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Mathematica Demonstration for Project Based Materials Science Course

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Mathematica Demonstration for Project Based Materials Science Course

Abstract:

This project-based materials science course integrates experimental design, computational modeling, and peer-reviewed publication using AI-powered tools like Mathematica. The course enhances traditional materials science instruction by emphasizing programming, modeling, and AI/machine learning applications. By combining hands-on experiments with computational modeling, students develop a deeper understanding of material behavior and gain critical engineering skills.

Students design and test experimental systems while creating interactive Mathematica simulations submitted for peer-reviewed publication. Through this process, they engage with AI and machine learning tools to analyze data and predict material behavior. Teams are intentionally diverse, working on experiments related to mechanical properties, phase transitions, and microstructural analysis. The integration of computational and experimental work fosters deeper learning, critical thinking, and problem-solving.

A key innovation is the use of AI-driven modeling tools alongside open educational resources (OER), eliminating financial barriers from costly textbooks and software. Students publish their simulations on the Mathematica Demonstrations platform, gaining professional feedback and experience with scholarly publication. The course structure promotes engagement, teamwork, and equity, ensuring all students—particularly those from underrepresented backgrounds—actively participate and build confidence in both experimental and computational research.

Preliminary results suggest improvements in student performance, engagement, and preparedness for careers involving AI and data-driven engineering. In particular the cohort showed a statistically significant improvement in overall course grade from a class average of 80% to 87% with a p-value of 0.005. Additionally, by creating diverse groups there was an improvement in the publication rate of Mathematica Demonstration projects and student surveys illustrated this approach made students more comfortable with AI tools. This model offers a scalable approach for integrating experimental work, AI modeling, and OER into engineering education, with future work focusing on long-term impacts on student retention and success, especially among underrepresented groups in STEM.

Introduction:

The integration of artificial intelligence (AI) is transforming engineering education by reshaping how students engage with complex scientific concepts. This paper introduces a novel project-based materials science course that integrates experimental design, computational modeling, and peer-reviewed publication opportunities. Leveraging AI-powered tools such as Mathematica, the course equips students with essential skills in programming, modeling, and the application of AI and machine learning—competencies increasingly critical in modern engineering practice [1, 2].

Central to the course is a project-based framework in which students design, execute, and analyze experimental systems while creating interactive Mathematica simulations. These simulations enable students to model material behavior, generate predictive insights, and visualize experimental outcomes. By utilizing industry-standard tools, students gain hands-on experience with technologies prevalent in both research and professional environments [3, 4].

To ensure a collaborative and inclusive learning experience, teams are purposefully composed with diverse backgrounds, addressing evidence that diversity enhances problem-solving and educational equity [5, 6]. Students explore fundamental materials science topics, including mechanical properties, phase transitions, and microstructural analysis. The course also emphasizes open educational resources (OER) to eliminate financial barriers, promoting equitable access to advanced learning tools without relying on costly textbooks or proprietary software [7, 8]. Additionally, students are encouraged to publish their findings and models on the Mathematica Demonstrations platform, providing early exposure to scholarly communication and valuable peer feedback.

Project-based learning (PBL) has been shown to improve engagement, retention, and the development of critical skills such as teamwork and communication [9, 10]. Incorporating AI and computational modeling into PBL enhances student understanding and prepares them for real-world challenges that demand both technical and analytical proficiencies [11, 12]. AI-integrated learning environments are particularly effective at fostering cognitive engagement and active learning, especially in courses with real-world applications [13, 14].

Moreover, diverse team structures are integral to the course, aligning with research that demonstrates their role in fostering inclusivity and reducing performance gaps for underrepresented students [15, 16]. Such approaches address systemic inequities in STEM education, building confidence and enhancing the participation of historically marginalized groups [17, 18]. Initial results indicate that this course structure significantly increases student engagement, academic performance, and equitable outcomes.

Overall, this course represents a transformative model for integrating experimental research, computational modeling, and OER in a project-based framework. By promoting engagement and equity, the approach addresses critical challenges in engineering education. Future efforts will focus on assessing long-term impacts on retention and career readiness, particularly for underrepresented groups in STEM [19, 20].

Course Structure:

A traditional lecture-based introductory Materials Science and Engineering course often incorporates laboratory activities such as XRD experimentation, tensile testing, and hardness testing. While these activities offer valuable hands-on experience, they are typically pre-designed, limiting student engagement in experimental design and data analysis. Even final projects, which may require students to design experiments, frequently lack a focus on computational modeling—a critical skill in modern engineering. It should also be noted that this is the introductory level Materials Science course with pre-requisites of Calculus III, Chemistry, and at least an introductory level of programming course (either Python or Matlab) and many other students are introduced to Mathematica in at least one other course.

To address these gaps, this course introduces an innovative framework that integrates an open educational resource (OER) textbook, YouTube-based Mathematica programming tutorials, and AI-driven computational tools. The OER textbook provides theoretical foundations while linking to curated video tutorials that teach advanced programming in Mathematica and the use of AI tools for engineering problem-solving. These resources empower students to build strong computational and analytical skills, seamlessly integrated with their experimental work.

Laboratory activities retain traditional materials testing components but emphasize student autonomy and computational analysis. Instead of performing pre-designed experiments, students use Mathematica's AI tools to analyze data and refine experimental designs. For instance, after tensile or hardness testing, students utilize AI-driven tools for curve fitting, trend analysis, and predictive modeling, bridging physical experimentation with computational analysis. This iterative process develops their programming skills, critical thinking, and ability to apply AI and machine learning tools effectively.

The course culminates in a final project where students design, model, and execute their experiments. Beyond conducting physical tests, they create computational models and simulations in Mathematica, which serve as the basis for a Mathematica Demonstration. This platform enables students to publish their work for review by Mathematica Demonstration reviewers and public dissemination, providing insights into the scientific communication and revision process and aligning their education with professional engineering practices.

The project based aspect of the course is conducted as seen in Figure 1.

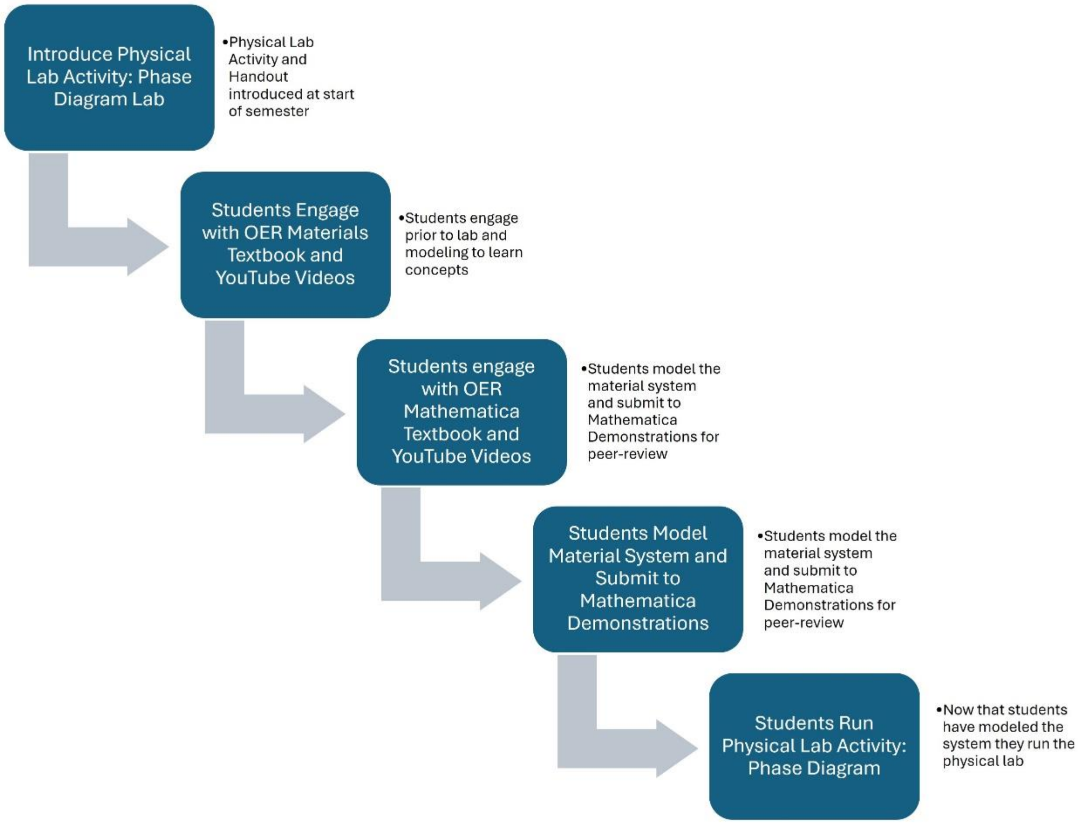

Figure 1: Flow schematic of the Mathematica demonstration project. Students are introduced at the beginning of the semester to the physical lab that they can conduct and all the materials for the physical lab and required background information are provided at the start of the semester. Students then engage with OER textbook and YouTube videos first related to the concepts of the lab and then to Mathematica and AI tools. Then students will model the physical lab activity and develop a Mathematica Demonstration that will be submitted for peer-review by Mathematica Demonstration reviewers for publications. The students then run the physical lab activity.

The students are introduced to several physical Materials Science and Engineering lab activities at the beginning of the semester and provided with lab handouts and background information. The students then select one of the lab activities and then engage with OER content related to the physical lab activity. This involves both an OER textbook as well as recorded YouTube videos. Once this is done the students can move to modules of the OER textbook and YouTube videos that prepare them for the Mathematica aspect of the project as well as the AI related tools that Mathematica offers. With this preparation the students will then begin to create their Mathematica Demonstration which models aspects of the physical labs and the students will then submit the Mathematica Demonstration for peer review from Mathematica Demonstration reviewers for publication. Once the Mathematica Demonstration is submitted the students can then move to completing the physical lab with the idea that these previous scaffolded steps enhances not only the understanding of the physical lab but many Materials Science and Engineering concepts in general.

To determine the efficacy of this approach two cohorts of students were compared. The first cohort termed Pre-AI Project consisted of a sample size of 25 students and the second cohort is the Post-AI Project with a sample size of 14. The final grade distribution of the two cohorts can be seen in Figure 2 where the Pre-AI cohort achieve a mean grade of 80% and the Post-AI cohort achieved a mean of 87%.

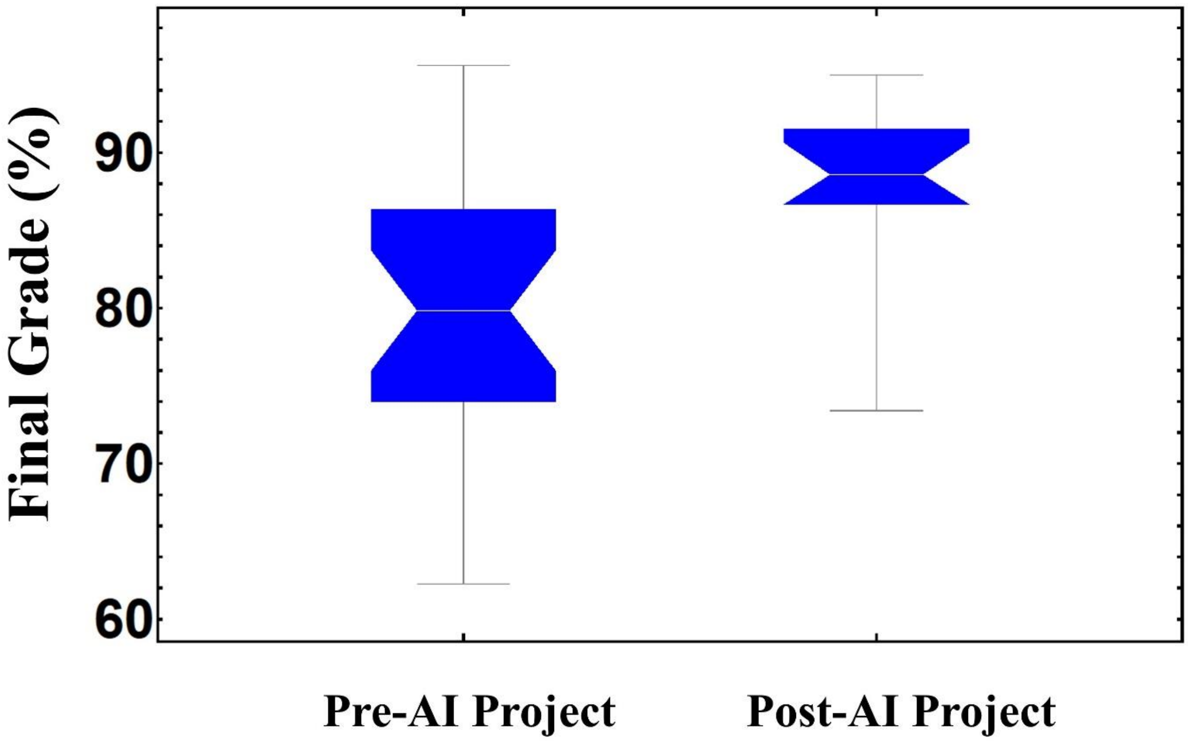

Figure 2: Final grade distribution of pre and post AI project student cohorts. The 95% confidence interval can be visualized between the notches. A t-test comparison was performed on the two cohorts which yielded a p-value of 0.005 which indicates a statistically significant difference between the cohorts. Therefore, a statistically significant increase in the grades was observed for the two cohorts and the primary difference in the courses is the implementation of a Mathematica based modeling final project utilizing AI tools.

The analysis of student performance reveals a significant improvement in final grades for the cohort of students who completed the Mathematica modeling project, which heavily utilized AI tools, compared to the cohort engaged in a traditional experimental approach for their final project. This shift toward higher grades is particularly noteworthy given that the syllabus, grading rubrics, and assignment weightings remained consistent across both cohorts. The only substantial difference lay in the integration of Mathematica modeling, AI tools, and the use of open educational resources (OER), including an interactive textbook and linked YouTube tutorials, in the redesigned course.

The improved outcomes suggest that the Mathematica modeling project provided students with a unique advantage in understanding and applying materials science concepts. By engaging with computational modeling throughout the semester, students had the opportunity to repeatedly practice and refine their problem-solving skills. This iterative learning process appears to have translated into better performance on problem sets and exams, which were designed to assess a comprehensive understanding of course material.

In addition to the benefits of modeling and AI tools, the OER textbook and YouTube video resources played a crucial role in supporting student learning. The OER textbook provided accessible explanations and integrated problem-solving exercises that aligned closely with the course objectives. These resources ensured that students could revisit concepts and practice independently outside of class. Moreover, the linked YouTube tutorials complemented the textbook by offering visual and step-by-step demonstrations of Mathematica programming and AI tool usage. Feedback from students indicated that these resources were particularly helpful in demystifying complex computational tasks and making advanced modeling techniques more approachable.

When considering the final grades as a composite indicator of overall student performance, the cohort utilizing the Mathematica modeling project consistently outperformed the traditional cohort. This finding highlights the synergy between the OER resources and the hands-on, AI-driven modeling project. The accessibility of the textbook and videos allowed students to build foundational skills at their own pace, while the modeling project encouraged the application of these skills in a creative and exploratory manner.

These results underscore the importance of integrating high-quality OER resources and computational tools into engineering education. The alignment of these resources with active learning projects not only improves academic outcomes but also equips students with practical skills in computational modeling and AI that are increasingly valuable in professional and research settings. Future iterations of the course will continue to refine the integration of these components to maximize student engagement and performance.

We conducted a t-test to compare the final grades of the cohort that completed the Mathematica modeling project, which incorporated AI tools, with those of the cohort that completed a traditional experimental final project. The results yielded a p-value of 0.005, indicating a statistically significant difference between the two groups at the 95% confidence level. This finding confirms that the cohort utilizing AI-driven modeling achieved statistically higher grades compared to their counterparts in the traditional course design.

The statistically significant improvement suggests that the integration of AI tools and computational modeling in the course had a meaningful impact on student performance. These results are particularly compelling as they demonstrate that the redesigned course not only enhances student engagement and learning outcomes but also leads to measurable improvements in academic achievement. The structured approach to introducing Mathematica modeling and the iterative application of AI tools likely contributed to this success by fostering deeper understanding and application of materials science principles.

The relationship between team diversity and the success of student projects was analyzed over two consecutive years of the implementation of the Mathematica AI project, with notable differences observed in both the diversity of student groups and their publication rates. In Year 1 (Y1) of implementation of the Mathematica projects students were encouraged to form their own groups and this resulted in project groups that were not diverse. To quantify the diversity of the groups we calculate the Simpson Diversity Index (SDI) [21] which is defined as:

$$Simpson\ Diversity\ Index = \frac{\sum_{d=1}^{D} \frac{Unique\ Categories\ in\ Dimension_d}{Total\ Categories\ in\ Dimension_d}}{D}$$

Where D is the total number of dimensions. The dimensions, D, that we considered gender, ethnicity, and major. The number of possible categories in gender was male, female, and non-binary, for ethnicity the categories were white, black, hispanic, asian, and indigenous, and for major the majors the categories were mechanical, electrical, civil, computer, and management. A value of 0 indicates no diversity and a value of 1 would indicate very diverse. The Simpson Diversity Index is a useful indicator due to the simplicity of the output, the fact that it allows for comparisons to different populations or in this instance student groups, and accounts for number of categories and their relative representation [22-23]. However, like any metric and particularly diversity metrics it is sensitive to sample sizes, treats all categories as equally distinct, and does not account for cultural, historical, or systemic differences between categories. In the first year, the average Simpson Diversity Index for all the groups calculated as 0.34, as seen in Table 1, reflecting limited representation across diversity dimensions such as gender, ethnicity, academic backgrounds, and technical skills. For that Year 1 cohort, a sample size of 14 students, the less than half of the projects were able to be published.

Table 1: Impact of Diversity of Project Groups and Percent of Projects Published

	Simpson Diversity Index	Percent of Projects Published
Year 1	0.34	42%
Year 2	0.88	67%

The low diversity within teams appeared to hinder collaboration and innovation, reducing the likelihood of successful project completion at a publishable level.

In the second year, with a sample size of 26, deliberate efforts to create more diverse teams resulted in a significant increase in the average Simpson Diversity Index to 0.88. These efforts included a structured approach to team formation, ensuring representation across multiple diversity metrics. Alongside this improvement in diversity, the percentage of student groups successfully publishing their Mathematica Demonstrations rose to over 67%. Feedback from Mathematica Demonstration reviewers, experts in not only the topic but the Mathematica programming language and AI tools, noted that the demonstrations produced by these more diverse teams exhibited greater originality and technical depth, suggesting that increased diversity fostered a broader range of ideas and problem-solving strategies.

The data indicates a strong correlation between higher diversity scores and improved publication success. Teams with more diverse compositions appeared to leverage their varied perspectives to address complex modeling challenges more effectively. This finding is consistent with prior research, which highlights the positive impact of diverse teams on creativity and performance in STEM education and professional contexts.

While the improvements in both diversity and publication rates are encouraging, the results also suggest areas for further exploration. For example, some teams with high diversity scores still faced challenges related to communication or integrating differing levels of technical expertise. Addressing these issues through targeted training and team-building activities could further enhance the effectiveness of diverse teams. It is also important to consider the relatively small sample size on the effect of percent of projects that were published. However, this evidence seems to suggest that the diversity of the groups had a significant impact considering both Year 1 and Year 2 samples were relatively small.

These findings underscore the importance of fostering diversity within team-based learning environments. Beyond promoting equity, diverse teams are better positioned to achieve professional-level outcomes, as evidenced by the increase in successful Mathematica Demonstration publications. Future efforts will focus on sustaining and expanding diversity initiatives while exploring additional metrics to assess the long-term impact of these changes on student learning and career readiness.

Additionally, this cohort was given a survey of the following questions with a scale of 1-5

1. Q1: How confident are you in your ability to use Mathematica's AI tools to model material behavior?
2. Q2: How well do you understand the role of AI tools in analyzing and modeling material properties?
3. Q3: How would you rate the ease of learning and applying Mathematica’s AI-driven modeling tools in your coursework?
4. Q4: How comfortable are you using AI tools in Mathematica to troubleshoot and refine your material behavior models?
5. Q5: To what extent do you feel that using AI tools in Mathematica has improved your understanding of material behavior and modeling concepts?

The average results of the student survey can be seen in Table 2.

Table 2: Student Survey Question Results

	Q1	Q2	Q3	Q4	Q5
Year 2	4.1	4.3	4.6	4.0	4.5

Student feedback on the use of Mathematica's AI tools and their impact on learning outcomes was overwhelmingly positive, as reflected in survey responses. Across all questions, the average student rating exceeded 4 on a 5-point scale, indicating a strong overall satisfaction with the course's integration of these tools. Two areas stood out particularly in the feedback: the ease of using Mathematica's AI features and the tools' impact on students' understanding of material behavior, which received average scores of 4.6 and 4.5, respectively.

Students frequently highlighted the intuitive interface and user-friendly design of Mathematica's AI tools, which allowed them to engage deeply with complex computational modeling tasks without feeling overwhelmed. Comments from students suggested that the tools' ease of use enabled them to focus more on conceptual understanding and problem-solving rather than struggling with technical hurdles. This accessibility likely contributed to their enthusiasm and willingness to explore advanced modeling techniques.

The impact on their understanding of material behavior was another notable highlight. Many students reported that the AI-driven simulations helped them visualize and predict material properties in a way that traditional methods could not achieve. By directly linking theoretical concepts to dynamic, real-world applications through AI modeling, students gained a more profound and practical grasp of materials science principles.

These high ratings and positive feedback underscore the value of integrating user-friendly computational tools like Mathematica into engineering education. The combination of ease of use and meaningful learning outcomes demonstrates the potential for such tools to enhance both student engagement and academic success in STEM fields.

Conclusion

This study demonstrates the effectiveness of integrating AI-driven computational tools and project-based learning into materials science education. By leveraging Mathematica's advanced modeling capabilities and fostering collaborative, diverse team environments, the course not only enhances technical proficiency but also prepares students for the increasingly AI-driven landscape of engineering. The incorporation of open educational resources further supports inclusivity, enabling students from all backgrounds to access high-quality learning materials and tools.

The results indicate significant improvements in students' understanding of core materials science concepts, their proficiency in computational modeling, and their confidence in using AI tools. The successful publication of Mathematica demonstrations and positive peer-reviewed feedback highlight the professional relevance of this approach, bridging the gap between academic learning and industry practices. Furthermore, the emphasis on diverse team formations and equity-focused pedagogy aligns with the broader goals of fostering inclusivity and reducing performance gaps in engineering education.

Future work will focus on scaling this model to other courses within the engineering curriculum and investigating long-term impacts on student retention and career pathways. By continuing to innovate with AI tools, computational modeling, and project-based frameworks, this pedagogical approach has the potential to redefine engineering education and empower students to excel in an increasingly complex and technology-driven world.

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