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Computational Modeling in Materials Science and Engineering: Student Responses to a Restructurated Introductory Course

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Abstract: This paper reports student perceptions of a redesigned introductory materials science and engineering (MSE) course based around computational atomistic models embedded in a novel interactive digital textbook. Atomistic models can foster principled understanding of MSE phenomena by foregrounding how material structures and properties emerge from atomic interactions and can be used to engage students in active, inquiry-based learning. Students completed an end-of-course survey with Likert-style and open-ended questions. A large majority of students reported feeling that the course was more engaging than other STEM courses, that they learned more than in other courses, that the course was equally or somewhat more challenging than other courses, and that they had a positive experience with the interactive textbook. Open-ended questions revealed that most students preferred active model-based learning compared to video lectures, because they were engaging and helped with understanding. However, some students found the computational models confusing. Students also had positive experiences with the interactive textbook and appreciated that the content on the platform was well-organized, easy to navigate, and exactly reflected the requirements of the course. Overall, the findings show it is feasible to radically redesign introductory MSE around computational modeling while maintaining positive student experiences.

1. Introduction

This paper reports on student perceptions of an introductory materials science and engineering (MSE) course redesigned to center around computational models and taught with a novel interactive textbook with the computational models embedded. This redesign is in response to two trends. First, computation is transforming MSE, and the curriculum should reflect that fact. Second, computation and computational representations can be harnessed to create powerful tools for learning. This paper is a continuation of the work presented in [1] which described the redesigned course without reporting on any student results. The background section of this paper summarizes the theoretical foundation for the course redesign and the methods section briefly describes the redesign itself, but refer to [1] for more details. The focus of this paper is student perceptions and reactions to the redesigned course as a whole rather than focusing on content-based learning outcomes. We made this choice for two reasons. First, given the magnitude of the changes we made to the course—redesigning it entirely, engaging students in explorations of computational models throughout, and authoring/using an interactive textbook—it was entirely possible that students would be overwhelmed or have other negative reactions. Therefore, it was important to demonstrate the feasibility of this kind of radical change to the curriculum. Second, as we redesigned the content of the course around computational models, we also redesigned assessments to require deeper conceptual understanding, making it difficult to compare student learning outcomes to prior years. It is still possible to evaluate student learning in relation to our new assessments, but this requires in-depth qualitative analysis which could not fit in this paper due to space limitations. Future work will investigate student learning outcomes as well as how our assessments evolved to require deeper conceptual understanding.

2. Background

2.1 Computation in MSE

The impact of computation on science and engineering has been dramatic. The advent of digital computers has been described as "the second metamorphosis of science" because computational modeling and experiments provide a new way to generate knowledge about nature, complementing experimental and mathematical methods from the first metamorphosis which initiated the scientific revolution [2], [3]. In addition to the vast calculations computers enable, computational representations also support a different (complementary) way of thinking compared to classical mathematical representations, emphasizing procedural "how to" knowledge compared to more descriptive "what is" knowledge of most classical mathematics [4].

MSE is no exception to the trend of computation transforming science and engineering, and there is widespread agreement that undergraduate and graduate education should reflect these changes [5], [6], [7]. Recently, the Materials Genome Initiative argued that computation is one of the three competencies that the next generation of the MSE workforce would need to master [8]. On the theoretical side, computation allows scientists to model "real, complex materials as they are" [9], by modeling interactions of many atoms and allowing larger scale patterns to emerge. The procedural focus on *how* atoms interact can help researchers "to gain insight into a physical system and then obtain a new theoretical understanding" [10] compared to only focusing on macrolevel descriptions.

2.2 Restructurations for Learning

The term *restructuration* refers to the ways that new representational forms change the way we think and learn [11], [12]. A classic example is the transformation from Roman to Hindu-Arabic numerals, which enabled much more powerful ways of thinking about and manipulating numbers [12]. Computational representations can provide similarly dramatic changes in how we think and learn [11], [12], [13], [14]. One reason is the procedural nature of computational knowledge discussed above. In the context of MSE, the focus on *how* things happen combined with the calculation power of computers enables the modeling of materials starting from atomic interactions. Since all materials phenomena ultimate emerge from atomic interactions, the same core computational model can be used to understand many phenomena. This "one-to-many" property of computational models makes them powerful tools for understanding the atomic mechanisms underlying materials phenomena and unifying understanding of various phenomena together [15]. Additionally, the perspective of *emergence*—how large-scale patterns arise from many micro-level interactions—is a powerful lens for understanding not only many phenomena in MSE, but many phenomena across the sciences [11], [12], [16]. It is a "powerful idea" in the language of constructionist learning theory [13] and an important cross-cutting concept in the language of the Next Generation Science Standards [17], [18].

A significant body of research has investigated the benefits of computational restructurations for understanding emergent phenomena, including in physics [19], chemistry [20], [21], [22], biology [23], [24], probability [25], social sciences [26], [27], and materials science [15]. There have been calls to integrate computational modeling, and the perspective of emergence it highlights, across K-16 STEM curricula in general [28], [29] and specifically to make "one-to-many" computational models the backbone of the MSE curriculum [15]. However, prior work on computational restructurations have only designed learning interventions for specific topics within a subject. The course redesign reported in this paper is the first time that a project rooted in restructuration theory has taken on the task of redesigning an entire course.

2.3 Prior work

In [1], we described the course redesign in detail, including conceptual explanations of the computational techniques used, but we did not report on student results of any kind. This paper focuses on student perceptions of the course, and future work will address content-based student learning outcomes for the reasons discussed in the introduction.

3. Research Questions

Given the magnitude of the changes we made to the introductory MSE course, we chose to focus on student perceptions to assess the feasibility and desirability of our approach. Our research questions are:

1. Is it feasible to redesign the introductory MSE curriculum to center around computational models while maintaining positive student experiences of the course?
2. What were student perceptions of the redesigned course, the interactive textbook, and the computational models?

The goal of answering the first research question is a kind of existence proof. We simply want to demonstrate that it is possible to radically change the introductory MSE course to center around computational models—considered by many to be an advanced topic—and maintain positive student experiences with the course. Our goal in this paper is not to compare our restructurated course to more traditional courses (see future work section). The goal of the second research question is to gain qualitative insight into student perceptions of the course to learn what they did and did not find valuable.

4. Methods

4.1 Setting and Participants

The setting of this design-based research is an introductory materials science and engineering (MSE) course taken by approximately 100 students each term at a large private university. The course serves both MSE majors and other engineering majors with about three quarters of the students coming from other majors as part of their engineering requirements. The only prerequisite is one introductory chemistry course.

4.2 Structure of the Course

The course has two 80-minute lecture periods per week and one 50-minute recitation led by teaching assistants. Students were assigned pre-lecture exercises, which usually consisted of interacting with one or more computational models and answering questions to complete before each lecture. Lecture periods usually consisted of three segments of 20-30 minutes: (1) lecturing on the content covered in the pre-lecture exercises, (2) a period of active-learning usually comprised of another model-based inquiry task, and (2) a final short lecture on that topic. See [1] for more details on the structure and content of the course.

4.3 NetLogo: Computational Modeling Tool and Example Models

NetLogo [30], the main computational modeling tool used in the course, has unique affordances which make it ideal for introductory MSE course despite not being specifically an MSE tool. It is an agent-based modeling platform designed to be "low threshold" and "high ceiling" [31], meaning that it is easy to get started, even for users with no programming experience, while not being limiting for advanced users. The "low threshold" design of NetLogo allowed sophomore MSE students to learn the syntax of NetLogo and code a new model in a single 2.5 hour session [15]. NetLogo models can be interacted with while they are running, enabling various interactions which support conceptual understanding. Additionally, there is a browser-version, NetLogo Web [32], which enables students to use the software without downloading anything, making it much easier to implement in a large classroom.

We were able to create models for the large majority of topics in the course using just two techniques: molecular dynamics and random walk. The one-to-many nature of these techniques [15]—that one technique can be used to model many phenomena—helps to emphasize the common principles and mechanisms underlying many MSE topics. Figure 1 shows two example models from the course, one for each of these techniques. On the left is a model of chain-growth polymerization. Each "agent" represents a molecule which executes a random walk without overlapping with each other. When a monomer collides with a radical, they bond, after which their random walk is also restricted to prevent their bond from breaking. Students can explore how changing the numbers of monomers and initiators changes the molecular weight distribution and the speed of the reaction. On the right of Figure 1 is a molecular dynamics model in which the bonds between atoms are visualized and students are able to adjust the size of an impurity atom to see how it affects lattice strain and the overall energy of the material. For more examples of models we created in the course as well as a brief conceptual explanation the computational techniques, see [1].

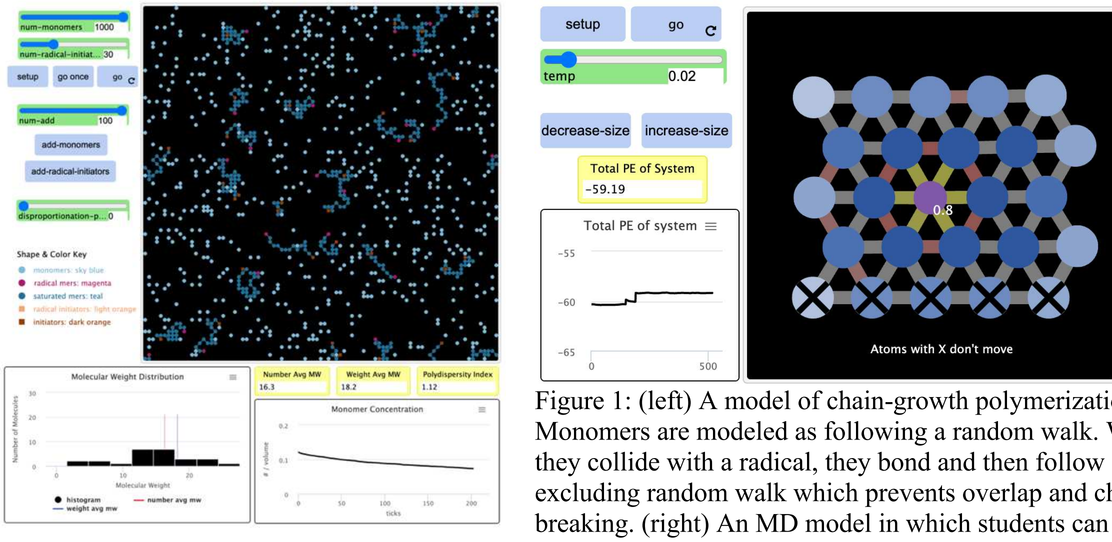


Figure 1: (left) A model of chain-growth polymerization. Monomers are modeled as following a random walk. When they collide with a radical, they bond and then follow a self-excluding random walk which prevents overlap and chain breaking. (right) An MD model in which students can explore substitutional impurities by changing the size of one of the lattice atoms and seeing how it changes the energy of the material and the strain on the lattice.

4.4 Interactive Textbook

An important aspect of the course redesign was authoring a new interactive textbook to align with the course by the first and second authors. It was hosted on a platform called Morfli[1] (pronounced more-flea) designed by the first author with the intention to integrate all the course content in one place including computational models, explanations, and exercises. Morfli makes it easy for the authors to edit and add content. For students, they are able to interact with the NetLogo models, answer questions, and read surrounding explanatory material all in one place.

Since we authored the textbook from the outset in an interactive digital medium, we were able to foster more active learning than a typical textbook in two important ways. First, we embedded interactive computational models throughout the text. Second, we often require students to explore a model and attempt to answer questions about it before providing additional explanation, in line with research on The Learning Cycle [33], [34], [35] and related pedagogical approaches [36], [37], [38], [39] which show that active exploration before explanation improves learning. We combined these ideas with the constructionist idea of "microworlds"—interactive computational models that embed important concepts from a learning domain [13]—to produce "constructionist learning cycles." The textbook contains 15 chapters, 30 embedded computational models, and over 300 embedded questions for students to answer. For most of the questions, students are able to view a solution immediately after submitting their own answers, allowing them to check their understanding.

4.5 Data and Analysis Methods

[1] https://www.morfli.com/

Data for this study come from an end-of-course survey in the spring of 2024 which included several questions about their experience with the course overall and their perceptions of Morfli and the embedded NetLogo models. Seventy-eight students completed the survey. Table 1 shows the four Likert-style questions on the survey. The results of these questions are reported in tables and bar charts. Table 2 shows the four open-ended questions along with the methods used to analyze them. Inductive bottom-coding was used to identify certain types of responses and categorize them. We first did a round of open coding using "descriptive coding" [40]. Next, we conducted "pattern coding" [40] on the initial codes to reduce the number of codes to a smaller number of categories representing key themes in the data. Following Hammer and Berland [41], the codes developed are not treated as data to be quantified but as claims about the data. The raw written responses are the data, and codes are claims made about the data. The code are reported in the results section along with enough examples of data for each code that readers can decide for themselves if they agree with the coding scheme [41], [42].

Table 1: Likert-style questions on the end-of-course survey

Question	Response Options
Rate your experience using Morfli (the interactive textbook) in this course.	5: It was great 4: It was good 3: It was okay 2: It was kind of bad 1: It was really bad
How engaging was this course compared to most other engineering, science, and math courses you have taken?	Much more engaging Somewhat more engaging About the same Somewhat less engaging Much less engaging
How challenging was this course compared to most other engineering, science, and math courses you have taken?	Much more challenging Somewhat more challenging About the same Somewhat less challenging Much less challenging
How much do you think you learned in this course compared to most other engineering, science, and math courses you have taken?	Much more Somewhat more About the same Somewhat less Much less

Table 2: Open-ended questions on the end-of-course survey

Question	Analysis Methods
About how much time did you spend doing pre-lecture exercises per class using	First, the amount of time the student reported was recorded. If they reported a range, both the low and high end were recorded and then averaged. Most students did not report

Morfli? What about video lectures? Did you prefer the video lectures or model-based exercises more and why?	separate times for Morfli exercises vs video lectures. For those who did, the minimum time of the two was recorded as the low end and the maximum of the two was recorded for the high end and then averaged. 57 responses had numerical information about how much time they spent. The rest either didn't answer or gave non-numerical answers such as "Not enough time, I wish I did more." Next, each response was coded for whether the student preferred video lectures, model-based exercises, or both. 66 responses included this information. Finally, the remaining "why" of student answers were coded qualitatively. First, the answers were open coded resulting in 20 codes. 57 responses received at least one of these qualitative codes. The remaining answers only reported on timing and which type of pre-lecture exercise they preferred. Next, similar codes were combined, and some were split to differentiate between whether they were referring to video lectures or Morfli exercises. For example, initially responses were coded with "easier to review." This code was then split because some students found the Morfli exercises easier to review and some the video lectures. After this, any codes with fewer than three responses were removed. An additional round of code combination and splitting was carried out after which any opposing codes were grouped together but not combined into a single code (e.g., some students found the video lectures more convenient and some the Morfli exercises). After this, any codes or code groups with fewer than five responses were ignored, as the goal was to identify major themes in the data.
What did you like about Morfli?	First, the answers were open coded resulting in 15 codes. 72 responses received at least one of these qualitative codes. Next, codes were grouped into two main categories: (1) regarding the content on Morfli, and (2) regarding functionality of Morfli which was further divided into (a) interactive functionality and (b) other functionality. One code did not fit into either of these categories making it its own category. Only codes which appeared at least 5 times in the data are reported.
Share any ideas you have for improving Morfli.	First, the answers were open coded resulting in 25 codes. 52 responses received at least one of these qualitative codes. The other 24 of the remaining responses were either blank or said things like "n/a" or "it works well," and two were

	irrelevant to the question. Next, codes with only one response were removed and the rest were grouped into four main categories: (1) regarding the content of the course hosted on Morfli, (2) suggestions for new features, and (3) suggestions for improvements to existing features.
Do you think the NetLogo computational models used in class and pre-lectures helped you learn? What did you like? What didn't you like?	Each response was coded for whether the student felt the NetLogo models helped them learn or not. A third category of "somewhat" emerged from the data. 72 of the 78 responses could be coded into one of these three categories. The remaining 6 responses did not contain enough information. The remainder of reach response was then open coded for reasons they liked or didn't like the NetLogo models resulting in six initial codes for liking the models and six for disliking. These codes were then refined, and some were merged resulting in four codes for liking the models and five for disliking. Note, that even students who said they thought the models helped them learn might have had some complaints about the models and vice versa.

5. Results

The results section begins with the students' overall perceptions of the course and the interactive textbook as reported in Likert-style questions followed by the time students spent on pre-lecture exercises. Then, major themes in student perceptions from open-ended questions are reported.

5.1 Overall perceptions of the course

Tables 3-6 below show the results of student answers to the Likert-style questions about the course and the interactive textbook (Morfli). A large majority of students, 81%, thought the course was more engaging than other courses STEM courses they had taken, while 14% thought it was about the same and only 5% thought it was somewhat less engaging (Table 3). Regarding perceptions of learning, a large majority, 72%, felt they learned somewhat or much more compared to other courses, 23% thought they learned about the same, and only 5% thought they learned somewhat less (Table 4). Regarding how challenging the course was compared to other courses, the large majority thought it was fairly typical—87% thought it was somewhat less challenging, about the same, or somewhat more challenging—while 13% thought it was much more challenging (Table 5). An overwhelming majority of the students, 98%, rated their experience with Morfli as okay, good, or great with a large majority, 80%, in the latter two higher categories (Table 6).

Table 3: Response to the question, “How engaging was this course compared to most other engineering, science, and math courses you have taken?”

Rating	Respondents	Percentage
Much more engaging	33	42%
Somewhat more engaging	30	39%
About the same	11	14%
Somewhat less engaging	4	5%
Much less engaging	0	0%

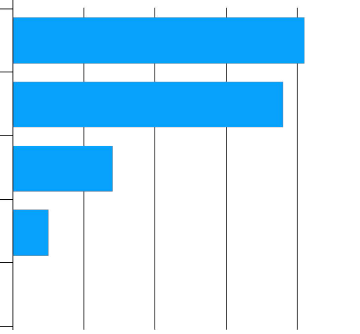


Table 4: Response to the question, “How much do you think you learned in this course compared to most other engineering, science, and math courses you have taken?”

Rating	Respondents	Percentage
Much more	36	45%
Somewhat more	21	27%
About the same	18	23%
Somewhat less	4	5%
Much less	0	0%

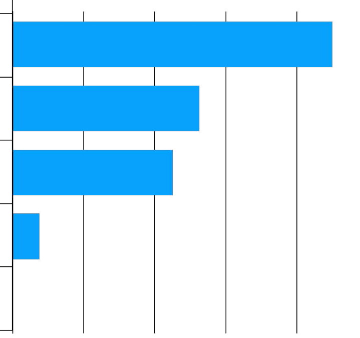


Table 5: Response to the question, “How challenging was this course compared to most other engineering, science, and math courses you have taken?”

Rating	Respondents	Percentage
Much more challenging	10	13%
Somewhat more challenging	34	43%
About the same	24	31%
Somewhat less challenging	10	13%
Much less challenging	0	0%

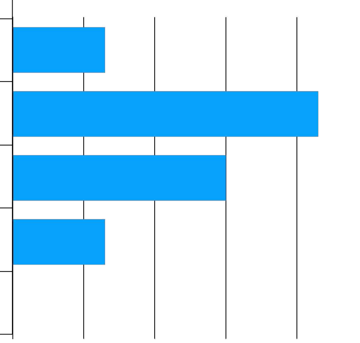
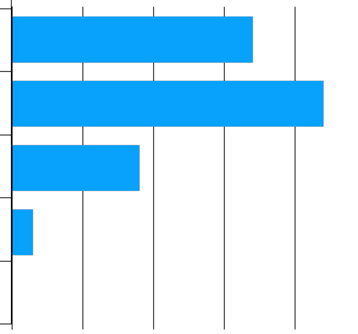


Table 6: Responses to the question, "Rate your experience using Morfli in this course"

Rating	Respondents	Percentage
5: It was great	27	35%
4: It was good	35	45%
3: It was okay	14	18%
2: It was kind of bad	2	2%
1: It was really bad	0	0%



5.2 Time Spent on Pre-lecture Exercises

The average time students reported spending on pre-lecture activities was 45 minutes, the median was 35 minutes, and the minimum and maximum were 10 minutes and 3 hours respectively. A median time of 35 minutes for pre-lecture activities is totally reasonable, given the expectation that students spend a total of around 10 hours per week on a course.

5.3 Preference of model-based pre-lecture exercises vs videos

Of the 78 students who responded to the survey, 66 provided responses with a clear answer to this question: 41 students (62%) preferred the model-based pre-lecture exercises, 19 students (29%) preferred video lectures, and 6 students (9%) said they like a combination of both. Table 7 displays the two main categories of reasons that students preferred model-based exercises in order of how commonly they appeared: (1) they were more interactive, engaging, or fun, (2) they helped students understand or visualize the concepts better. Table 8 displays the one main category found for why students preferred video lectures: they found them easier to understand and/or found the models confusing.

Students were also asked in another question whether they thought the NetLogo models helped them learn, what they liked about them, and what they didn't like about them. Of the 72 students who answered whether they thought the models helped them learn, 65 (90%) said yes, five (7%) said somewhat, and two (3%) said no. Student responses regarding what they did and didn't like resulted in similar themes as the previous question. Students liked that NetLogo models were interactive or engaging and thought they helped them visualize phenomena and understand them better. On the negative side, students sometimes thought the model were confusing or not enough explanation was provided. Given the similarity of these responses to the previous question, specific examples are not included here for space considerations.

Table 7: Reasons students gave for preferring model-based pre-lecture exercises

Code	Count	Examples

Interactive/ engaging/ fun	22	“I liked the model-based exercises because it allowed me to adjust the initial and future conditions and see the results very easily.” “pre-lecture exercises I think helped more than the video lectures because I was actually applying the knowledge.” “The models were just fun to play around with.” “I enjoyed the model-based ones more since I could interact with them and try out things beyond what was asked in the assignment.”
Better understanding/ visualization	13	“i really really liked model based exercises because i was able to gain better intuition for the concepts and i could picture the simulation during a test when i needed to.” “I liked the model exercises because it helped visualize the concepts” “Model-based; greatly increased my understanding of whatever the topic was and provided a different angle than just lecturing.” “I prefer the model-based exercises as they allow me to play around with them and have a better grasp of the material.”

Table 8: Reason students preferred video lectures

Code	Count	Examples
Videos easier to understand or models were confusing	13	“I liked the video lectures because they explained everything.” “I preferred the video lectures more because learning from a person ensured I related more to the content and understood it better.” “I liked the video lectures more because the model exercises were a little more time consuming and harder to understand.” “The video lectures were always very nice. Some of the models were a bit confusing, so I usually prefer videos.”

5.4 Questions Related to Morfli

The following summarize the main takeaways from each category of what students liked about Morfli (their suggestions for improvement are below):

1. Many students thought that the content on Morfli reflected the course content and was well organize, clear, comprehensive for the needs of the course, and concise. The codes with example responses supporting this claim are shown in Table 9.
2. Students enjoyed the NetLogo models, general interactive nature of Morfli, and the fact that solutions to questions were immediately available after submitting an answer. The codes with example responses supporting this claim are shown in Table 10.

3. Students found Morfli easy to use and navigate and specifically appreciated that due dates for assignments were very prominent. The codes with example responses supporting this claim are shown in Table 11.
4. Students appreciated the extent to which everything was in one place on Morfli including text, questions and models. Example responses supporting this claim are shown in Table 12.

Table 9: Reasons students like the content of the course hosted on Morfli

Code	Count	Examples
Well organized, structured and focused	16	"I liked the organized structure and content." "There's a lot of info and it's easily accessible and well sorted.." "It was organized into smaller sections and chapters."
Morfli content reflected the course content	11	"Morfli reflected what was shown in class…" "I liked that it was written by the instructor so all of the information was important which I never feel was the case I felt when reading textbooks for my other classes." "I liked how everything I needed to know was on it. It ensured that I was not questioning if a concept would be tested or not." "I liked that the "textbook" for this class was customized so that it only contained info that we were supposed to know and not just random information too."
Clear content	8	"It was very easy to use and the content was clear and concise." "Content was straightforward and simple to understand. Callister is a bit too dense in my opinion." "I liked that it was like a textbook, but easy to read and easy to use. It's conveniently split up, and definitely used it a lot to study for the exams. I just read all the Morfli chapters from front to back, which really helped me understand all the content." "It was not hard to understand like a lot of other textbooks."
Comprehensive content	7	"The information on there was really comprehensive and easy to understand." "It was a good source of info, learned a lot from it and it was everything I needed to learn." "I liked that it was written in such a way that you could actually read every word on every page and it had just the right amount of material for our class. Didn't have to judge whether something was

		getting too complicated and should be skipped to focus on stuff that would more likely actually be covered in class.”
Content was concise	7	“It was very easy to use and the content was clear and concise.” “It had just the right amount of information, enough to feel like I understood the content while still being able to go and read it all.” “…most of the information was presented in a concise manner.”

Table 10: Codes related to Morfli's interactive features

Code	**Count**	**Examples**
Liked the models	13	“I really enjoyed the models that we used.” “Simulations was the best part.” “…the models were useful…” “The models were fun to play with.”
General interactive	8	“I liked that it tested your knowledge at every step.” “I liked how it was interactive.” “I liked the interactive exercises.” “The exercises were productive and helped me interact with the content.”
Immediate Solutions	4	“I liked the feedback and answers right away.” “I liked that we were able to see the solution after answering.” “I also liked that after answering questions you could easily check your answer instead of having to wait for a key to be released. i could immediately correct my mistake in my head instead of proceeding with the incorrect assumption.” “I liked how you could change your answer after submitting, made it much lower stress, and the ability to see the answer and correct yourself was very helpful to ensure you were going down the right track which was nice.”

Table 11: Codes related to ease-of-use

Code	**Count**	**Examples**
Easy to use and navigate	22	“It was very easy to use…” “It was very convenient to use, especially when reviewing.” “It was easy to access all the information.”

		"It's a great platform and very intuitive, no major complaints!" "I like the setup of the course and how easy and intuitive it is to use."
Clear due dates	8	"The due date times are all there." "I liked that it gave me exactly what I needed to do and by when..." …I also liked how the assigned questions appeared on the home page and indicated when they were due, and if they were completed or not." "…the task list on the home page is really nice to make sure nothing is missed…"

Table 12: Stand-alone code about the platform having everything in one place.

Code	Count	Examples
Everything in one place and well-integrated	10	"How everything was in one place." "I liked how the question software was embedded into the textbook." "I enjoyed how the exercises could be interwoven into the textbook, and they built off of each other." "I love how Morfli helps students see simulations, read the textbook, and do homework, all in the same place."

Only 52 students of the 78 responses suggested improvements for Morfli. The other 26 either left this question blank or wrote things like "n/a" or "none," or "Overall I thought it was very solid." The responses for what students thought could be improved about Morfli were coded and these codes grouped into four broad categories. Any code which had only one response and was not able to be categorized into one of these categories was removed. The broad take aways from the four categories are:

1. The most common responses were the mention of typos (12 responses) and that the content in Morfli wasn't complete (9 responses). These were grouped into one category because they relate to the course not being finished and polished.
2. Students had various suggestions on how to improve the content of the course on Morfli. None of these suggestions appeared more than five times, indicating that there were not any glaringly obvious problems. Some suggestions included: shortening the sections, providing more external resources, including more videos, and improving the descriptions of models.
3. Seven students expressed frustration with the questions in the course which required students to submit an image. This aspect of the platform can be improved.
4. Students had a few suggestions for new features for Morfli. The only suggestion that occurred more than once (three times) was for a commenting system, which is now being developed.

6. Discussion

This project reports on student perceptions of a major redesign of the introductory MSE course at a large private university to center around computational models. The redesign was rooted in the idea of *restructurations*, that the way we represent knowledge can have a profound impact on thinking and learning. Although a large literature on computational restructurations exists, this project was the first to attempt a full course redesign. It was not obvious at the outset that it would be feasible to do this without overloading students in a large lecture-based course. We have shown that with the right tools and pedagogy, not only is it feasible, but the response from students was overwhelmingly positive.

The core of the course's restructuration is using "one-to-many" computational techniques to represent and model materials science phenomena. Each computational technique can be used to model many phenomena, and each one embeds "powerful ideas," in the language of constructionism, and important "cross-cutting concepts" and "core disciplinary ideas", in the language of Next Generation Science Standards. Molecular dynamics (MD) is the most common computational technique in the course which is based on the core concepts of Newton's laws and interatomic force/energy interactions. From the relatively simple rules of modeling each atom as a point mass which exerts a force on surrounding atoms, phenomena such as crystal structure, energy of point defects, mechanical properties, and dislocations emerge. Thus, in addition to foundational Newtonian physics, MD simulations continuously highlight the emergent nature of materials phenomena.

The core tools used for the course were NetLogo and an interactive textbook platform called Morfli. NetLogo is a computational modeling platform designed to be "low threshold" and "high ceiling." NetLogo code is relatively easy for novices to understand, and it enables the models to be interactive in real time as they run. The custom interactive textbook used to deliver the computational models enabled models, surrounding explanatory content and exercises to all be on one platform. This made it easy to engage students in more active learning than a typical course.

Specifically, we used the constructionist learning cycle, a combination of constructionist microworlds with the original learning cycle, for designing activities around computational models. The learning cycle is based on the idea that students must go through a constructivist process to learn "science concepts of considerable explanatory power" [35, p. 78] but that most students will not discover these ideas on their own without some direct instruction. The learning cycle thus consists of three stages: (1) exploration, in which students explore a phenomenon on their own, (2) concept development/term introduction, in which the instructor helps students interpret their findings from the exploration and eventually introduces the scientific terms of the phenomenon, and (3) concept application, in which students apply the concept to a new situation. The constructionist learning cycle, introduced here, retains these three stages and uses computational microworlds (interactive computational models) in the exploration and/or the concept application stages. The overall approach is meant to strike a balance between student-driven exploration of models and the targeting of specific learning outcomes.

Based on the Likert-style questions, the answer to our first research question is that it is feasible to restructurate the introductory MSE course around computational models and maintain positive student experiences. Students had overwhelmingly positive experiences with the course, the interactive textbook, and the computational models. The large majority of students rated the course as more engaging than most STEM courses they had taken and their experience with the interactive textbook as good or great. A large majority also thought they learned more than in a typical course while only a small minority found it much more challenging than a typical course.

Student responses to open-ended questions, revealed a number of important themes about student perceptions to the novel aspects of the course, specifically the interactive models and the interactive textbook. Most students preferred the model-based pre-lecture exercises over video lectures. The main two reasons for this preference were that they were (1) more interactive, engaging, or fun and (2) they helped students understand and visualize concepts better. For the minority of students who preferred video lectures, the main reason was they found videos easier to understand or found the models confusing. This suggest that that although the model-based exercises worked well for most students, additional scaffolding might be needed for some students.

The reasons students liked the interactive textbook fell into four broad categories. First, students thought that the content was clear, well organized, concise, and comprehensive for the needs of the course. It was feasible to make the interactive textbook concise while still comprehensive with respect to the course because it was designed text specifically for our course, enabling us to cover everything we wanted without having superfluous material. The platform we used allows instructors to edit the text which would enable other instructors to adapt the text to be concise yet comprehensive with respect to their courses. Second, students enjoyed the interactive nature of Morfli, including both the embedded NetLogo models and the fact that solutions were immediately viewable after submitting answers to a question. These are features obviously not available for static textbooks. Third, students felt the interactive textbook was easy to use and helped them keep track of when pre-lecture assignments were due. Finally, students appreciated that the interactive models, explanatory text, and exercises were all in one place. In an age when software products are proliferating, students appreciate having a single website contain all these elements in one place. The main suggestions for improvements were very minor relating to typos in the text and that they wished the content of the interactive textbook was finished (at the time of the course, a few course topics had not yet been completed).

6.1 Limitations and Future Work

The study has a number of limitations. First, the students are from a selective private university. It is possible that the positive results reported here will not generalize to other student populations. Second, we did not collect data from a control group because our materials and questions evolved over a number of iterations, making it difficult to compare between groups. Third, this study does not study student learning outcomes. We plan to conduct future work to address these limitations by working with another professor to collect data on student learning and perceptions prior to using our materials and then again after implementing a version of our materials.

7. Conclusion

Basing the introductory MSE course around computational models aligns it with the larger trend of increasing computation in the field and—when using the right tools—harnesses the powerful learning affordances of computational representations, as described in restructuration theory. We redesigned the introductory MSE course using two main technological tools—NetLogo and Morfli—and one main pedagogical approach, the constructionist learning cycle. NetLogo is an easy-to-use yet powerful modeling platform which enabled to us to create interactive models and embed them in an online interactive textbook. Morfli is an interactive textbook platform which made it easy to engage students in constructionist learning cycles in which they first explore a computational model of a phenomenon, answer questions about it, and then receive explanations before further applying the new concepts. Our findings demonstrate that, at least with these tools and pedagogy, it is feasible to develop an introductory MSE course based around atomistic computational models and for the large majority of students to have very positive experiences with it, both in terms of engagement and perceived learning.

8. References

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