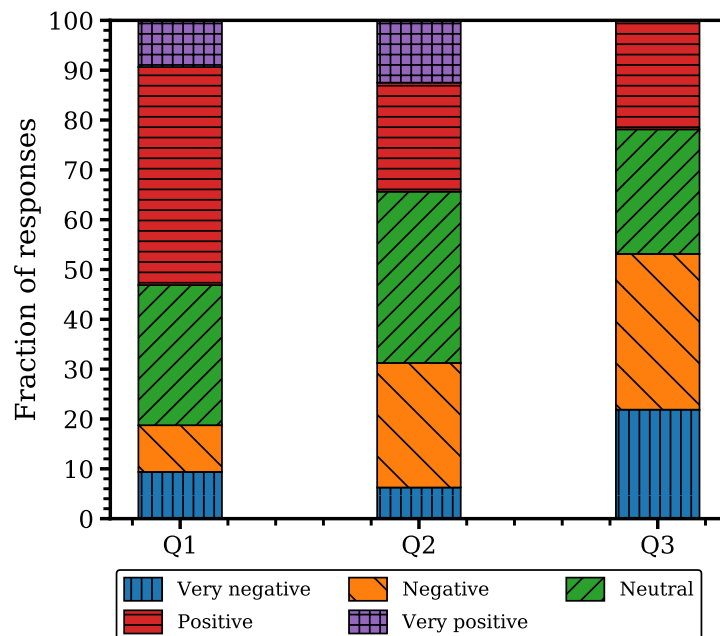


Figure 2: Students' perception of the influence of computational modules on their learning experience. Details of Q1, Q2, and Q3 are described in the text.

We also asked graduating students about their confidence (Very comfortable — 1 2 3 4 5 — Very uncomfortable) in using different software packages to solve materials science problems (see Fig. 3 for results). Similar questions were asked at the end of the courses that incorporate computational modules. We find that students have highest confidence in using MATLAB for numerical analysis, followed by OOF2 (FEM), LAMMPS (MD), and OVITO (visualization). The students have lowest confidence in using Quantum Espresso (DFT) and Thermo-Calc (Calphad).

This correlates with frequency of usage: MATLAB is frequently used throughout the curriculum, also outside of SIIP courses. Students are exposed first to MATLAB in CS 101 in their first year, which explains the high level of confidence in the entry survey for MSE 201, their first SIIP course. OOF2 is used in sophomore- and junior-year courses (MSE 206 and 406) while three junior courses incorporate MD simulations (MSE 401, 402, and 406). On the contrary, students only experience Thermo-Calc once in MSE 201, which is a sophomore course. Students express significantly higher confidence in using Thermo-Calc at the end of MSE 201 ( $2.87 \pm 0.95$ ), but the confidence seems to decay over time ( $3.28 \pm 1.44$ ). We believe that this occurs because students are not exposed to it later in the curriculum.

Lastly, students are least comfortable with using DFT, despite it being used in modules for MSE 201 and 304. While MSE 304 is not a required junior-level course, the majority of the responses

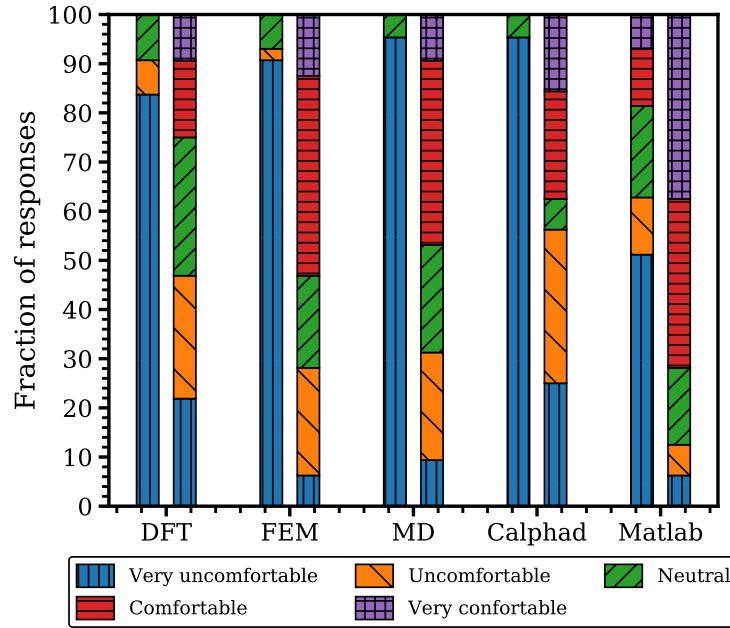


Figure 3: Students' perception about their confidence in using computational tools at the entry survey of MSE201 (left bars) and in their senior year (right bars).

( $\approx 80\%$ ) are from students who had taken the course. Comparing the confidence levels ( $3.34 \pm 1.24$ ) with those in the final surveys of MSE 201 and MSE 304 ( $3.30 \pm 0.88$  and  $3.51 \pm 1.25$ , respectively), we find that they are comparable. This rules out frequency of usage as contributor; further investigation is required to understand why students are least comfortable with DFT. Generally, we conclude that repetitive usage throughout the curriculum can help boost students' confidence. Also, the graduating students' confidence in using those computational tools is significantly improved compared to their confidence as sophomores.

## 5.2 Research and job hunting experience

To understand how exposure to computation affects undergraduate students' choices of their research career, we asked the following question:

- Your past experiences with computational modules motivate you to choose a computational research topic (Strongly agree — 1 2 3 4 5 — Strongly disagree)

The responses are shown in Table 3.

	Strongly agree	Agree	Neutral	Disagree	Strongly disagree
Fraction	6 %	16 %	22 %	19 %	37 %

Table 3: Students' perception of the influence of computational modules on their desire to conduct computational research in the future.

Approximately 22 % of the graduating senior students indicate that their experience with computational modules motivates them to choose a computational research topic in the future. We plan to ask their future/acquired jobs and their original tendency in a future survey to better clarify the influence of computational modules on this topic.

Next, we asked students about their perception of the influence of computational modules on their job hunting process with the following three questions:

- Q1: Your past experiences with computational modules are considered as advantage in your resume  
(Strongly agree — 1 2 3 4 5 — Strongly disagree)
- Q2: Your past experiences with computational modules prepare you for more job/internship opportunities  
(Strongly agree — 1 2 3 4 5 — Strongly disagree)
- Q3: Your past experiences with computational modules help you stand out in the job interviews/job hunting  
(Strongly agree — 1 2 3 4 5 — Strongly disagree)

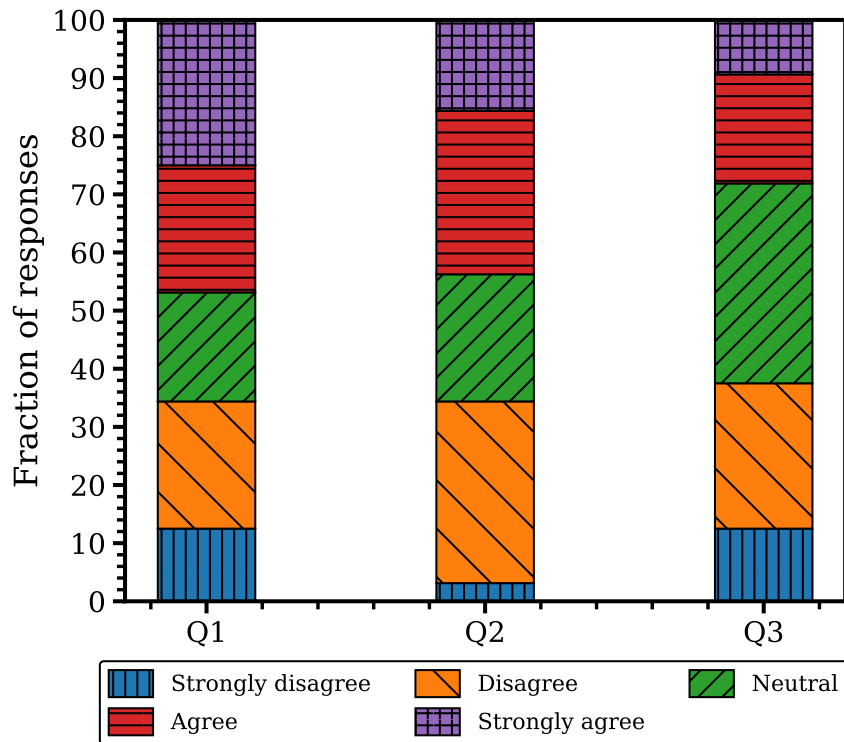


Figure 4: Students' perception about the influence of computational modules on their job hunting experience. Specifically, Q1, Q2, and Q3 are about resume, job opportunities, and interviews, respectively.

Figure 4 shows a small positive edge in student perception when it comes to resume and job opportunities, but no difference when it comes to the interview process. About 47 % of senior

students consider their experience with computational modules an advantage in their resume, while 34 % disagree, with an average of  $2.75 \pm 1.37$ . Similarly, 44 % of them indicate that their experience with computational modules prepares them for more job opportunities, while 34 % disagree, with an average of  $2.78 \pm 1.14$ . Lastly, approximately 28 % of the students feel that their experience with computational modules helps them stand out in the job interview/hunting process, while 38 % disagree, with an average of  $3.13 \pm 1.14$ . Further quantification of the influence of computational modules and computational training on the job hunting process will require insights from employers and graduated students. Nonetheless, our data suggests a potential direction for further refinement of the computational modules by better aligning our modules with post-graduate needs.

### 5.3 Attitude towards computational tools

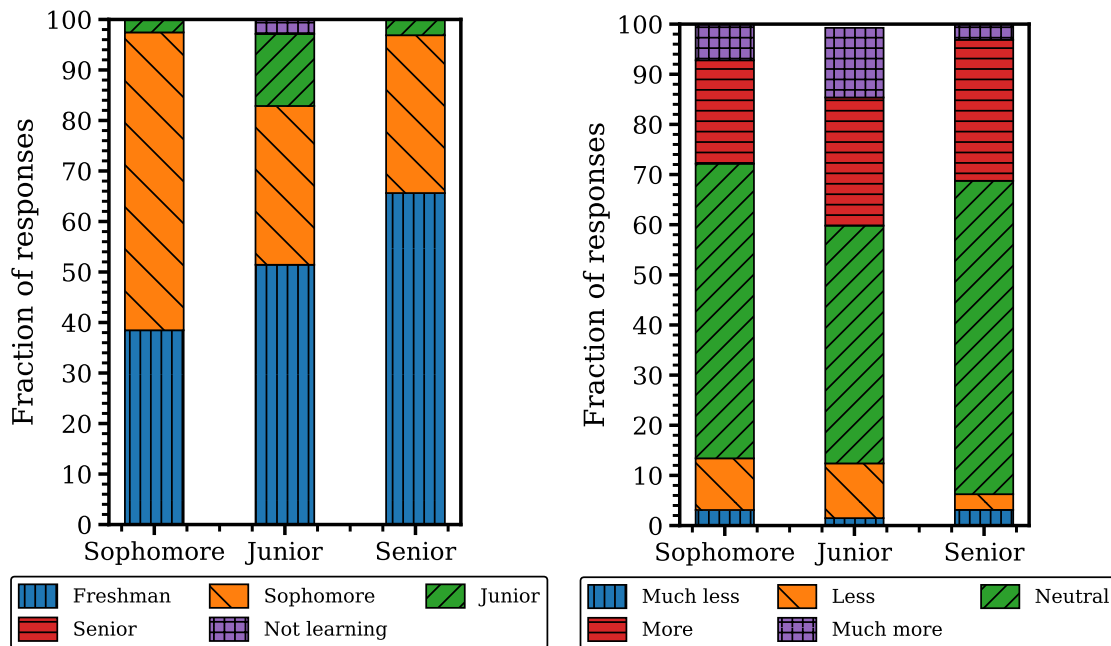


Figure 5: Left panel: Students' perception about when is the best time to start learning computational tools. Right panel: Students' perception about the current amount of computation in the curriculum.

Currently, for each course, we have two computational homework assignments and one to two short lectures detailing the specific computational tools used. The 2018 end-of-semester surveys for sophomores (MSE 201 and 206) and juniors (MSE 304 and 406) show that students are generally satisfied with the amount of computation in these courses (see Fig. 5), which is consistent with our earlier data [7, 10]. Our current survey for senior students again confirms this. The survey results also suggest that students want to have computation in the curriculum as early as freshman year, consistent with what is reported in the literature [10]. More than 90 % of students think that the computational instruction should start before junior year, slightly favoring freshman year. Furthermore, the survey results also suggest that more senior students want earlier

exposure to computation, with two thirds of the senior students want to have computation in their curriculum in freshman year. With students' desire to have earlier exposure to computation in the curriculum and the potential benefit of frequent exposure discussed earlier, we are exploring whether more computation can be included in the first year, e.g. in the course "Introduction to MSE" (MSE 182), in addition to CS 101.

## **6 Feedback from faculty members**

We distributed a survey to faculty members in the MSE department, asking about their intentions and difficulties encountered when using the computer-based teaching techniques, including iClicker, lecture recording, online homework/exam, and computational modules. Instead of using 5-point Likert type questions, we provided multi-choice questions and also collected direct responses. We received responses from 15 courses and 9 of them are from non-SIIP courses (see Table 1 for details). The results for each technique are summarized in Table 4 and discussed below.

### **6.1 iClicker**

The survey responses show that 8 out of 15 courses use iClicker and their major purposes are to track attendance (8/8), gauge students' understanding (8/8), provide a short break for students to digest (6/8), and to work through questions (7/8). Feedback shows that using iClicker creates an interactive learning environment (4/8) and helps the instructor to control the pace (2/8), as well as identifying knowledge gaps in real time (3/8). We find that the instructors' goals are indeed supported by the students' perception in usefulness of iClicker questions ( $2.11 \pm 1.02$  for MSE 304), which is consistent with the literature [17].

### **6.2 Lecture recording**

Our survey results show that lectures are recorded in 8 out of 15 courses. The major goals are to help students review the course content (5/8), to provide flexibility for students (3/8), to substitute lectures (3/8), and to provide supplementary lectures (3/8). Further feedback shows that lecture recording to substitute lectures is used only in rare circumstances (2/8). Some faculty mentioned that it is helpful for students who miss lecture (3/8). Our feedback also indicates that "missing sound track" is an issue encountered in rare occasions.

### **6.3 Online homework/exam**

The survey results show that 11 out of 15 courses use online homework/exam. The major goal is to speed up the grading process (9/11) and to provide flexibility for students (8/11). Most faculty members also find it useful for tracking students' performance (7/11) and some use it to help students master the course material better (3/11). One response mentions that none of the records

get lost, and another two point out that the online homework/exam provides immediate feedback to students. However, from our feedback we also conclude that there is a steep learning curve for instructors when implementing such a system well into an existing course, indicating that better technical support is needed.

Table 4: Provided options in the survey (multiple choice) and responses from the department faculty members. There are in total 15 responding courses.

iClicker	
Options	Number of responses
Track attendance	8
Gauge conceptual understanding	8
Work through questions	7
Provide short break for students to digest	6
Review previous lectures	4
Summarize today's lecture	2
I don't use it at all	7
Lecture recording	
Options	Number of responses
Help students review the course content	5
Substitute lecture	3
Provide flexibility for students	3
Provide supplementary lectures/instructions	3
I don't use it at all	7
Online homework/exam	
Options	Number of responses
Speed up the grading process	9
Provide flexibility for students	8
Track student's performance	7
Help students master the material	3
I don't use it at all	4
Computational modules	
Options	Number of responses
Add computational perspectives to the course content	8
Expose students to computational approaches/tools	7
Provide visualization for problems	2
Help students understand abstract mathematical equations	0
I don't use it at all	7

#### 6.4 Computational modules

Lastly, 8 out of 15 courses use computational modules. The major goal is to add a computational perspective to the course content (8/8) and to expose students to computational tools (7/8). A small fraction of instructors uses computational modules to provide visualization for problems

(2/8). Our feedback also indicates that computational approaches are increasingly important for course topics, e.g., materials characterization, electrical ceramics, and there is a strong need to include them in the course. The instructor of the Thermodynamics course (MSE 401) shares feedback that computational modules (here: MD) provide atomistic insights into some of the complicated thermodynamics concepts. One of the instructors points out a dilemma of incorporating computational modules: All of the already existing course material is important and including computational modules inevitably diverts time from that material.

## **6.5 Influence on non-SIIP courses**

We also note that there are some non-SIIP courses, that adopt the above-mentioned computer-based teaching techniques. More specifically, non-SIIP course instructors have started to adopt these techniques since 2014, the year the original SIIP project started. We also find that all of the responses for non-SIIP courses are not involved in any of the SIIP courses. This suggests that our curriculum reform also has a broader impact on non-SIIP courses, but the small sample size prevents us from further quantification.

## **6.6 Discussion**

In summary, the three computer-based teaching techniques that are implemented in the SIIP courses lead to positive feedback from department faculty who used them. These techniques make the learning environment more interactive, provide better flexibility for both students and instructors, and provide quicker grading and immediate feedback to students. The biggest challenge identified here is the steep learning curve of using computer-based techniques, embodied by technical issues. Dedicated technical support in the department and better documentation of all previous files would help instructors to adopt these useful teaching techniques. This is supported by our feedback that for computational modules, where we have a dedicated teaching assistant, technical issues are rarely a concern. Another issue is to incorporate computational modules into existing, densely packed syllabi, since this might replace important topics by the computational content. In order to achieve a synergistic integration, we will put future emphasis on better integrating computational modules with the existing content. At the same time, they should be designed such that existing course materials is supplemented and broadened.

## **7 Conclusions**

Since the survey data from 2009 shows the need for workforce with computational training experience [1], more and more MSE departments incorporate computational modules/course into their curriculum [2]. In response to this, our department has reformed the undergraduate curriculum by integrating computational modules into core courses. This transformation has been in a stable state since 2017. In this work, we confirm that our computational curriculum is indeed stable by demonstrating a consistent trend of improving students' confidence in using

computational tools. Our survey on department faculty shows that their major goals are to provide computational perspective to the course and expose students to computational techniques, regardless of their ties to the original SIIP project. At the same time, the survey for graduating students shows that within our current curriculum students become comfortable with using several computational tools to solve problems in materials science. However, we also identify three aspects that require further investigation: We find that there is little to no positive edge in student perception regarding the influence of computational modules on their job search. A more quantitative measure will require surveys of employers and alumni. We also find that students are least comfortable with the quantum mechanics based method (DFT), despite similar frequency of repetition throughout the curriculum. We plan to investigate whether the difficulty of a topic affects students' perceived confidence in using it. Lastly, we find that students not necessarily found it easier to memorize the course content related to computational modules and we plan to investigate whether better integration of the computational modules is needed.

## Acknowledgments

This work was supported by the College of Engineering and the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign as part of the Strategic Instructional Initiatives Program (SIIP), by a National Science Foundation CAREER Award to J.A.K. (Grant No. 1654182), by a NSF CAREER Award to R.M. (Grant No. 1654065), by a NSF CAREER Award to C.L. (Grant No. DMR-1554435), by a NSF CAREER Award to A.S. (Grant No. DMR-1555153), and by a NSF Grant to P.B. (Grant No. DMR-1709857). Any opinions, findings, and conclusions or recommendations expressed in this material are those of the authors and do not necessarily reflect the views of the National Science Foundation.

## References

- [1] K. Thornton, S. Nola, R. E. Garcia, M. Asta, and G. B. Olson, "Computational materials science and engineering education: A survey of trends and needs," *JOM*, vol. 61, no. 10, p. 12, 2009.
- [2] R. A. Enrique, M. Asta, and K. Thornton, "Computational materials science and engineering education: An updated survey of trends and needs," *JOM*, vol. 70, pp. 1644–1651, Sep 2018.
- [3] M. Borrego and C. Henderson, "Increasing the use of evidence-based teaching in stem higher education: A comparison of eight change strategies," *J. Eng. Educ.*, vol. 103, no. 2, pp. 220–252, 2014.
- [4] C. Henderson and M. H. Dancy, "Barriers to the use of research-based instructional strategies: The influence of both individual and situational characteristics," *Phys. Rev. ST Phys. Educ. Res.*, vol. 3, no. 2, p. 020102, 2007.
- [5] C. Henderson, A. Beach, and N. Finkelstein, "Facilitating change in undergraduate stem instructional practices: An analytic review of the literature," *J. Res. Sci. Teach.*, vol. 48, no. 8, pp. 952–984, 2011.



- [6] C. Henderson, M. H. Dancy, and M. Niewiadomska-Bugaj, "Use of research-based instructional strategies in introductory physics: Where do faculty leave the innovation-decision process?," *Phys. Rev. ST Phys. Educ. Res.*, vol. 8, no. 2, p. 020104, 2012.
- [7] A. Kononov *et al.*, "Computational curriculum for MatSE undergraduates," in *2016 ASEE Annual Conference and Exposition*, ASEE, 2017.
- [8] R. A. Mansbach, G. L. Herman, M. West, D. R. Trinkle, A. Ferguson, and A. Schleife, "Work in progress: Computational modules for the matse undergraduate curriculum," in *ASEE Annual Conference & Exposition*, 2016.
- [9] R. Mansbach *et al.*, "Reforming an undergraduate materials science curriculum with computational modules," *J Mater Educ*, vol. 38, pp. 161–174, 2016.
- [10] X. Zhang *et al.*, "Computational curriculum for matse undergraduates and the influence on senior classes," in *2018 ASEE Annual Conference & Exposition*, (Salt Lake City, Utah), ASEE Conferences, June 2018. <https://peer.asee.org/30213>.
- [11] P. Giannozzi *et al.*, "Quantum espresso: a modular and open-source software project for quantum simulations of materials," *Journal of Physics: Condensed Matter*, vol. 21, no. 39, p. 395502 (19pp), 2009.
- [12] S. Plimpton, "Fast parallel algorithms for short-range molecular dynamics," *J. Comput. Phys.*, vol. 117, no. 1, pp. 1–19, 1995.
- [13] A. Stukowski, "Visualization and analysis of atomistic simulation data with ovito—the open visualization tool," *Modelling and Simulation in Materials Science and Engineering*, vol. 18, no. 1, p. 015012, 2009.
- [14] A. C. E. Reid, R. C. Lua, R. E. García, V. R. Coffman, and S. A. Langer, "Modelling microstructures with oof2," *IJMPT*, vol. 35, no. 3-4, pp. 361–373, 2009.
- [15] J. O. Andersson, T. Helander, L. Höglund, P. Shi, and B. Sundman, "Thermo-Calc & DICTRA, computational tools for materials science," *Calphad*, vol. 26, no. 2, pp. 273–312, 2002.
- [16] MATLAB, *version 8.4.0 (R2014b)*. Natick, Massachusetts: The MathWorks Inc., 2014.
- [17] J. E. Caldwell, "Clickers in the large classroom: Current research and best-practice tips," *CBE—Life Sciences Education*, vol. 6, no. 1, pp. 9–20, 2007.