Materials Science Students' Perceptions and Usage Intentions of Computation

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Abstract

Over the last several decades computational methods have increasingly played a central role in Materials Science and Engineering (MSE) for characterizing structure, simulating processes and predicting materials' response. To align with this shift, an MSE department at a research university in the U.S. Mid-Atlantic region launched a curricular innovation to inculcate students with a basic facility with computational methods and to leverage computing proficiency to increase student comprehension of core MSE concepts. In this study we investigate the impact of this curricular innovation on students' (a) perceptions regarding the utility of integrating computation in their studies and their future careers; (b) perceptions regarding their own abilities to implement computation for solving problems relevant to MSE; and (c) intentions regarding the use of computation in their studies and future careers.

Results of this study suggest that the specific nature and context of students' previous experience with computation can have a measureable effect on students' perceived abilities to use it as a tool to solve problems in science and engineering as well as perceived utility for their academic courses and future careers. These two constructs can potentially determine future intentions of use or future intentions to seek additional training.

Background and Motivation

Over the last several decades Materials Science and Engineering (MSE) as a discipline has embraced the integration of computational methods for characterizing structure, simulating processes and predicting materials' response. This change has been most notable in academia with the establishment of "computational materials science and engineering" (CMSE) as a recognized sub-discipline. Survey research indicates a consensus in the field that adequate training in modeling and simulation of materials is critical for both undergraduate and graduate students in MSE academic programs to prepare students for careers in basic research, engineering and material development.

To align with this shift, an MSE department at a research university in the U.S. Mid-Atlantic region launched a curricular innovation to inculcate students with a basic facility with computational methods. The curricular innovation consists of a new course entitled "Computation and Programming for Materials Scientists and Engineers" (*CPMSE*). The course's primary learning goal was for students to apply algorithmic thinking and computer programming toward the solution of engineering and scientific problems relevant to MSE. The course was designed according to the How People Learn framework as embodied by an inverted lecture/homework delivery method that required students to watch lectures outside of class, respond to on-line quizzes and come to class prepared to engage in active learning[1]. The creation of this new course was also coupled with the integration of computational learning modules in the major's six core courses to simultaneously reinforce CMSE skills and foundational MSE concepts. The central premise for introducing this curricular approach is that students learn disciplinary topics and scientific computing better when the topics are taught in an integrated manner rather than by learning each topic separately [2].

To this date the department has completed the first delivery of the *CPMSE* course and has integrated the additional learning modules in three of the six core MSE courses. In this study we report the results of students' perceptions of computation and the computational modules as part of the following three foundational courses: Structure of Materials (Structures), Physical Chemistry of Materials I: Thermodynamics (Thermodynamics) and Biomaterials I (Biomaterials). The research questions driving this study are:

1. What are students' perceptions regarding the utility of integrating computation in their studies and their future careers?
2. What are students' perceptions regarding their own abilities to implement computational methods commonly used to solve MSE problems?
3. What are students' intentions regarding the use of computation in their studies and future careers?

Review of the Literature

Computation is an essential engineering research and development tool for the analysis and design of solutions to modern technological needs[3]. Higher education, however, is not keeping pace by equipping undergraduate engineering students with the computational literacy needed to solve problems in existing or emerging application fields [4-7]. Current educational strategies at the undergraduate level frequently treat computing as a narrow technical tool that is applied in isolation from related disciplinary topics [8,9]. However, the power of computational thinking is best realized in domain-specific and professionally relevant contexts [4]. Computational literacy in engineering requires knowing when, why, and how computation methods work and don't, and applying or modifying existing numerical methods or methodologies to successfully solve problems or design solutions in different engineering fields [10]. To develop computational literacy effectively in current and future engineers requires infusing computation across disciplinary curricula.

A frequently used method for integrating computing into the engineering curriculum has been through the development of introductory programming courses e.g., [11,12-16] introduction to engineering courses, [17,18] or numerical analysis courses [12] designed for all engineering majors. A second more-focused scheme has integrated computing through projects and exercises as part of disciplinary courses [19-21]. And a third approach has focused on developing specific courses in computational science and engineering [22]. Other forms for integrating computation have centered on the use of tutorials and online modules [23-25]. Some instances have infused computing modules in more than one course [26-28], vertically integrating problem-based learning scenarios that link across courses [19,29-31] and other implementations throughout the entire curriculum [32-35]. Assessments of these implementations have mostly concentrated on student-user metrics, student comments/feedback (reported by the instructor), instructor perspectives, and student self-reporting of perceptions and learning [13-15,19,20,22,23,35], and, to a lesser extent, assessments have also focused on student performance [21]. The focus of our study centers on student acceptance of computation in their studies and future careers. To this end, we have adopted and adapted the Technology Acceptance Model as the theoretical foundation to guide this investigation.

Theoretical Framework

Technology Acceptance Model (TAM), adapted from the Theory of Reasoned Action [36] and originally developed by Davis [37], proposes that an individual's acceptance of technology is determined by (i) perceived utility and (ii) perceived ease of use. TAM has been applied to the study of adoption of different technologies such as word processors, e-mail, WWW, GSS, and hospital information systems [38]. We are applying this model to the study of adoption of computation as a technology as well as a common practice.

Design/Method

The research design used a pre-post test design that included open questions and a Likert-survey aimed to measure predictors of future behavior according to the Technology Acceptance Model (TAM). The desired future behavior is the integration of computation (e.g., algorithm design, modeling and simulation, data visualization) in students' future studies and eventually in their future careers.

Participants and Procedures

Participants of this study include 154 engineering students from Structure of Materials (28), Physical Chemistry of Materials I: Thermodynamics (33) and Biomaterials I (93). Students completed two learning modules integrating computation with the course's core concepts in the Structures course, three modules in the Thermodynamics course, and one in the Biomaterials course. Twelve students were enrolled in two of these courses during the semester. Students were asked to respond to the survey at the beginning and at the end of the semester. The analysis presented in this paper was conducted exclusively with all complete data (i.e., including pretest and posttest scores), which consisted of 93 responses.

Data Collection

According to TAM, the elements that predict future behavior are perceived utility (2 questions), perceived ease of use or ability to do or perform (8 questions) and future intention to use (2 questions). We developed survey questions to identify how students' perceived these constructs as related to computation (see Table 1). For each of the questions we used a Likert-scale response and we scored our responses as follows: strongly disagree (1), disagree (2), undecided (3) agree (4) and strongly agree (5).

Table 1. Survey questions grouped by constructs of the TAM

TAM	ID	Statements
Ability to do	Q1	I have the ability to design an algorithm.
	Q2	I have the ability to write a computer program.
	Q3	I have the ability to use a computer to solve a set of linear equations.
	Q4	I have the ability to visualize data using a computer.
	Q5	I have the ability to create a computer representation of an atomic or molecular structure.
	Q6	I have the ability to numerically solve an initial value problem.
	Q7	I have the ability to implement a numerical model based on a simple partial differential equation.
	Q8	I have the ability to implement a graphical user interface.
Utility	Q9	I feel computation (data visualization, modeling and simulation algorithm design) will be useful in my studies.
	Q10	I feel computation (data visualization, modeling and simulation algorithm design) will be useful in my career.
Intention to use	Q11	I intend to purposefully seek courses that will allow me to increase my knowledge about computation.
	Q12	I intend to use computation (data visualization, modeling and simulation algorithm design) in my future career.

Data Analysis

The data analysis started by computing a composite score for each of the three constructs being measured herein called ability to do, utility and intention to use. These composite scores were computed and plotted for all pretest and posttest scores. Then, analysis of these scores were performed grouping students responses according to two different variables including (a) number and nature of previous courses in computing students have taken, and (b) number of core disciplinary courses where students were exposed to the curricular innovation. Inferential statistics was then used to identify significant differences between pretest and posttest scores for the two variables. Scores from 1 to <2.5 were interpreted as negative perceptions or intentions to use. Scores from 3.5 to 5 were interpreted as positive perceptions or intentions to use. Scores from 2.5 to <3.5 were considered neutral. In Tables 2 to 5 in the section below we have highlighted in red negative results and we have bolded positive results.

Results

Results describe students' perceptions of computing in terms of ease or ability to do, level of perceived utility and intention to use. Here we report comparisons of pretest and posttest scores of student responses by (a) computing courses students had previously completed, and (b) number of core disciplinary courses in which students were exposed to the curricular innovation.

Previous Computing Background

In Figure 1 we first present a comparison of data for students who completed the *CPMSE* course (N=9) vs. those who did not. The CPMSE course is primarily taken by freshmen and was offered the semester before students enrolled in one or more of the 3 core MSE courses in which the computational modules were integrated. The course was designed using the How People Learn framework and employed an inverted classroom delivery method as detailed in a previous publication [1]. Among those who had not enrolled in *CPMSE* we have further distinguished between those not having taken a previous computing course (N=9), having taken one previous computing course (N=36), having taken two previous computing courses (N=26) and having taken from 3 to 4 computing courses (N=13).

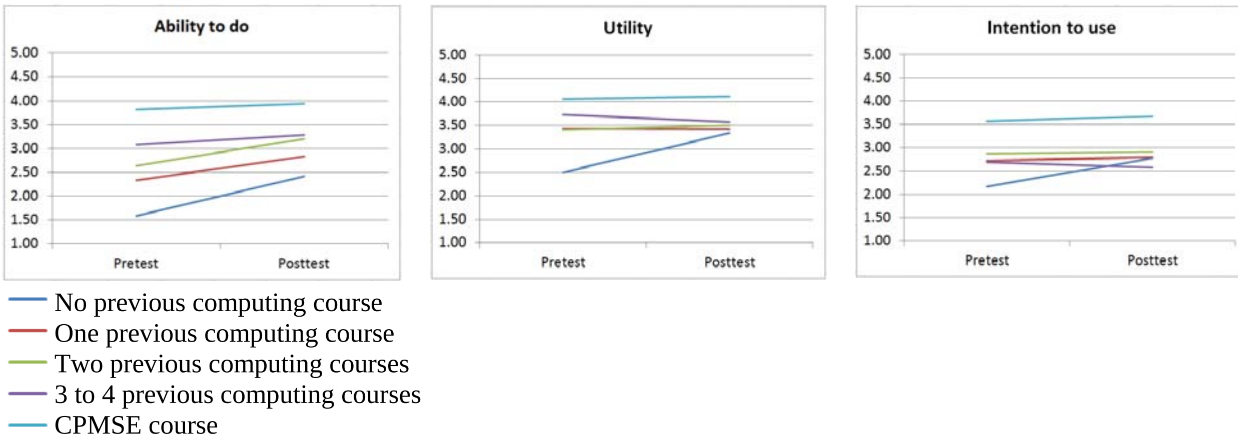

Figure 1. Pretest and Posttest scores of students perceived ability to use computation, perceived utility in their studies and future careers, and intentions of future use of computation grouped by previous computing background.

As shown in Table 2, survey results document that students who completed the *CPMSE* course demonstrated significant higher positive perceptions at the *beginning of the semester* on their abilities to use computation to engage in programming and algorithm design as well as to solve specific MSE relevant science and engineering problems ($F = 16.84$, $P = 2.76e-10$). They also had significant higher positive perceptions of the utility of computation in their academic and future careers ($F = 3.369$, $P = 0.013$), and consistent positive perceptions in their intentions to continue to use computation and seek further training in computation ($F = 2.088$, $P = 0.0891$).

Survey results also show that at the beginning of the semester students who had not taken any previous course in computing had the most negative perception on their ability to utilize computation to solve specific problems in science and engineering, the utility of computation in their academic courses and future careers, and intentions to seek further training in computation. A Tukey test used to compare the students who had taken the *CPMSE* course and those who had not taken any previous computational course showed significant differences for perceived ability ($p < 0.001$) and utility ($p = 0.0081$). Students who had not taken any previous computational courses showed the largest gains in these scores at the end of the semester after which they had been exposed to computational modules. In the three dimensions of the TAM, however, these students only became less negative or changed from negative to neutral in their perceptions or intentions of future use.

Table 2. Pretest and Posttest scores of students perceived ability to use computation, perceived utility in their studies and future careers, and intentions of future use of computation grouped by previous computing background.

	Pretest Scores						**Posttest Scores**					
	Ability to do		Utility		Intention to use		Ability to do		Utility		Intention to use	
	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.
No previous computing course (N=9)	1.58	0.42	2.50	1.35	2.17	1.09	2.42	0.80	3.33	1.32	2.78	1.06
One previous computing course other than *CPMSE* (N=36)	2.34	0.64	3.43	0.92	2.72	1.05	2.84	0.76	3.42	1.08	2.79	1.15
Two previous computing courses other than *CPMSE* (N=26)	2.64	0.83	3.30	0.98	2.87	1.02	3.20	0.63	**3.50**	1.22	2.90	1.21
3 - 4 previous computing courses other than *CPMSE* (N=13)	3.08	0.45	**3.73**	0.88	2.69	0.93	3.29	0.62	**3.58**	0.98	2.58	0.86
Exposure to the *CPMSE* course (N= 9)	**3.82**	0.44	**4.06**	0.73	**3.56**	1.26	**3.94**	0.43	**4.11**	0.65	**3.67**	0.94

On the other hand, students who were exposed to at least one programming course in the past indicated in the pre- and post-survey neutral perceptions of their ability to use computation to solve specific problems in science and engineering and of their intentions to use of computation in the future. However, in the pre- and post-survey these students indicated positive results on the utility of computation in their academic studies and their future careers. Scores from the three dimensions increased from pre- to post-survey measures; however these differences were not found to be statistically significant for utility and intention of use dimensions as show in the Table 3.

Table 3. T-test Pre- vs Post-survey scores of students perceived ability to use computation, perceived utility in their studies and future careers, and intentions of future use of computation.

TAM	**DF**	**T value**	**Pr > | t |**
Ability to do	92	-7.7624	**1.12e-11**
Utility	92	-0.7754	0.4401
Intention of use	92	-0.8888	0.3764

These data suggest the lasting impact of the *CPMSE* course on student attitudes. Portions of the survey used for this study were taken by students in *CPMSE* course at the beginning and end of the previous semester [1]. We present the results in Figure 2 below in terms of student self-reported abilities to: (1) design an algorithm, (2) write a computer program, (3) solve a set of linear equations with computation, (4) visualize data using a computer, (5) create a computer representation of an atomic or molecular structure, (6) numerically solve an initial value problem, (7) numerically solve a boundary value problem, (8) implement a numerical model based on a simple partial differential equation, and (9) implement a graphical user interface.

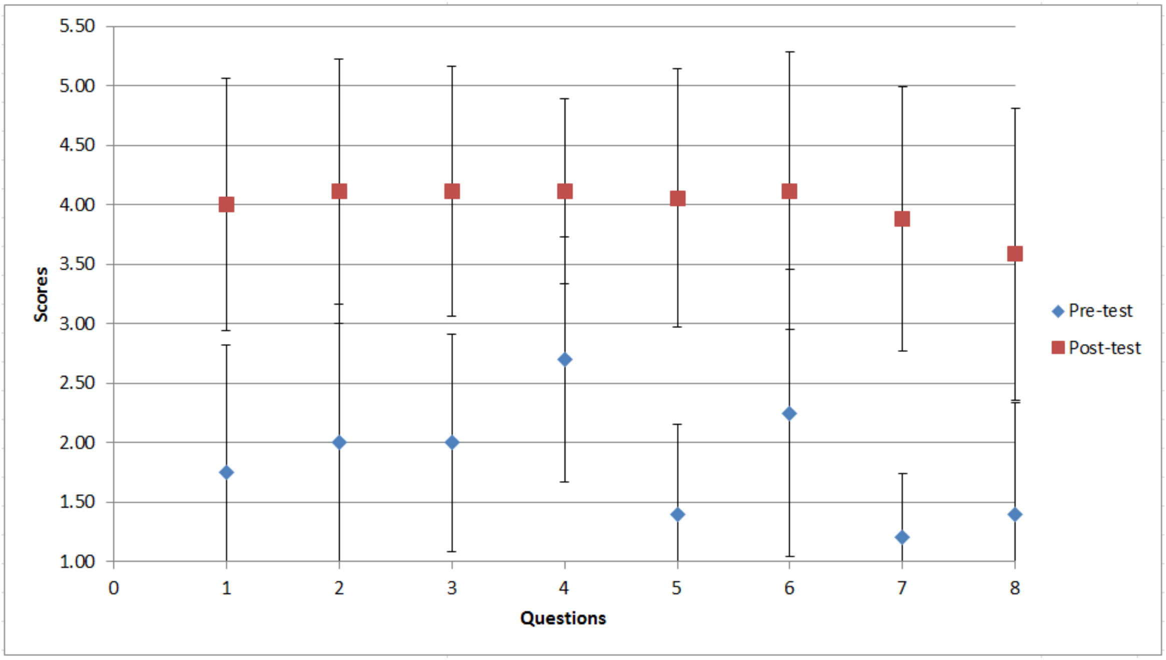

Figure 2. Previous semester *CPMSE* results on student perceived ability to complete a set of computation tasks.

These data also suggest that exposure to computational modules may be effective in increasing student self-perceptions regarding their abilities to use computational methods particularly for students who have not had previous computational exposure, but do not change student perceptions as much as exposure to a disciplinarily grounded programming courses.

Disciplinary Courses with Computational Learning Modules

To identify the impact of the computational modules integrated into the core disciplinary courses, pre- and post-survey scores were analyzed by the number of core disciplinary courses students enrolled. The number of students included in each category was as follows.

- 60 in the Biomaterials course
- 3 in the Structures course
- 18 in the Thermodynamics course
- 5 in the Biomaterials and Structures course
- 4 in the Biomaterials and Thermodynamics course
- 3 in the Structures and Thermodynamics course

Because some of the categories had very few students we conducted this analysis grouping students in two major categories: students who were exposed to computational learning modules in one disciplinary course (N=81) and students who were exposed to computational modules in two disciplinary courses (N=12). Results depicted on Figure 1 suggest a possible relationship between students' exposure to computing courses and positive student perceptions about computing utility, their ability to currently use computing, and plans to use computing in future professional and academic work.

Table 4. Pre- and Post-survey scores of students perceived ability to use computation, perceived utility in their studies and future careers, and intentions of future use of computation grouped by number of disciplinary courses students completed.

	Pretest Scores						Posttest Scores					
	Ability to do		Utility		Intention to use		Ability to do		Utility		Intention to use	
	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.	Mean	Std. Dev.
Exposure to core disciplinary courses. (N=81)	2.55	0.83	3.35	1.04	2.69	1.05	3.03	0.78	3.46	1.12	2.78	1.09
Exposure to two of the core disciplinary courses using computational learning modules. (N= 12)	2.89	0.87	**4.00**	0.56	3.42	1.06	3.33	0.69	**3.96**	0.84	**3.54**	1.12

Survey results suggest that students who were exposed to computational learning modules in only one of the core MSE disciplinary courses began with neutral perceptions on their ability to use computation to solve problems in science and engineering, perceived utility of computation for their academic courses and future careers and undecided intentions to use computation or seek for further training in computation in the future. The data in the previous section suggest that this is likely due to a lower degree of computational preparation within this group of students. Although students' perceptions in these three dimensions remained neutral, all of them showed an increased score in the post-survey scores.

Students who were exposed to two of the courses where students utilized computational learning modules remained neutral across the semester regarding their abilities to use computation to solve specific science or engineering problems despite rising for the post-test. These students also indicated positive perceptions of the utility of computation in their academic and future careers and the perception remained positive in the posttest score measure. Finally, student responses indicating their future intentions of use of computation changed from undecided to positive perceptions.

Table 5. Anova Pre- vs Post-survey scores of students perceived ability to use computation, perceived utility in their studies and future careers, and intentions of future use of computation grouped by number of disciplinary courses students using computational learning modules.

TAM	DF	F-Value	P-Value
Ability	4	2.657	**0.0381**
Utility	4	1.364	0.253
Intention of use	4	0.192	0.942

The p-values on Table 5 suggest that the number of modules had a significant impact on students' perceived ability to use computation. On the other hand, student perceived utility and future intention of use was not influenced by the number of modules due to their high pretest value.

Limitations of the Study

This study has the major limitation that the results presented regard student perceptions rather than capability. However, understanding student perceptions are important for identifying acceptance of technology for learning purposes and in this case, intentions of future use of computation.

Discussion and Conclusion

Advances in computing contribute to science and engineering discovery, innovation, and education by facilitating collection, representation, processing, storage, analysis, simulation, and visualization of ever increasing amounts of experimental and observational data. Computing, as both fundamental knowledge and a technical skill, is therefore required to contribute to and compete in our fast-changing, global society. Therefore, understanding undergraduate students' perceptions and usage intentions of computing is an important research endeavor that can suggest future adoption. Specifically, in this study we have investigated students' (a) perceptions regarding the utility of integrating computation in their studies and their future careers; (b) perceptions regarding their own abilities to implement computation for solving MSE problems; and (c) intentions regarding the use of computation in their studies and future careers.

Results of this study suggest that previous experience in programming courses has a larger impact on students' attitudes about computational science than individual modules integrated into core disciplinary courses. This is not surprising as these courses immerse students in computational methods more than core courses which focus more on foundational disciplinary content. The biggest impact was measured for a computation and programming course taught within the context of the discipline, the *CPMSE* course described above, which incorporated active and project-based learning. The data suggests that changes in student perceptions while taking this course persisted into the following semester. Similarly, this course proved more effective in increasing student perceptions and intentions regarding computation than taking multiple non-*CPMSE* computing courses. Also, although students' perceptions regarding utility and intention of use did not show significant increase from the pretest to the posttest, they did not decrease either. And both of them showed a reasonable positive score during the pretest (Utility = 3.43, Intention of Use = 2.78).

The results of this study can be explained through the lens of the literature in self-efficacy. Previous research about student self-efficacy has identified that students' confidence in their abilities to complete a variety of tasks, specifically mathematical-related tasks in courses at the college level, predicted their future interests in mathematics courses [39]. We believe that this may also be the case with exposure to computation.

Implications of this study relate not only to the integration of computation earlier and often in the engineering curriculum, but also to the integration of computation into disciplinary courses. This is consistent with recommendations from the National Research Council arguing that the power of computational thinking is best realized in domain-specific, personally-relevant contexts [4]. And that learning computing within a science-and-engineering domain can be more successful than learning each knowledge domain separately [2].

Future Work

Future work will include collecting data for three different core MSE courses offered in a subsequent semester that include computational learning modules. Data on surveys conducted in these courses will allow us to identify if (1) gains made in previous semesters persist and (2) if student perceptions saturate or accelerate with increased exposure to computational modules. The researchers are also collecting data on student performance in these courses using direct quantitative and qualitative measures of student learning (e.g., matched pre- and post-module quizzes, think-aloud) to explore if students perceptions correlate with student mastery of disciplinary content.

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