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Incorporating the Use of a Materials Database into a Materials Science and Engineering Freshman Course

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Incorporating the use of a materials database into a Materials Science and Engineering freshman course

Abstract

Over the past years, our team has taken a concerted effort to integrate computational modules into courses across the undergraduate curriculum, in order to equip students with computational skills in a variety of contexts that span the field of Materials Science and Engineering. This effort has proven sustainable during the recent period of online transition of many courses, illustrating one of the benefits of computational modules. The most recent addition to our set of modules included a visualization component that was incorporated into our introductory freshman course for the first time in Fall 2019. Students can perform this module either using local computer labs, access those resources remotely, or via their own computers. In the Fall of 2020, we modified this module and expanded it towards the utilization of a materials database to teach students how to search for materials with specific properties. The results were then interfaced with the previously existing visualization module to connect the atomic structure and symmetry of materials with their properties and to compare them with experimental results. We implemented a more detailed survey to learn to what extent students gained the capability of using databases for future research and education. We will also use these responses to further develop and improve our existing modules.

Introduction

Materials databases store crystallographic structures and other properties of a large number of materials which have been investigated in materials science and engineering. Databases are developed since it is getting difficult to find the appropriate data from accumulated knowledge about materials. A demand for organized databases increases with the beginning of a new era in data science and to date, various databases in the materials science and engineering field have been created. Crystallographic databases are popularly used to find crystallographic information, including atomic structure, point and space group, and density. Inorganic crystal structure database[1], Crystallography open database[2], Cambridge Structural Database[3], and American mineralogist crystal structure database[4] are examples for such crystallographic databases. In addition, there are property-targeted databases such as the refractive index database[5] and Polymer Property Predictor and Database[6]. The Materials Project[7] is a materials database consisting of materials information from first-principles density functional theory high-throughput calculations, and is one of the projects in the context of the materials genome initiate.

Since databases contain diverse information, materials science and engineering academia starts to

incorporate materials databases into the curriculum. To this end, these databases were able to assist education: Nandhakumar *et al.* indicate that database software can improve student's learning experience at the higher-education level by engaging independent and effective learning[8]. Materials science and related fields have also attempted to exploit diverse databases in undergraduate courses or outreach programs. Tchoua *et al.* demonstrate the integration of a database with a course and show that students can learn how to review the literature and contribute to creating the database during the course[9]. Materials databases can also be utilized in courses about materials selection, where students screen the materials for specific criteria and find the appropriate materials[10]. Students can study the structures and bonding of molecules and compounds and chemical reaction pathways through crystallographic databases[11]. Especially, Cambridge Structural Database (CSD) develops a teaching subset to provide representative molecules and show chemical functional groups with teaching materials, activity examples, and exercises[12]. Graduate students have been involved in developing further database functions, and they can draw their thesis research topics related to those works[13].

As a reply to the demand for students with database skills, we integrated a materials database into our freshman course this year, for students to have a chance to experience on their own how the database can be exploited. To this end, we modified a new computational module on crystal visualization that was introduced to our freshman course in 2019[14]. This module helps students to understand and learn the atomic structure of materials and projections on crystallographic planes. Students experienced the connection between theory and experiments by comparing their answers with scanning transmission electron microscope images. This year, we added database-related exercises into this computational module, to expand the students' experience towards a materials database. The updated module included the interface between the materials database and a visualization program. Students were requested to find a material from the database, download a crystallographic file, and open it through a visualization program. We designed a survey questionnaire to check their perspective on general computational modules in the curriculum, the difficulty of each module, quality of instructions, potential utilization, and feedback for the module's future development. In this paper, we present and discuss the survey results from the students in the freshmen course and find a way to provide a better experience to students based on their feedback.

Course Details and Computational Module

The course we focus on here is an introductory class for freshmen in the department of materials science and engineering. The goal of MSE 182 is for first-year students to experience broad topics in materials science and engineering. Students are expected to learn diverse topics and interdisciplinary subjects in materials science and engineering. One of the crucial subjects is understanding the crystal structure of materials, which is the basic concept to understand how materials are constructed. The computational module for this class helps students learn crystallography of materials. Crystal structures and crystallographic planes are subjects for students to establish the ability to think three-dimensionally about visualization of materials and distinguish different atomic arrangements.

A traditional way to learn atomic structure is drawing with pencil and paper. Since paper is a two-dimensional medium, it is not easy for first-year students to learn three-dimensional atomic

e) The scanning transmission electron microscope (STEM) acquires images that represent 2D projections of 3D crystals, much like the ones you drew in the gumdrop activity. Below are 3simulated STEM images of silicon in the diamond structure. In these images, bright dots represent the positions of atomic columns. Using the information you obtained using your OVITO simulations, identify which two are imaged along the [110] and [111] directions, which are also called zone axes, and state which is which.

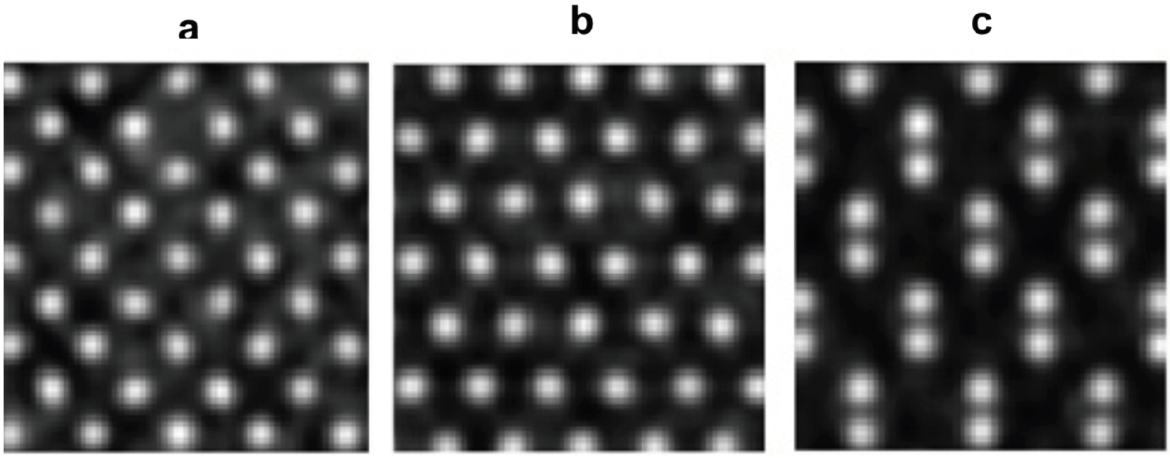

Figure 1: Screenshot of exercise about the scanning transmission electron microscope integrated with the OVITO visualization program.

configurations using this approach. Contemporary research institutes and industries mostly use computer programs to visualize those crystal structures. Their demand for recruits with this skill is increasing. Thus, another goal of MSE 182 is to expose undergraduates to modern approaches and frontiers in materials science and engineering by using software to solve materials science problems.

In 2019, we first introduced the computational module using OVITO[15] for atomic visualization to make students familiar with work experience on three dimensional visualization on a computer. The original objective of this module is to make students familiar with three-dimensional structures and the visualization program. The instructor provided a handout about the visualization program and a crystallographic file of the silicon lattice structure. For exercises, students were asked to sketch specific projected atomic planes along with specific directions. The instructor also provided scanning transmission electron microscope (STEM) images, and students were trained to distinguish the plane index by rotating and comparing the atomic configuration through a visualization program (see Fig. 1).

This year, we included an additional aspect into the module, using the Materials Project[7] as a materials database to interface it with the OVITO program. The objective of the database add-on module is that students experience the materials database. Materials database can provide various materials case studies with crystal structures. Thus, the addition of a materials database can improve the achievement of learning objectives of MSE 182 by exposing students to various examples. The instructor developed one additional handout on materials databases to deliver their

Use the attached handout on Materials Database to:

1. On the Materials Project, click Fe (Atomic No. 26) and press the search button. You will see several listings because Fe can occur in several different crystal structures. On the list, find the "Materials ID" mp-13 and open it.
    a) Find the crystal system and lattice parameters *written on this webpage* and record them
    b) Using the lattice parameters *written on the webpage*, identify the crystal system of this crystal structure.
    c) Using the built-in viewer on this page, see if you can rotate the crystal structure so that you see a square pattern and sketch the arrangement of atoms you see.

Figure 2: Screenshot of exercises on identifying the structures of pure iron phases implemented using a materials database.

meaning and importance. Instead of offering crystallographic files, students were instructed to find target materials through the database by identifying the crystal system and lattice parameters on the web page (see Fig. 2). After that, students should download the crystallographic file of selected materials and open them using the OVITO program. In addition to sketching atomic planes and comparing them with STEM images, students were asked to implement OVITO's built-in function to determine each atom's coordination number.

Survey Details

The survey questionnaire developed in 2019 focused on collecting the students' general perspective on computational modules since this survey was carried out for several courses with computational modules in the department of material science and engineering. There were two specific inquiries focusing on the freshmen course, to check students' level of comfort with the computation module compared to conventional methods of teaching the material. We included the same questions in 2020 to compare the freshmen students' perspective between both years. These questions 1 to 9 are listed below.

- Q1: Do you think computational tools are important for materials science and engineering? (Very unimportant 1 ... 5 Very important)
- Q2: Do you think computational materials science skills are important for your post-graduation career? (Very unimportant 1 ... 5 Very important)
- Q3: Should there be more or less computational material in MatSE classes? (Much less 1 ... 5 Much more)
- Q4: In general, do you think the computational experiences you have had in MatSE classes are beneficial to you? (Not Beneficial at All 1 ... 5 Very Beneficial)
- Q5: What do you think is the best time to start learning computational skills in MatSE classes? (Freshman, Sophomore, Junior, Senior)

- Q6: Do you think the computational modules help you understand the related course materials in MatSE 182? (Strongly disagree 1 ... 5 Strongly agree)
- Q7: Do you understand the objective of the computational modules? (Don't understand very well 1 ... 5 Understand very well)
- Q8: If you were asked to visualize and compare different crystal structures, how comfortable would you be using drawing (pencil and paper)? (Very uncomfortable 1 ... 5 Very comfortable)
- Q9: If you were asked to visualize and compare different crystal structures, how comfortable would you be using OVITO (or similar software)? (Very uncomfortable 1 ... 5 Very comfortable)

In 2020, we designed additional questions about the updated computational modules to evaluate how effectively the newly inserted exercises on materials databases were implemented. The first three questions ask about the difficulty of each program and its interface. Students indicate which module may require more instructor support next time. The next two questions are about satisfaction with the length and clarity of the instructions. Based on the results from these questions, the written instructions will be updated in future years. We create four questions investigating the utilization of the current module and similar programs. These questions also check whether students might potentially use such software in the future. Lastly, we check whether students want more or less exercises with these computational modules.

- Q10: How difficult to find the target information through web interface of the Materials Project? (Very difficult 1 ... 5 Very easy)
- Q11: How difficult to download the structure from Materials Project and open the crystallographic file in the OVITO program? (Very difficult 1 ... 5 Very easy)
- Q12: How difficult to analyze the structure through the OVITO program? (Much difficult 1 ... 5 Very easy)
- Q13 and Q14: How would you rate the instructions for computational modules in MSE 182? (Very vague 1 ... 5 Very clear)
- Q15: How comfortable would you use OVITO or any visualization programs to solve the problems? (Very uncomfortable 1 ... 5 Very comfortable)
- Q16: How comfortable would you use Materials Project or any materials databases to solve the problems? (Very uncomfortable 1 ... 5 Very comfortable)
- Q17: If you were asked to find a material with specific properties in another class, would you use Materials Project or similar databases? (Not likely 1 ... 5 Very likely)
- Q18: If you were asked to analyze a material's crystal structure in another class, would you use OVITO or similar visualization programs? (Not likely 1 ... 5 Very likely)
- Q19: Do you think MSE 182 needs more/less exercises for different materials to study atomic structures with computational modules? (Much less 1 ... 5 Much more)

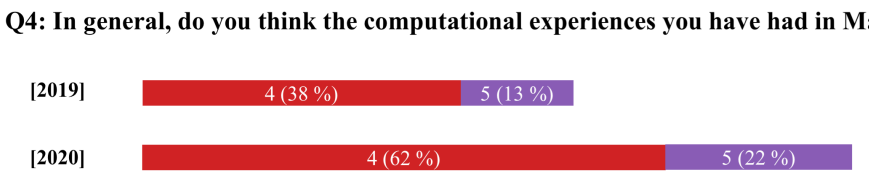

Figure 3: Statistics of students' positive answers on question 4 from MSE 182 course. Answers are scaled from 1 (Not beneficial at all) to 5 (Very beneficial). The number of total responses in 2019 and 2020 is 82 and 47, respectively.

Results and Discussion

Students' general perspectives on computational skills in 2019 and 2020 did not change largely after we updated the computational module, and the results show that students have positive opinions in general about the importance of computational skills in materials science. The total number of responses in 2019 and 2020 is 82 and 47, respectively. The overall aspect of answers is almost not changed except for question 4, which will be discussed later (see Fig. S1 and S2). Around 90 % of the students think computational tools are essential for materials science and engineering in both years. Almost the same number of students agreed that computational skills are important for their post-graduation career. More than half of the students want more computational material in their MatSE classes. Around 60 % of students consider their freshman year to be the best time to learn computational skills in MatSE classes. Fewer than 20 % of students felt it was difficult to understand the objective of the computational modules.

Unlike questions 1 to 7 about the general perspective on computational skills, questions 8 and 9 in both years are specifically related to the freshmen course; here, our survey results indicate that students' perspectives on visualization of materials structures through hand drawing and computer programs were not largely changed. Students still felt that hand drawing is easier than using OVITO or similar programs to visualize and compare crystal structures. Current exercises are working with relatively simple atomic structures, such as BCC iron and silicon, that are not difficult to be drawn by hand. Thus, the difficulty of learning a new visualization program is more demanding than simple drawing by hand. Adding more complex structures to the module may increase the students' perception of the advantages of visualization software compared to hand drawing. However, it will be important to balance the difficulty of class exercises by providing structures which are appropriate for first-year students who are new to crystal structures and more complex structures that more clearly demonstrate the advantages of visualization software.

Question 4 is asking about whether students expect to benefit from computational experiences in MatSE classes. We found an apparent positive change of answers from 2019 to 2020 shown in Fig. 3. 51 % (38 % of beneficial + 13 % of very beneficial) of students in 2019 think these experiences are beneficial to them, compared to 84 % (62 % of beneficial + 22 % of very beneficial) in 2020. In detail, a large portion of students who answered 3 is reduced, and it is absorbed to answer 4 comparing 2019 and 2020. The unusual situation of 2020 might affect the perspective of students on computational modules. Overall, on-site laboratory experiences are reduced due to the COVID19 pandemic, while the amount of computational modules increases. This might give a positive impression on computational experiences and change the perspective of

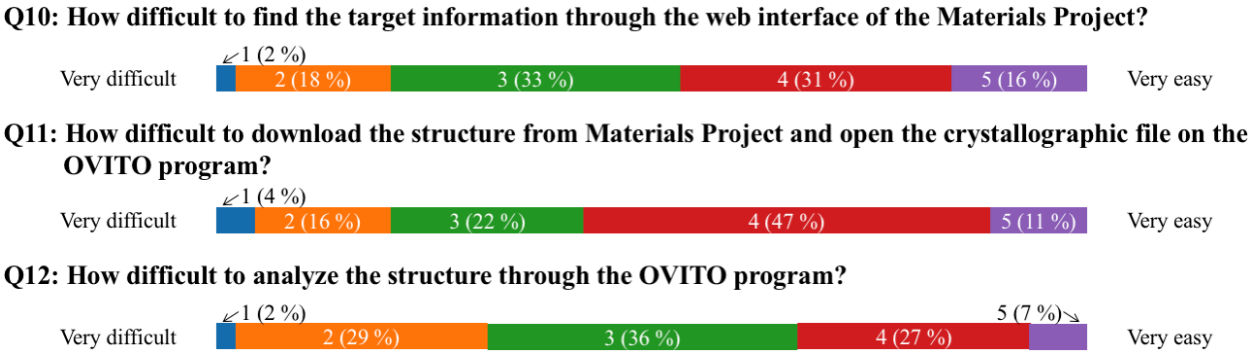

Figure 4: Statistics of students' answer on question 10 to 12 from MSE 182 course. The number of total responses in 2020 is 47.

first-year students.

Starting with question 10, we designed the questionnaires for the newly adopted module (see Fig. S3 and S4 for whole results). Questions 10 – 12 inquire about the difficulty of each module and their interface, and the results shown in Fig. 4 present that OVITO is the most difficult module. 20 % (2 % of very difficult + 18 % of difficult) of students feel that the Materials Project and its interface with OVITO are difficult. More students of 31 % (2 % of very difficult + 29 % of difficult) said that the OVITO program is hard to use for analyzing structures. Difficulty during the class exercise directly connects to the comfortableness to exploit the program. From replies to questions 15 and 16, 27 % and 33 % students answer that they are uncomfortable to use Materials Project and OVITO, respectively. This result indicates that we might need to update the OVITO program exercises to achieve better performance.

We prepare questions 13 and 14 to check the quality of provided instructions to implement each module, and the results confirm that the length and clarity of our instructions are appropriate. In terms of length, 26 %, 58 %, and 16 % of students said the instruction were short, appropriate, and long, respectively. The instruction is moderate in length, and it might need to balance the portion of short and long answers. Better balance might be achievable by adding short notes for challenging steps next time. 13 % of the students found the instructions to be vague. These students can get support from additional communication channels with the instructor or computational teaching assistant through e-mail and office hours, and we aim to reduce that number.

We also checked the potential usage of each computational module for related subjects in another class and the results indicate that there are some students willing to use OVITO in spite of not being fully comfortable with it. In Fig. 5, questions 17 and 18 show that more than half of the students want to use modules in another class. By comparing reply from question 12 in Fig. 4 and question 18 in Fig. 5, reduced negative answers in question 18 indicates that some students are willing to use OVITO although they are uncomfortable with it. The result from question 19 gives insight into how we can improve the current computational module. 80 % (60 % of more + 20 % of much more) of students want more exercises with different materials to study atomic structures with computational modules. This indicates that students want more exercises to develop more familiarity with computational modules. These results indicate that a key next step is simply to

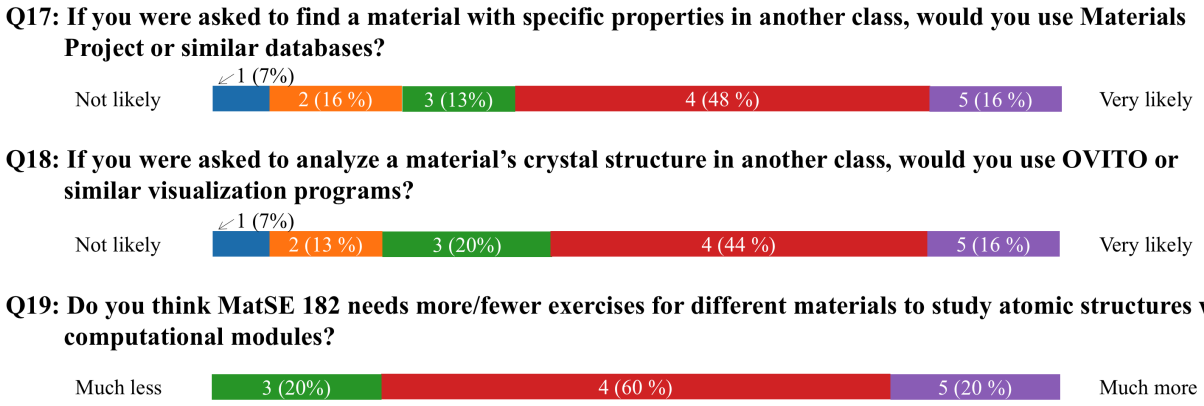

Figure 5: Statistics of students' answers on questions 17 to 19 from MSE 182 course. The number of total responses in 2020 is 47.

expand the number of exercises that utilize the computational modules, and that this adjustment should increase both the students' comfort level and willingness to use materials databases and visualization software in other classes.

Conclusions

As the importance of materials databases increases, we incorporated one into a computational module in a freshmen course in the department of materials science and engineering. The original computational module was designed to train students in three-dimensional visualization of materials' atomic structures. After the update, students now also locate the target materials in the materials database, distinguish the materials based on lattice parameters and unit cell, and download a crystallographic file. Students learned how to open the crystallographic file through a visualization program and characterize the structure using the coordination number and atomic configurations on projected planes. We surveyed students' perspectives on general computational modules over two years and explicitly conducted designed questions focusing on the freshmen course. During the unusual situation in 2020, students' attitude to computational experiences in MatSE classes became more positive, along with the change of the computational module. Some students feel it challenging to analyze the atomic structure through the OVITO program, but they want to use it for related subjects in other classes. The solution for this discrepancy is suggested from the reply to another question, that students want more exercises with the current module. More exercises might make students familiar with current modules, reduce the difficulty of usage, and increase their willingness to use them for related topics in other classes or after graduation.

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Supplementary materials

All survey questionnaires are listed in Sec. .

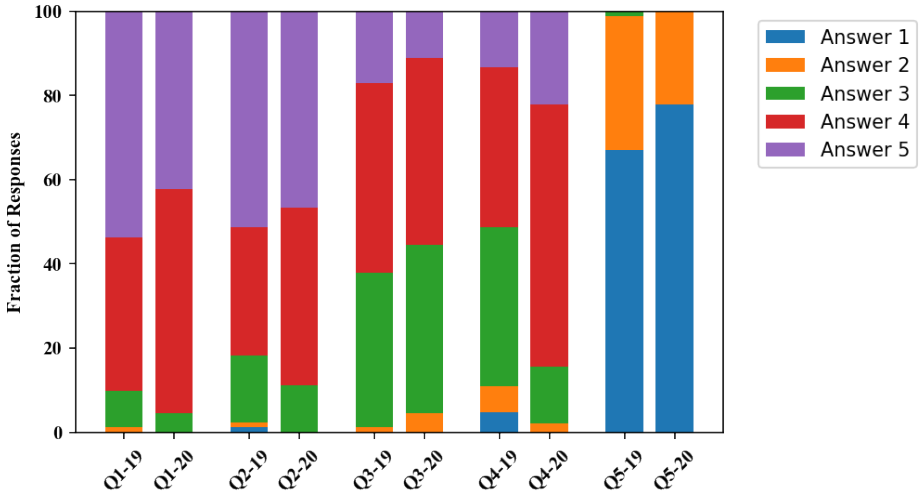

Figure S1: Statistics of students' answers on questions 1 to 5 from MSE 182 course. The number of total responses in 2019 and 2020 is 82 and 47, respectively.

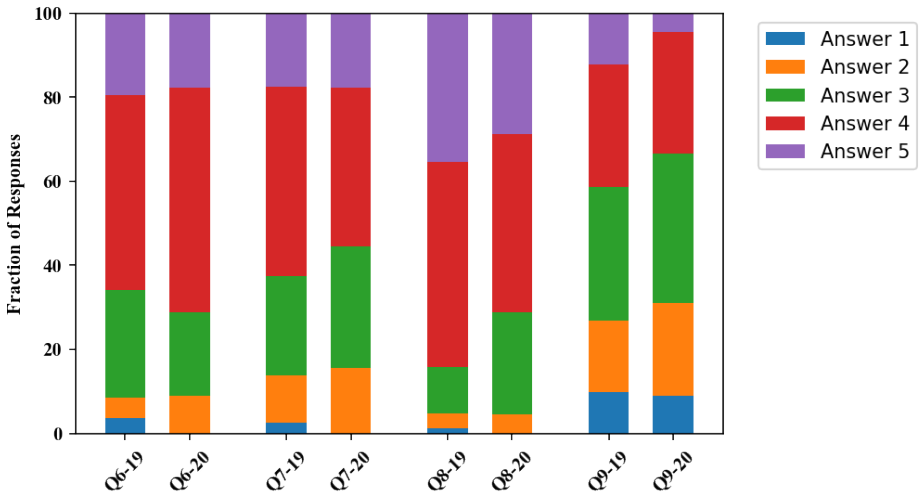

Figure S2: Statistics of students' answers on questions 6 to 9 from MSE 182 course. The number of total responses in 2019 and 2020 is 82 and 47, respectively.

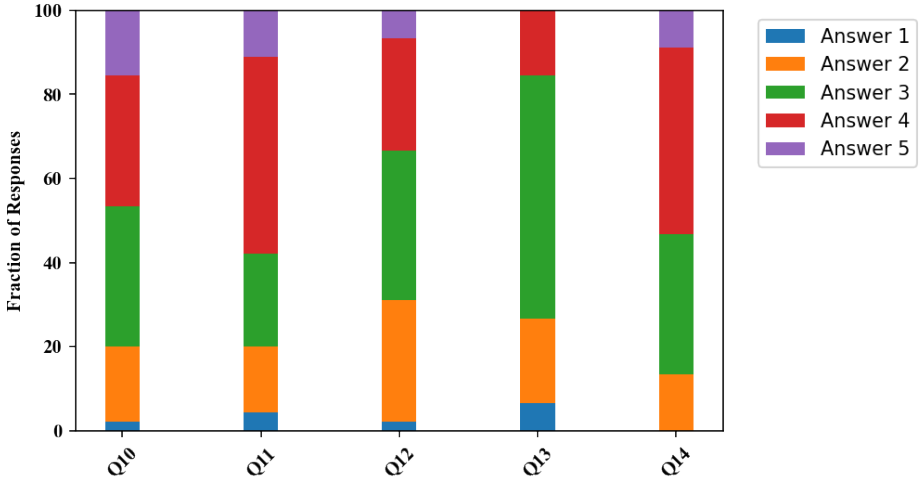

Figure S3: Statistics of students' answers on questions 10 to 14 from MSE 182 course. The number of total responses in 2020 is 47.

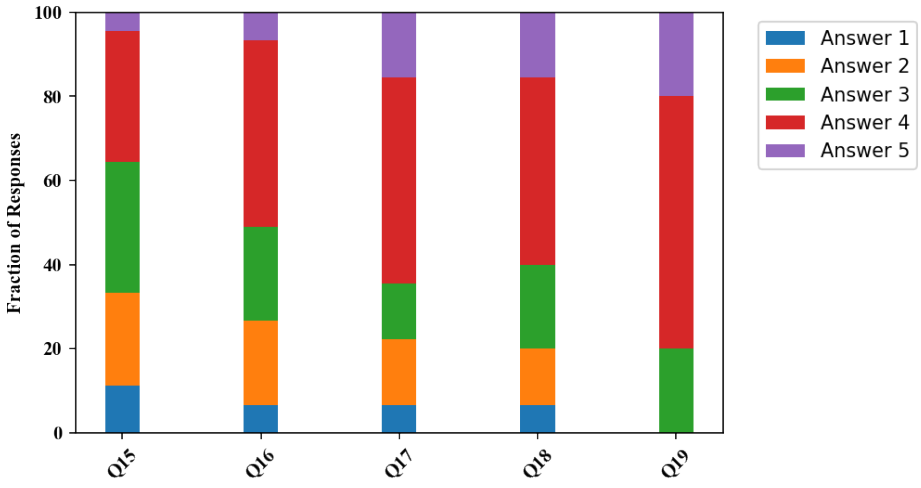

Figure S4: Statistics of students' answers on questions 15 to 19 from MSE 182 course. The number of total responses in 2020 is 47.