The Future of Engineering Education
2024 Annual Conference & Exposition
Oregon Convention Center
Portland, OR . June 23 - 26, 2024
ASEE
Paper ID #44272

Integrating Computational and Physical Lab Modules in Materials Science and Engineering

Jonathan R. Brown, The Ohio State University

Jonathan Brown (B.S., M.S. Mathematics, New Mexico Institute of Mining and Technology; Ph.D. Materials Engineering, New Mexico Institute of Mining and Technology) is an Assistant Professor of Practice in the Department of Materials Science and Engineering at The Ohio State University. His background is in computer simulations and theory of polymer glasses and block copolymers for energy applications. He teaches introduction to materials science and engineering and computational materials science courses.

Dr. Elvin Beach, The Ohio State University

Integrating Computational and Physical Lab Modules in Materials Science and Engineering

Abstract

Computational tools play an ever-expanding role in the careers of practicing engineers. As such, in addition to physical labs, our program requires all undergraduate students to take a two-semester sequence in computational materials science called "modeling and simulation" (or ModSim) focusing on practical programming skills and use of commercial CALPHAD and FEA software. These courses are taught in the spring semesters of the sophomore and junior years and formatted as hands-on computational laboratory courses. Originally, the physical lab and ModSim courses were delivered as separate sequences each loosely tied to what the students were learning in their lecture courses. However, while the application of physical labs to engineering practice is clear, students often did not connect what they were learning in ModSim to their future careers, as the computational labs were often written to reinforce basic MSE concepts or fit the capabilities of the computational software. In response to this, we have written two modules in the lab and ModSim sequences that directly make connections back and forth between the sequences. In the first, students are tasked with designing an aluminum alloy to meet certain strength, conductivity, and ductility requirements both physically in the lab and computationally using CALPHAD software, and in the other, students simulate a Jominy end quench hardenability test using CALPHAD and FEA tools, then physically perform the test on steel samples as part of a lab to identify an unknown alloy. Summaries of these modules and how student perceptions of the course and their learning changed as a result of these modules are presented.

Introduction

Data-driven and computational approaches in materials science have been growing in importance for decades and are now considered key competencies for undergraduate materials science majors. Our undergraduate curriculum includes two required courses in modeling and simulation, "ModSim" for short, which are held in computer laboratories and allow for significant real time guided experience with programming and software. The content includes basic coding concepts related to solving materials science problems as well as practical skills in applying commercial software (specifically, MATLAB, Thermo-Calc, and COMSOL). However, despite the importance of these concepts and the tutorial and practice-based nature of the computer laboratory course design, we found that some students struggled to connect their experiences in these courses with their knowledge from the rest of the materials science curriculum. Related to this, we recognized a perception among students that computer labs are inherently different and less practical than experimental labs. We expect that revisiting similar topics in different contexts improves student learning and engagement and increase retention [1], [2]. Thus, to address these issues, between the spring 2021 and spring 2022 offerings we redesigned the ModSim sequence to add several specific connections between the systems studied across the physical lab sequences.

This work to integrate computational approaches in the materials curriculum is especially relevant to share with other departments across the country given the recent national emphasis, through the Materials Genome Initiative and other programs, in using computational tools to enable rational design of materials [3]. In one example, CALPHAD was applied to design a new, cheaper alloy used to manufacture nickels [4]. Computational tools are crucial towards the goal of inverse design of materials, that is, focusing on the set of properties required and then designing the structure and properties of the materials to meet that goal, rather than simply predicting properties of an already identified material [5], [6], [7]. Thus, we hope to share with other educators the impacts of our redesign; this requires us to investigate in further detail how our course design changes, which have already occurred, impacted students.

A key goal of the redesign was to include during the computational sequence frequent mentions and use of data that was familiar to the students from the physical laboratory sequence. Our expectation was that using data that the students themselves had gathered would make the computational results seem more tangible, allowing the students to see their relevance more clearly. Thus, whenever possible, where data was needed in ModSim exercises such as curve fitting, the data was provided by the physical lab sequence experiments. To delve into these issues in more depth, two course modules were specifically designed with close connections between the laboratory sequences. Specifically, in their junior lab, students designed, cast, and processed aluminum alloys to maximize physical and electrical properties; this lab is now revisited in the junior ModSim course where they use Thermo-Calc to model and iterate on their design. Also, in the junior ModSim course, students simulate a Jominy test to predict the hardenability of a steel alloy; this computational lab ties into a senior-level physical metallurgy lab where students identify steel alloys in part by performing Jominy tests. Additional details these are presented in the next section. Finally, we also include a general, qualitative description of student impressions and outcomes as well as quantitative data from student evaluations in response to these modules that may be relevant to inform similar redesign efforts elsewhere. The authors would be happy to share the detailed rubrics and assignments used to interested educators.

Computational-Physical Lab Modules

Module 1: Aluminum alloy design competition

The first major overlapping physical-simulation module is the aluminum alloy design competition. In the physical lab (which occurs first, in the autumn semester of their junior year) teams of students design an alloy, including the thermomechanical processing, in order to maximize conductivity, ductility, and strength. Then, in the simulation lab, students simulate their resulting thermomechanical processing in Thermo-Calc, and propose changes to their process based on these simulations to improve their alloys.

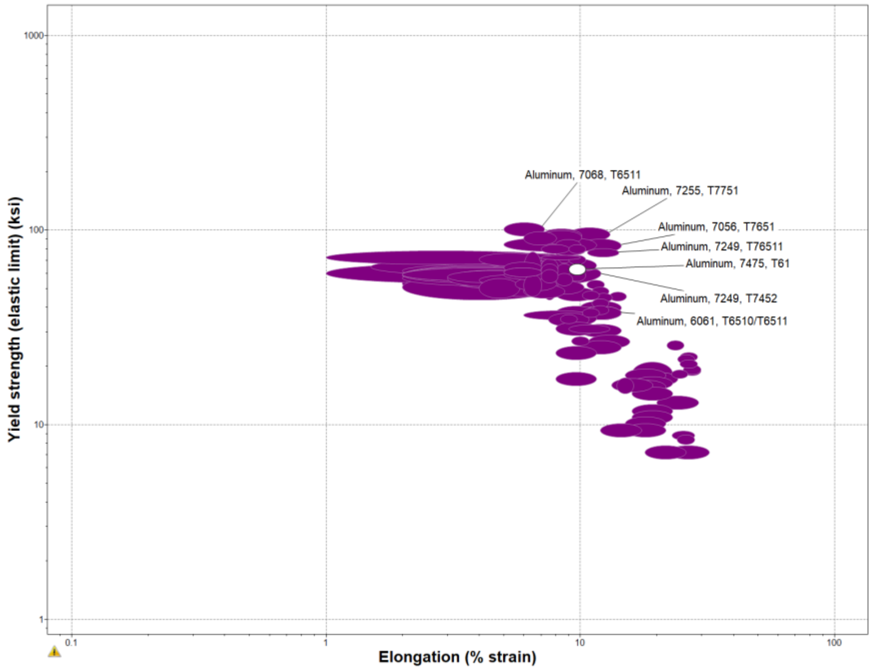
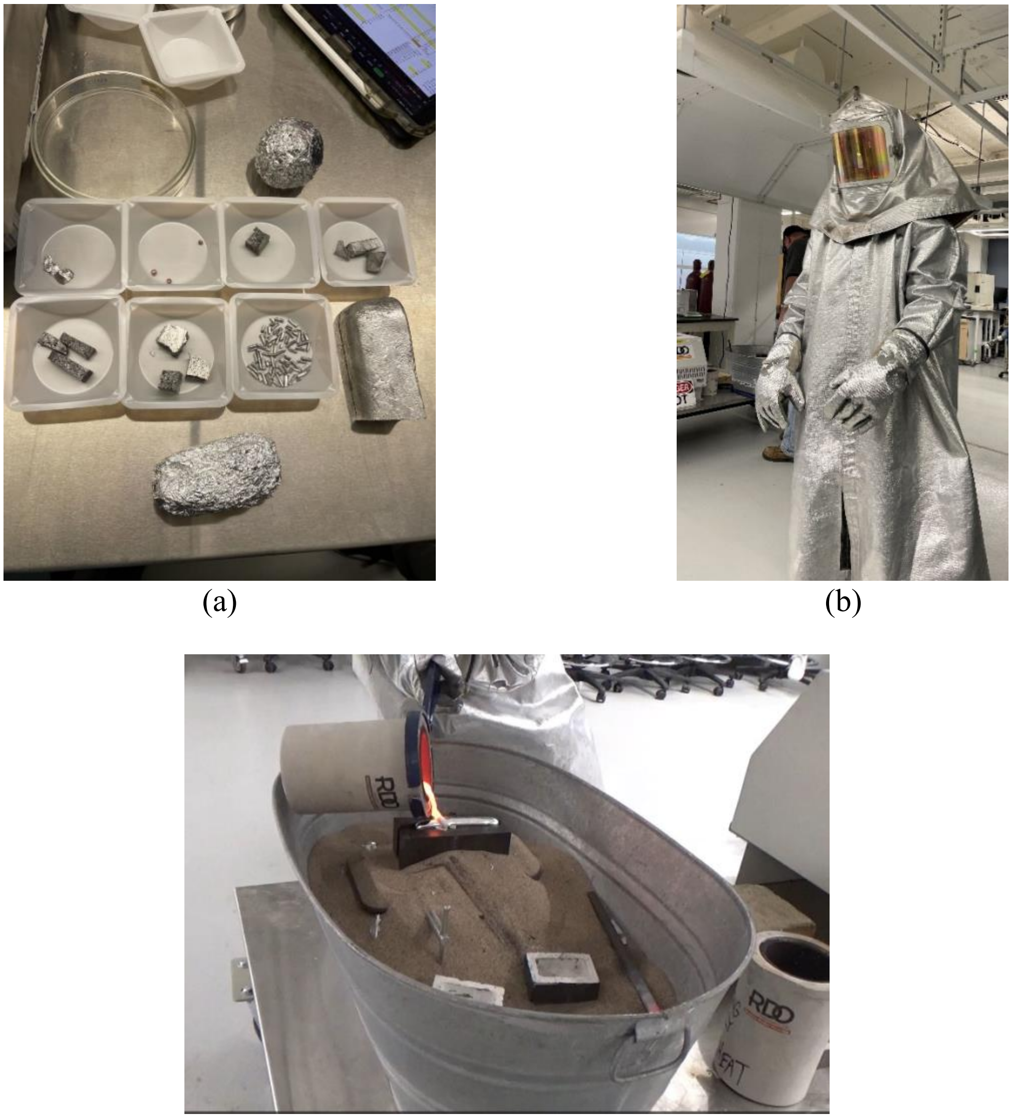


Figure 1. Example of an Ashby plot generated by the students as part of the materials selection process for the aluminum alloy design competition.

The aluminum alloy design competition is a seven-week module in the fifteen-week semester. Students are placed in teams of six to seven and tasked with materials selection, melting and casting their alloy, all thermomechanical processing, mechanical/electrical testing, and microstructural characterization. Teams start by using software to generate Ashby plots comparing various materials properties with the goal of selecting an alloy with the best combination of properties to win the competition. An example from a 2023 student team is shown in Figure 1 where the yield strength and elongation to fracture are compared. Student teams are allowed to modify the chemistry of their alloys within the competition limits (up to ten weight percent alloy content) but must justify why changes were made. The teams then weigh out all the components of the alloy, melt it in an induction furnace and pour two billets for processing. Figure 2 shows examples of the alloy components weighed out, students learning to wear safety gear and practice melting and pouring techniques and successful pouring of aluminum alloy billets.

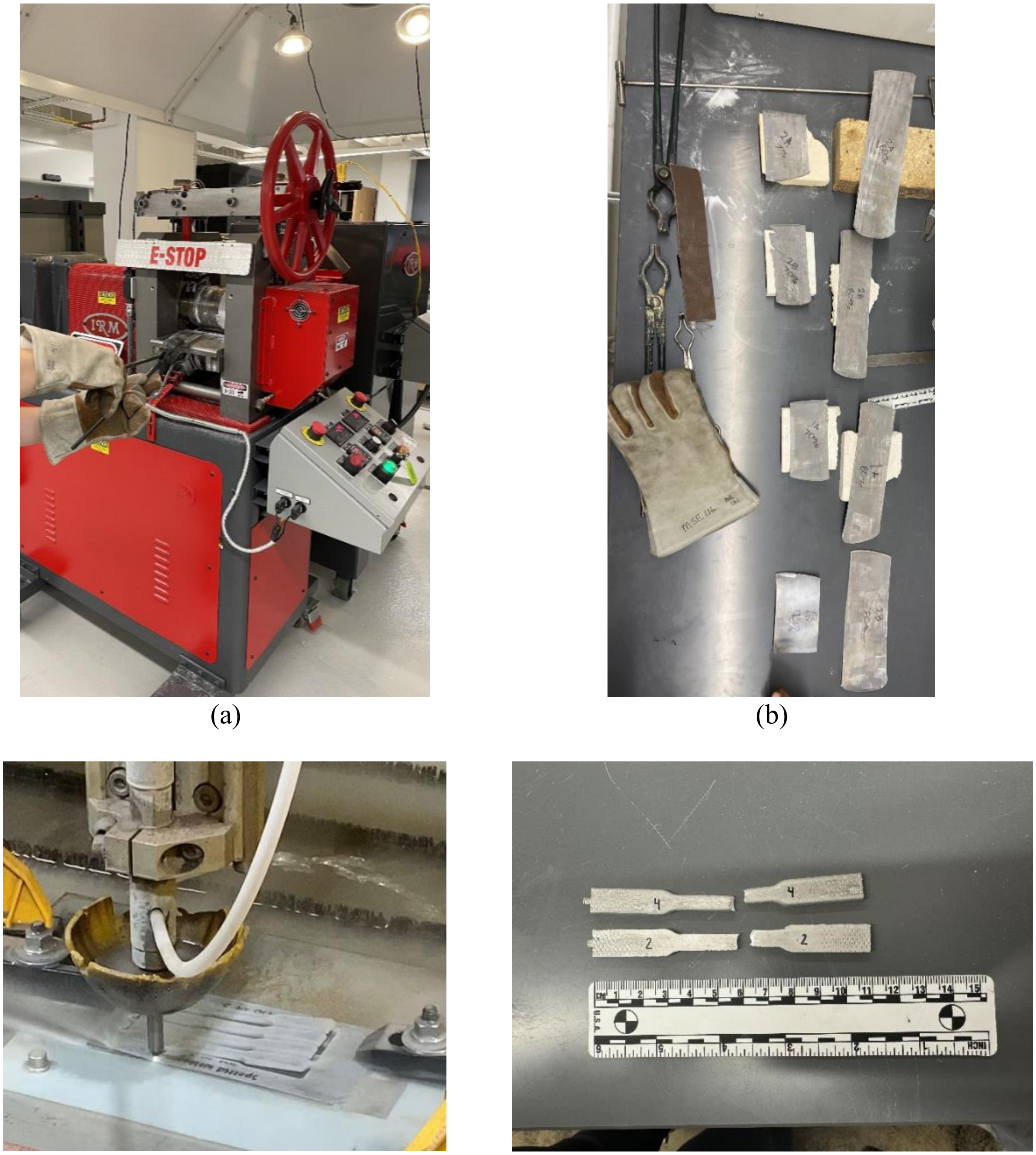


(a) (b)

(c)

Figure 2. Photographs showing (a) the alloying elements weighed out for addition to the melt, (b) students are trained and practice in full foundry safety gear prior to pouring their molten alloy, and (c) a student pouring molten aluminum into the mold.

Thermomechanical process design and execution requires planning and teamwork to complete everything in the allotted time period of 3 weeks (with the autumn break period built into the schedule). Student teams typically homogenize the billet, hot roll and cold roll the material to reach the required thickness (2-3mm final thickness from a 12.5mm original billet), solution heat treat and artificially age the sample. Photographs of students hot rolling and several hot rolled pieces of aluminum are shown in Figure 3 (a & b). The student teams then work with the machine shop to water jet cut tensile bars for mechanical testing and ultimately in the competition. Photographs of water jet cutting and tensile bars after testing are shown in Figure 3 (c & d). During the competition, student teams take samples for hardness measurements, microstructural analysis by optical microscopy, and performing electrical conductivity measurements.



(a) (b) (c) (d)

Figure 3. Hot rolling work is shown in (a) and (b) and the waterjet used to prepare samples for tensile testing is shown in (c) with tensile tested samples shown in (d).

The competition wraps up with a lunchtime competition where all of the student teams gather to spend some time socializing, eating, and discussing the upcoming competition. Electrical and mechanical testing of the final material submitted by the team are conducted in real-time with a score board up in the room to show results as they come in. The competition seems to motivate the teams, and during the past two years, the winner has been decided on the final tensile test making it an exciting event. Students are competitive and respectful to each other throughout the competition, which is part of the instructions provided in the beginning of the contest. The winning team has their photograph taken at a location of their choice in one of the laboratories and a plaque is placed in the processing lab documenting their accomplishment along with past winners.

The samples generated during the competition are used in the next laboratory exercise in this course when they are tested against three commercial aluminum alloys for corrosion resistance. The mechanical testing data generated during this laboratory is added to a spreadsheet of data that is also used in the first modeling and simulation laboratory for statistical analysis and linear regression work by the students the following year. In this way, the students are able to work with real data that has been generated in the labs they will work in and will contribute to the data in the following laboratory-based course.

For the computational lab, which takes place in the following semester (spring of the students' junior year), the students revisit the alloy competition on an individual basis (although they are encouraged to compare notes with their former teammates). This takes place at the end of a module where the students learn to use the commercial software Thermo-Calc to perform CALPHAD (CALculation of PHase Diagrams), and this acts as a mid-term project for the course over two weekly lab periods. Thermo-Calc includes the ability to calculate both equilibrium phase behavior and phase behavior that results from precipitation hardening (appropriate for an aluminum alloy); it also has models for predicting mechanical (*e.g.,* yield strength) and electrical (*e.g.,* conductivity) properties (among others) based on the calculated phase behavior.

The task the students are presented with has two parts:

1. Simulate the alloy they made in the physical lab including thermomechanical processing and compare the predictions of the yield strength and conductivity to what was found experimentally.
2. Modify their alloy (either in composition, processing, or both) to improve their "score" in the competition. However, there is no model for ductility in Thermo-Calc, so that element is neglected. An example student solution is shown in Figure 4.

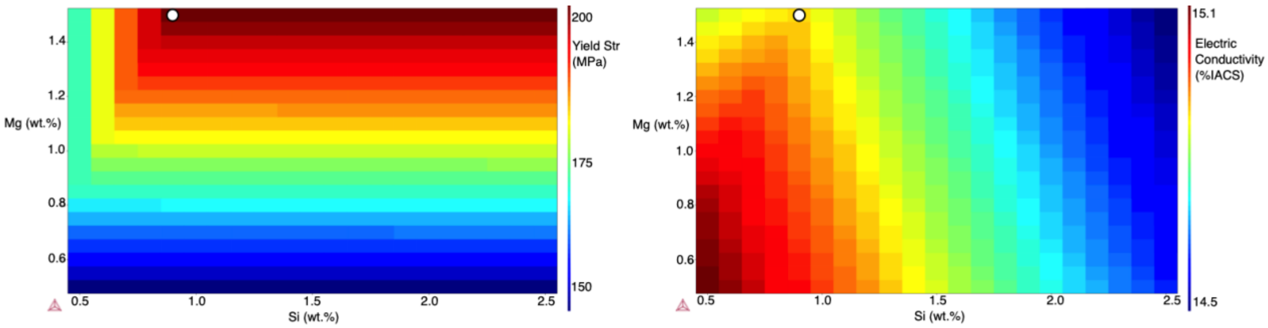


Figure 4. Example student solution to part 2 of the aluminum alloy computational lab. Here the student varied two compositional variables (wt.% Si and Mg) and calculated the predicted yield strength (left) and conductivity (right); the white circle indicates the proposed optimized composition.

As each student team has a different composition/process to simulate, this lab is considerably more open ended than previous ones, where the capabilities of CALPHAD software like Thermo-Calc were initially demonstrated through step-by-step tutorials and related problems. Here, the student must design and verify their own simulation procedure from scratch, based on what they learned in the previous labs, which is a much closer match to the reality of simulation work of a practicing engineer.

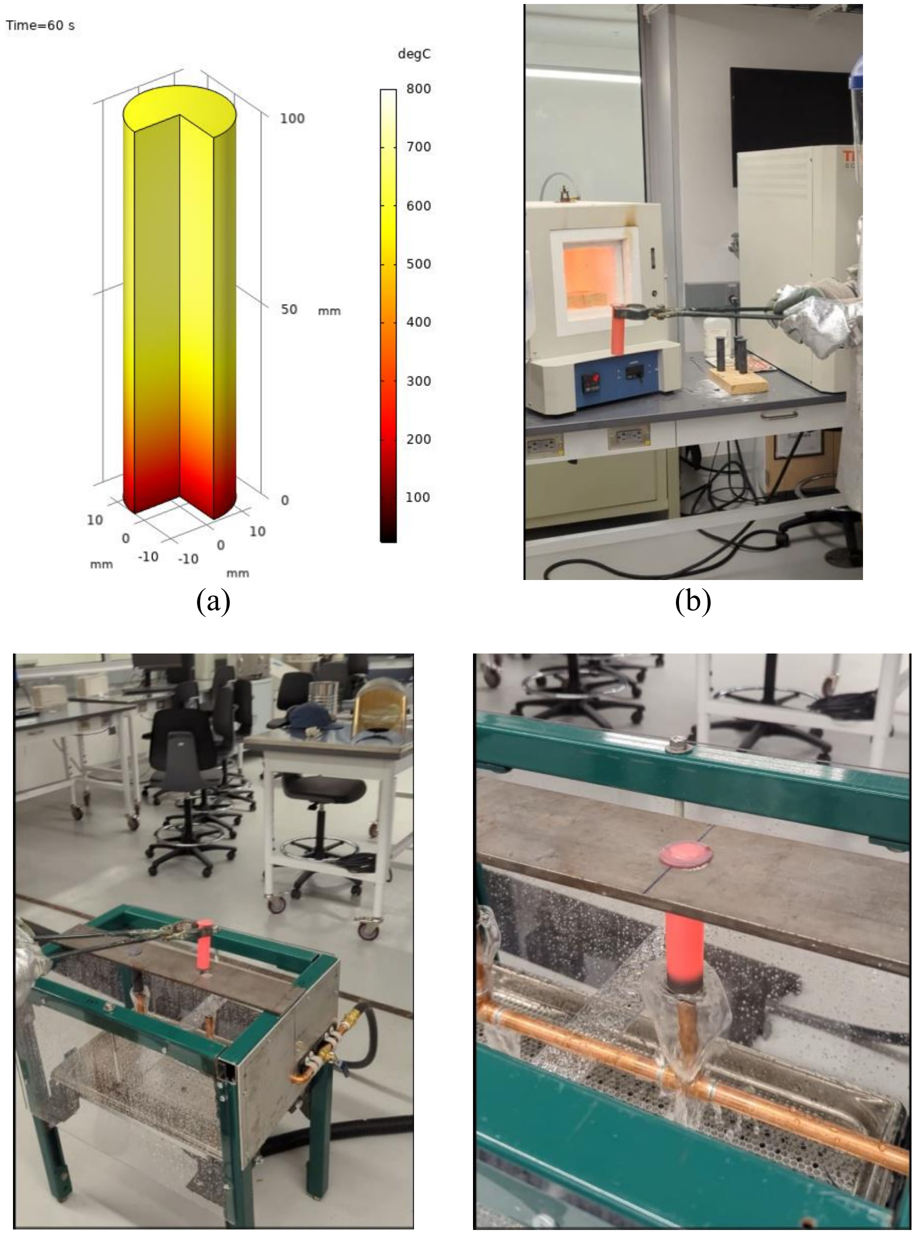
Module 2: Jominy test and steel bar identification

The second overlapping physical-simulation module is a simulation of a Jominy test followed by a physical lab where students are tasked to identify a steel alloy, in part by using a Jominy test. In this case, the ordering is reversed: the simulation lab is first (at the end of the junior year), and that is followed by the physical lab in the autumn semester of the senior year (in a popular but not required senior lab class).

The Jominy test computational lab occurs at the end of a series of labs covering finite element analysis (FEA) using COMSOL. Similar to above, this is a capstone project over the last two weeks of class after a sequence of labs where students are taught to use COMSOL via step-by-step tutorials and related challenge problems.

Here, the computational lab is somewhat less open-ended: students are all given the same steel composition to use (AISI 1045 steel), and the important physical parameters they need, but the detailed step-by-step directions for exactly how to perform the simulations required are not provided. As in the Thermo-Calc lab, the students must design the simulations themselves.

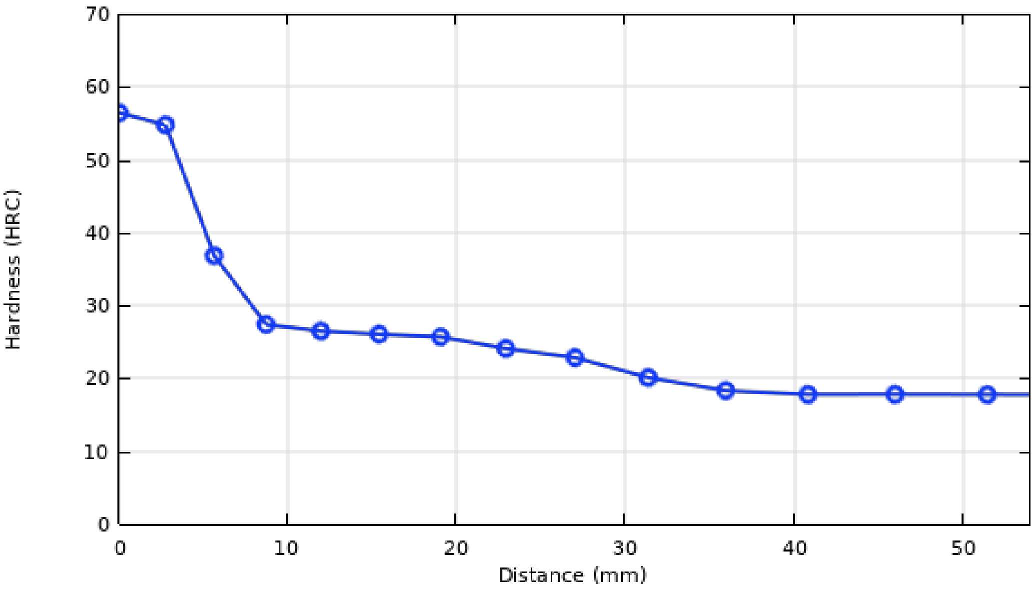
This lab brings together much of what was covered throughout the computational labs during the semester. Students must couple a heat-flow simulation, shown in Figure 5(a) along with related physical lab images discussed below, to a simulation of the phase transformations occurring in the steel as it cools. To do this, they first simulate the transformation dynamics of the 1045 steel in Thermo-Calc, creating a time-temperature transformation (TTT) data, which is used as an input to COMSOL simulations. The results can be used to predict the hardenability curve of the alloy as shown in Figure 6(a) together with analogous physical lab results.



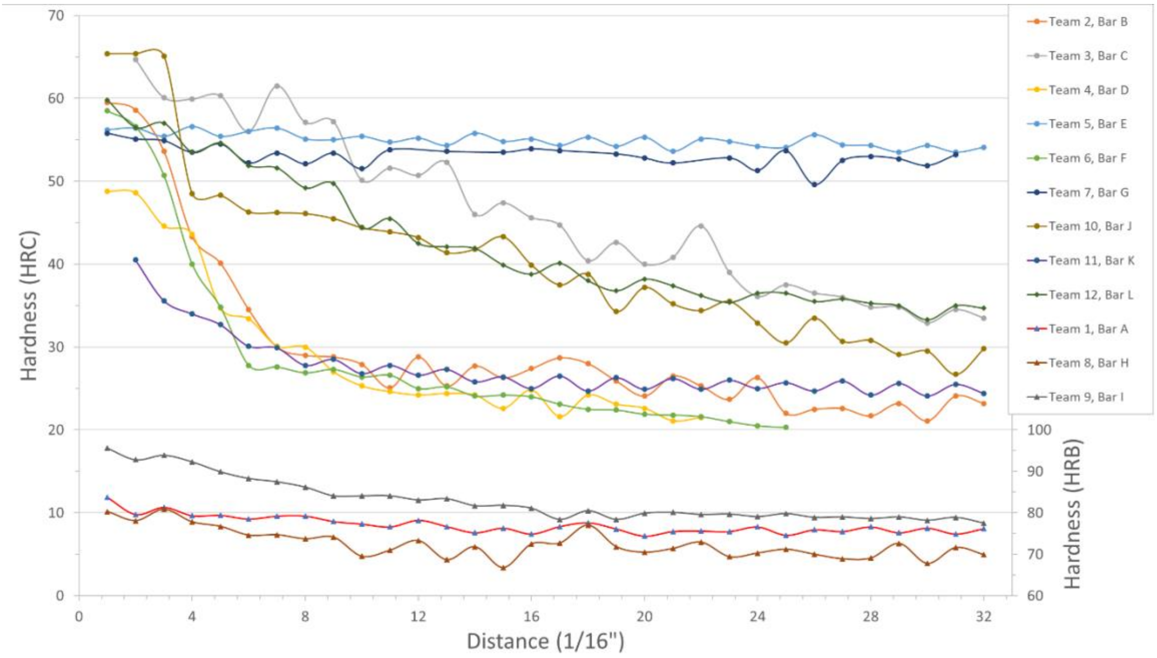
(a) (b)

(c) (d)

Figure 5. (a) 3D cutout showing temperature at the surface and interior of the simulated Jominy bar after cooling for one minute. Photographs of (b) a student removing a Jominy bar from the furnace, and (c) placing the Jominy bar in the quench stand, where (d) it begins to cool from the bottom.



(a)



(b)

Figure 6. Hardenability curves (a) from the simulated Jominy test of 1045 steel and (b) from all twelve student teams in the physical lab showing the hardness versus distance plots for the twelve unknown steel types after Jominy bars.

The physical lab course typically has twenty-four to twenty-seven students enrolled, and the first exercise in the lab is to determine the identity of an unknown steel Jominy bar using the Jominy end quench test, hardenability testing, and microstructural analysis at multiple locations along the bar. The twelve steel samples include three resulfurized steels of varying carbon content, two tool steels, two plain carbon steels, and the remaining steels are alloy steels of varying carbon and alloy content that provide sufficient differentiation in hardenability and microstructure that the student teams are able to successfully identify them. Photographs of the Jominy testing are shown in Figure 5(b-d) and an example of the hardenability curves generated by the students are shown in Figure 6(b).

The physical lab also has a weekly lecture component where the students and instructor talk about the results and hypotheses the students develop during the process. The final lab session for this involves the students presenting their evidence to the class and determining which alloy they think they have. The students must work together as a larger team to finalize the material identification and resolve any disputes on alloy identification using data. Only then are the alloys revealed; the students are generally successful in solving the puzzle.

Results and Discussion

Instructor observations

Discussions with students and their midterm feedback comments indicated that the aluminum alloy module was their favorite of the computational sequence, even though it was recognized as a difficult module. The related lab from the prior way the computational sequence was taught had not been as well liked.

We also found that, though it was not required, many students were able to apply the computational skills they had learned in the computational lab to model the system they worked on in the physical lab. We tried to encourage additional exploration in this area by offering significant bonus points if a team simulated all twelve compositions from the physical lab and included this in their report. However, as no teams have yet exercised this option, moving forward, the physical lab will be expanded to make this a required portion. Even without these additional requirements, based on informal discussions and observations, the students' simulations of some systems they had seen in the physical lab sequence seemed to give them a sense of efficacy in their ability to model systems and a sense that they had learned something applicable to their future careers.

Student evaluation data and comments

To quantitatively assess student experiences, we also analyzed student evaluation data. Specifically, average values by year of pertinent questions found on the standard Student Evaluation of Instruction forms are found in Figure 7, for both junior-level physical and computational lab evaluations. The physical and computational labs are taught at different times, but the first two data points on both curves are before the changes were implemented, while the remaining points are after.

Specifically, Figure 7 shows the students' average ratings on a 5-point Likert scale where students are asked to rate how much they agree with the statements (a) "This course was intellectually stimulating", (b) "The instructor encouraged students to think for themselves", and (c) "I learned a great deal from this instructor". For ModSim, the average value of the student ratings after the change is higher than before the change for all three questions (p=0.014, 0.027, and 0.033, respectively).

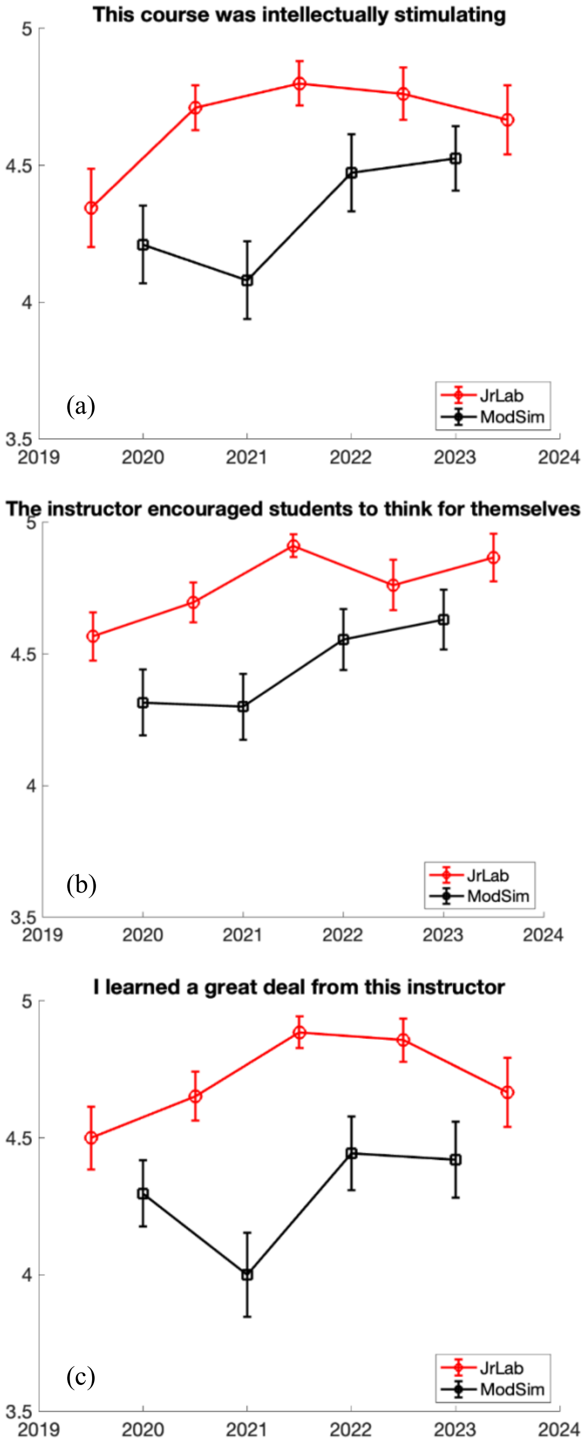


Figure 7. Results for three questions (a-c, questions labeled at top) on end of semester student evaluations for junior physical (red) and computational (black) labs. Points show the average agreement with the given statement on a 5-point Likert scale, and error bars show standard error.

Student comments also illuminate the reasons for their changes in perception. Most years, the majority of our undergraduates go directly to industry, not to graduate school, so that requires us to focus on industrially relevant uses of computational modeling to meet the needs of our students. Examples of comments that referred to utility of the material for their future careers (that included terms like "real life", "industry", or "useful") from each offering of ModSim are shown below (emphasis added):

Spring 2020:

- *Thermocalc was extremely useful and I learned a lot using it. Abaqus felt a lot less intuitive* and I felt like I'd never understand how to use it on my own without step–by–step instructions, but the final project really tied everything together. I enjoyed using MATLAB,

Thermocalc, and Abaqus with Excel and text files all to create a final product that had a direct application
- ***I wish that more of the course*** *was focused on coding (in free languages like Python, not MATLAB), and* ***contained more usable skills****.*
- *pretty unrewarding class with topics and programs that* ***will not be used in industry***
- *Things done in thermocalc and simulations done in abaqus were relevant to things I am learning in the major*.
- I really enjoyed the class and feel like I learned important applications.
- *labs were well written, understandable, and applicable to life after undergrad.*

Spring 2021:
- *I thought the labs in this course clarified concepts that we were taught in previous semesters but were confusing at the time so that has probably been the biggest takeaway for me.*
- *Overall the course was well organized and I learned useful skills*, but I do wish there was a broader scope of materials covered beyond metals

Spring 2022:
- *I liked that* ***every module was modeling a real life situation***. I liked the format of all the assignments. It was a lot but I don't know how else we really would have learned how to use the softwares. Almost everything we did I could see the purpose in.
- Overall I felt like this was a great way to apply prior mse knowledge.
- A lot of topics that I learned in thermodynamics and material processing are now more fully understood from the ThermoCalc and COMSOL labs.

Spring 2023:
- Great detail was added to ensure that the students understood what they were doing rather than just going through the motions.
- I loved MODSIM II and felt that ***I learned a lot of beneficial things for industry. I love how this course connected to other classes and information from the previous year*****.**

Before the changes, some students already felt the computational lab course was useful, while others did not see the utility or application to their careers of all or some of the content. After the changes, there were fewer comments about the lack of usefulness of the course, and a few specific comments praising the features we implemented in the new design. Note these were general end of course comments and students were not asked in this format specifically about the differences in design (which were imperceptible to most as they took the course in only one format without awareness of the past or future format). Overall, from these comments as well as informal discussions, we noticed that there was a more uniform perception amongst the students that the computational labs were relevant to their future careers or the rest of the content of the curriculum.

Conclusions

We were able to redesign our materials science and engineering lab sequence for close integration of multiple aspects of physical and computational labs. We chose several topics to introduce in both physical and computational labs, and then used a changing order of introduction of the concepts (physical led computational for one concept/system and then computational led physical for another concept/system). For example, students start by doing the physical alloy design lab the "hard way" without any assistance of relevant computational tools. They then experience how the simulation tool (that they have also already spent some time learning in a general context) can be applied to alloy design. They are able to understand and reflect upon how such tools would have helped them in the physical lab they completed the previous semester. In the next sequence, the order is reversed. Students are first given the computational tools, then are given a similar task in a physical lab. In this case, although it was not required, many students voluntarily used the simulation tools learned to answer the question in the physical lab. In addition to increasing engagement and helping to clarify the key concepts, this ordering helped to provide the bigger picture to the students of the different ways that modeling and simulation can be applied in the practice of materials design.

References

[1] S. A. Ambrose, M. W. Bridges, M. DiPietro, M. C. Lovett, and M. K. Norman, *How Learning Works: Seven Research-Based Principles for Smart Teaching*. John Wiley & Sons, 2010.

[2] J. M. Lang, *Small Teaching: Everyday Lessons from the Science of Learning*. John Wiley & Sons, 2021.

[3] A. Gillespie, "Materials by Design," *NIST*, May 2019, Accessed: Mar. 12, 2024. [Online]. Available: https://www.nist.gov/feature-stories/materials-design

[4] E. A. Lass, M. R. Stoudt, and C. E. Campbell, "Systems Design Approach to Low-Cost Coinage Materials," *Integrating Mater. Manuf. Innov.*, vol. 7, no. 2, pp. 52–69, Jun. 2018, doi: 10.1007/s40192-018-0110-2.

[5] R. Casukhela, S. Vijayan, J. R. Jinschek, and S. R. Niezgoda, "A Framework for the Optimal Selection of High-Throughput Data Collection Workflows by Autonomous Experimentation Systems," *Integrating Mater. Manuf. Innov.*, vol. 11, no. 4, pp. 557–567, Dec. 2022, doi: 10.1007/s40192-022-00280-5.

[6] J. Bishop, A. Clarke, and G. Wagner, "Integrated Computational and Experimental Methods for Additive Manufacturing," *JOM*, vol. 70, no. 8, pp. 1587–1588, Aug. 2018, doi: 10.1007/s11837-018-2966-1.

[7] R. L. Greenaway and K. E. Jelfs, "Integrating Computational and Experimental Workflows for Accelerated Organic Materials Discovery," *Adv. Mater.*, vol. 33, no. 11, p. 2004831, 2021, doi: 10.1002/adma.202004831.