A critical review of approaches to teaching artificial intelligence in undergraduate materials engineering

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Abstract

Software tools utilizing artificial intelligence (AI) through machine learning (ML) are becoming increasingly vital in Materials Science and Engineering (MS&E), particularly materials design and development. However, these tools are not yet widely integrated into undergraduate materials engineering curricula. This paper presents a critical review of existing approaches to introducing ML concepts to undergraduate students in materials engineering. Although Python-based frameworks such as Jupyter Notebooks, Scikit-learn, and Google Colab have been developed, their adoption remains relatively limited. Programming complexity and the unclear role of materials engineers in these exercises are likely reasons for this limited uptake. We propose greater emphasis on materials engineering domain knowledge and structured material data to enhance the application of ML in solving materials engineering problems, as required in industry. Additionally, there is a shortage of readily accessible, suitable datasets and tools for teaching ML to undergraduate MS&E students with minimal computer science (coding) background. Hence, more openly available real-world datasets for a range of materials engineering problems that could be used across various years of study would be beneficial in increasing adoption. The introduction of user-friendly AI software tools which do not require coding, would likely facilitate their integration into the classroom. A comparison can be drawn to the increased prevalence of finite element modeling software in engineering education over recent decades. We aim to engage the community in dialogue to foster ideas and encourage the adoption of AI tools in materials design and development within modern materials engineering curricula.

Introduction

Artificial intelligence (AI) is a broad term that refers to computers performing tasks that require cognitive functions. AI has existed since the 1950s, though it has undergone a boom in engineering applications, such as Materials Science and Engineering (MS&E), as recent significant improvements to computational speeds have made it more powerful [1, 2]. Machine learning (ML) generally refers to algorithms (e.g., linear regression, non-linear regression, random forest) that turn input data into output data, and in doing so, achieve AI goals. ML algorithms typically require tens to hundreds of data points. Deep learning can be considered a part of ML, and both fit in the broader term of AI. Deep learning algorithms (e.g., neural networks) typically work on thousands of data points and are, as such, used in 'big data' engineering applications.

AI-powered technologies are becoming more prevalent in daily life and the workforce, making it crucial to understand and adapt to using new large language model (LLM) tools, such as Chat Generative Pre-Trained Transformer (ChatGPT) in the classroom. Evidence suggests student use of ChatGPT can enhance academic performance, boost affective-motivational states, improve higher-order thinking propensities and reduce mental effort [3]. This evolving AI landscape encourages those in higher education to reassess goals, teaching methods, and assessment strategies. The impact of AI tools is far-reaching and has already caused educators to rethink Bloom's taxonomy (Table 1) to distinguish between distinctive human skills in the learning process and the role of generative AI (Gen AI) tools such as ChatGPT in the learning process.

Table 1: Bloom's Taxonomy comparison of human skills in learning and generative AI skills in learning. Adapted from [4] and the Oregon State University [5].

	Human Skills	**How GenAI Can Supplement Learning**
Create	Engage in both creative and cognitive processes that leverage human lived experiences, social-emotional interactions, intuition, reflection, and judgment to formulate original solutions.	Support brainstorming processes; suggest a range of alternatives, enumerate potential drawbacks and advantages; describe successful real-world cases; create a tangible deliverable based on human inputs.
Evaluate	Engage in metacognitive reflection; holistically appraise ethical consequences of other courses of action; identify significance or situate within a full historical disciplinary context.	Identify pros and cons of various courses of action; develop and check against evaluation rubrics.
Analyze	Critically think and reason within the cognitive and affective domains; justify analysis in depth and with clarity.	Compare and contrast data, infer trends and themes in a narrowly defined context; compute; predict; interpret and relate to real-world problems, decisions and choices.
Apply	Operate, implement, conduct, execute, experiment, and test in the real-world; apply human creativity and imagination to idea and solution development.	Make use of a process, model, or method to solve a quantitative or qualitative inquiry; assist students in determining where they went wrong while solving a problem.
Understand	Contextualize answers with emotional, moral or ethical considerations; select relevant information; explain significance.	Accurately describe a concept in different words; recognize a related example; translate to another language.
Remember	Recall information in situations where technology is not readily accessible.	Retrieve factual information; list possible answers; define a term; construct a basic chronology or timeline.

In addition to generative AI tools such as ChatGPT, undergraduate engineering students can now expect to encounter discipline-specific AI and ML tools in their studies and careers. In the context of MS&E, the use of domain-specific AI and ML tools has led to remarkable advancements in process-structure-property predictions, material design, and material discovery [2, 6]. ML models frequently take input (or training data) and can make predictions and find correlations within the data (Figure 1). These predictions and correlations can be used to optimize new materials for a specific application. In MS&E, AI and ML are often leveraged in a sequential learning loop that aims to lower the cost of material development and accelerate the time to market of new materials or products (Figure 2), whilst improving the performance of materials for given engineering applications, often making it more sustainable. Hence, current undergraduate students studying MS&E should now expect to encounter these tools in their careers [7].

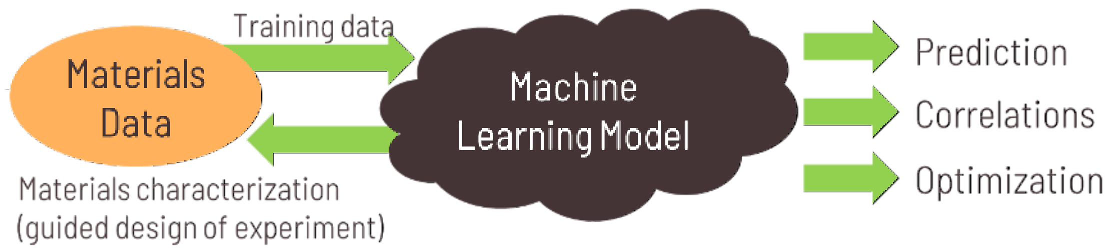

Figure 1: ML models help to predict properties, correlate properties and optimize properties in the materials design.

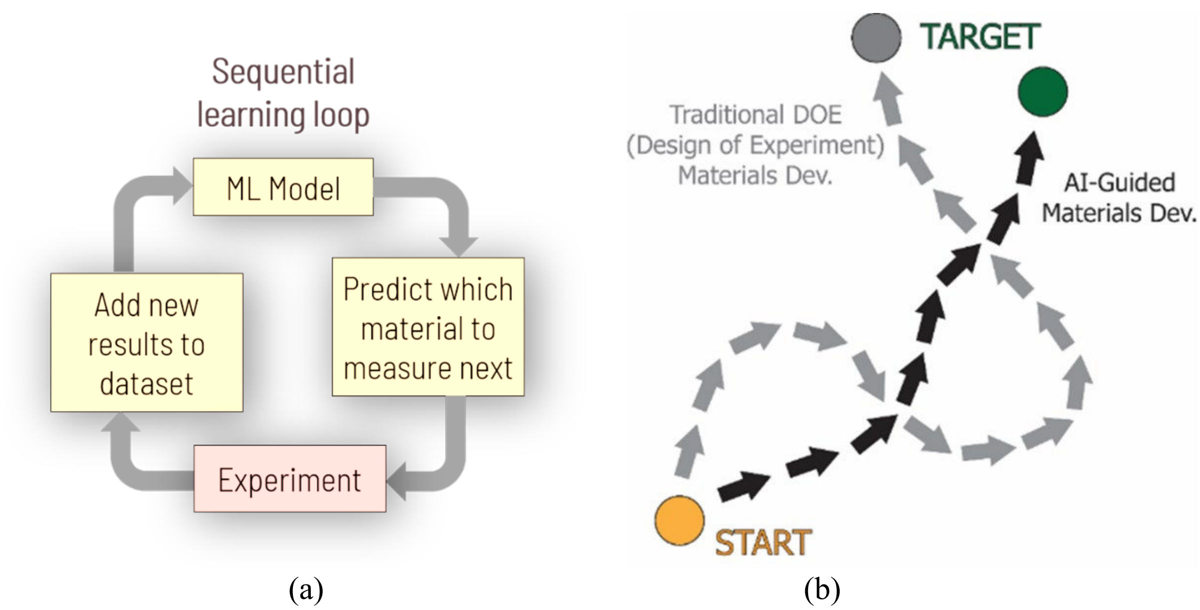

Figure 2: (a) Overview of sequential learning in materials design, and (b) AI-guided materials discovery saving time compared with the traditional design of experiment approach.

A wide range of MS&E and related industries are now applying AI and ML tools in the design and discovery of new materials and chemicals. For example, AI and ML tools have been used in materials development in applications such as batteries [8], ceramics [9], metal alloys [10-12], packaging [13], consumer electronics [14], adhesives [15], coatings [16], building materials [17], automotive [18], and aerospace [19]. The AI and ML software tools being used in these industries are often implemented by individuals with varying levels of programming skills [20, 21]. This highlights the growing recognition that AI and ML tools should be usable by those without deep expertise in the advanced mathematics and computer science required to develop these tools. MS&E graduates, for example, might encounter these technologies in their careers, much like they would encounter tools based on physics simulations, such as finite element modeling software. Therefore, there is a growing need to meaningfully incorporate AI and ML topics and tools into undergraduate MS&E curricula.

Similarly, AI and ML tools have been adopted in many areas where programming skills are typically not expected, such as in medicine [22] and business [23]. Moreover, initiatives like Artificial Intelligence for K-12 (AI4K12) aim to build AI literacy before students reach higher education [24].

In this work, we investigate the current approaches being used to teach AI and ML concepts to MS&E undergraduate students. We separate the variety of different approaches into two broad categories (Figure 3):

1. A computer-science-driven approach that places an emphasis on programming competency to develop and apply ML tools to materials engineering problems.
2. An engineering design-driven approach that places an emphasis primarily on the application of ML tools to an engineering problem.

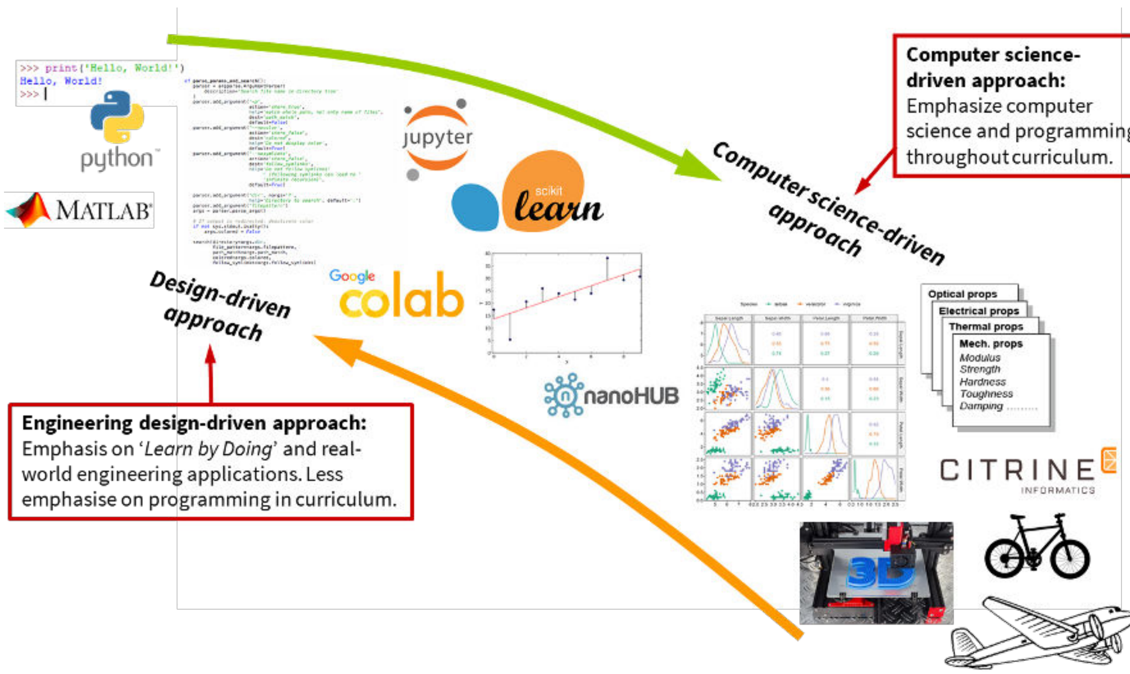

Figure 3: Overview of the two broad approaches to AI and ML teaching in the context of MS&E. Adapted from [25].

In subsequent sections, we outline the two broad approaches and discuss their advantages and disadvantages. We also assess the broad challenges associated with introducing AI and ML to undergraduate MS&E students, regardless of approach.

Computer-Science (Programming)-Driven Approaches

Computer-science-driven approaches to teaching AI/ML in engineering generally involve building a strong foundation in a programming language so that ML algorithms can be later implemented in solving a materials problem. This approach relies on establishing a base literacy in computer programming and data science topics. Python has been a popular choice as a programming language for this type of activity given its widespread use in science and engineering, as well as the numerous beginner-level open-source resources for learning the language [26].

The Python language also enables the use of Scikit-learn [27], also known as sklearn, an open-source ML and data modeling library. Moreover, Python codes can now be implemented inside of Jupyter notebooks. This approach allows for Python codes to be written, viewed and executed through a cloud-based digital notebook which can be supplemented with explanatory text and images to enhance students' understanding of code (Figure 4). Jupyter notebooks can often be run without edits to the code, however, they typically include designated points where changes can be made to investigate different aspects of ML models that could be changed. These digital notebooks have been popular for introducing learners to a variety of introductory computer science topics across a range of MS&E topics and case studies (published examples summarized in Table 2). They have also been used in the classroom in adjacent fields such as chemical engineering [28]. There are numerous published exercises designed to introduce students to the main steps in the data science and ML workflows, i.e. starting with initial data cleaning, data organization, and data querying and moving to analyzing material property predictions via various models (regression, random forest and neural networks), often including effective visualizations of ML model predictions (Figure 5) that could subsequently be used in materials design. Many of these Jupyter Notebooks are published on open-source repositories such as nanoHUB and GitHub. Moreover, students can go through the training Jupyter Notebook modules on a Google Collaboratory (Colab) cloud-based environment from their laptop or personal computer. The main advantage of this approach is that students can run modern AI techniques interactively, whilst avoiding the need to separately configure software packages and dependencies locally on their computers, since they can run notebooks shared by the instructor. This accessibility makes the approach particularly appropriate for the classroom [29].

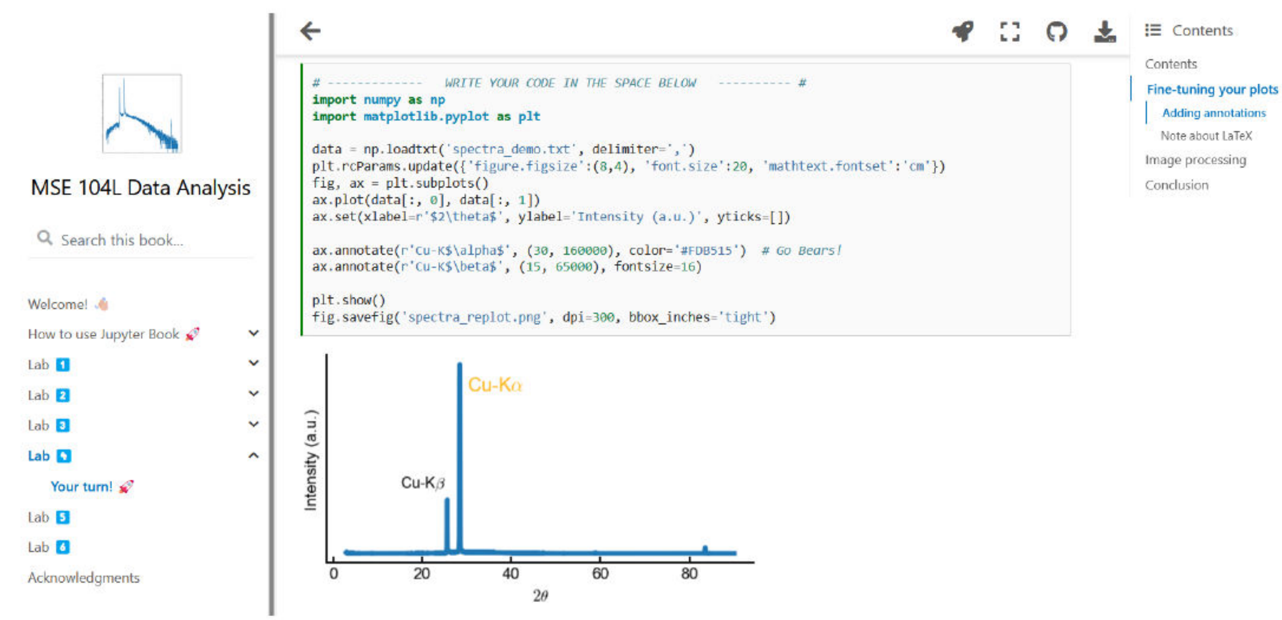

Figure 4: Screenshot of a page of the learning module in a Jupyter Notebook showing interactive links, editable python code and data visualization [30].

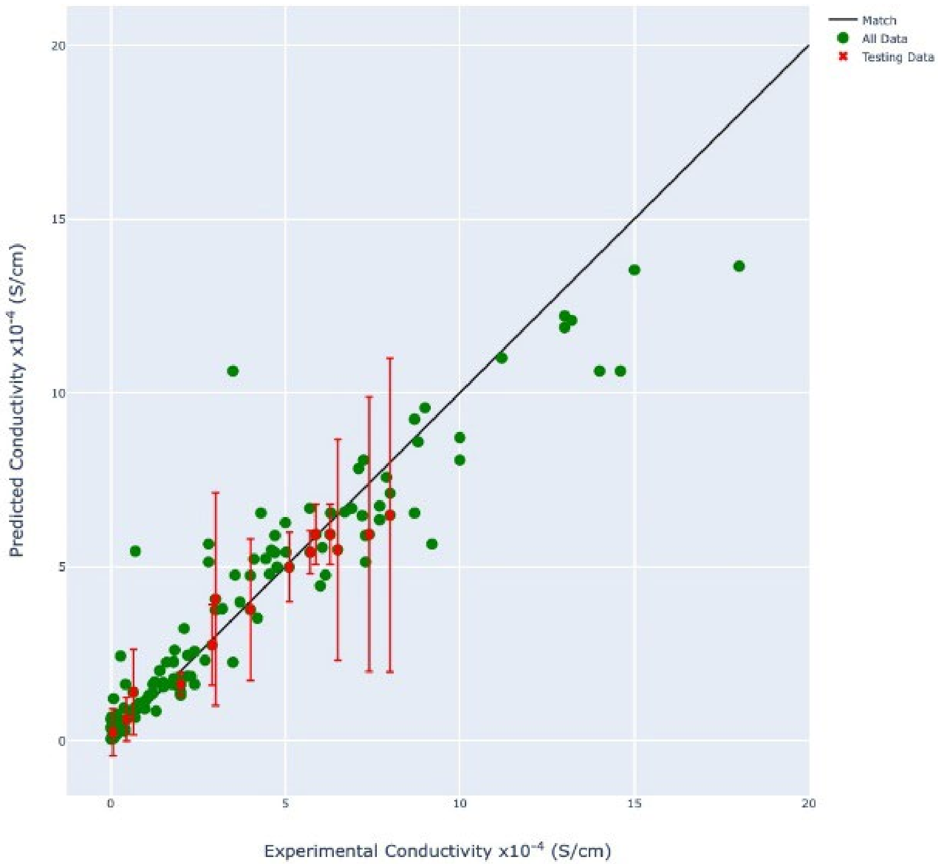

Figure 5: Visualization of material property predictions from an ML model [31].

Table 2: Published examples of computer-science-driven approaches to teaching AI/ML topics.

Computer Science and/or AI/ML Topics	Programming Language, Library, and Environment	MS&E Topic	Ref. (s)
Plotting, curve fitting, functions and correlations, annotations and clustering.	Python, Jupyter Notebooks.	Materials characterization laboratory (X-ray emission, X-ray diffraction, X-ray spectroscopy, scanning electron microscopy, transmission microscopy).	[30]
Data management, introduction to ML.	Python, Jupyter Notebooks.	Data-driven design of dielectric materials.	[32]
Introduction to ML models, ML frameworks, ensemble learning techniques in ML, performance metrics in ML.	Python, Scikit-learn.	Prediction of bulk modulus a perovskite material.	[33]

Data cleaning and organization, data splitting, classic ML models, neural network ML modeling, visualizing ML results.	Python, scikit-learn, PyTorch, Jupyter Notebooks.	Prediction of heat capacity for solid inorganic compounds.	[34]
Data inspection (importing, cleaning and evaluating data), feature generation, feature engineering, setup for ML model evaluation, fitting and evaluating default ML model, hyper parameter optimization, ML predictions and visualizing ML results.	Python, Scikit-learn.	Predicting materials for single-junction solar cells. Predicting wide band gap semi-conductors.	[31], [35]
Querying a dataset, obtaining features/descriptors from Matminer, processing and organizing data, generating ML models, active learning.	Python, Jupyter Notebooks.	Workflow to optimize the number of experimental samples required to reach the maximum bulk modulus from composition.	[35]
Querying a dataset, obtaining features/descriptors from Matminer processing and organizing data, regression models (neural network, random forest), active learning.	Python, TensorFlow, Jupyter Notebooks.	Predicting ionic conductivity of LLZO type garnets using compositional descriptors.	[35], [36]
Querying databases, organizing and plotting data, ML regression models (linear, neural network, neural network classification).	Python, TensorFlow, Jupyter Notebooks.	Predicting material properties like Young's modulus from a set of descriptors. Predicting the crystal structures of elemental metals through a classification exercise.	[35], [37], [38]
Image analysis, ML models (neural networks and convolutional neural networks).	Python, TensorFlow, GIMP (image editor)	Analyzing x-ray tomographic data	[39]
Quantum computing, high performance computing and ML models (neural networks).	Python, Jupyter Notebooks.	Quantum molecular dynamics (QMD), reactive molecular dynamics (RMD) in materials design.	[40]

Another unpublished example of AI/ML integration into undergraduate curriculum is the Computer Vision (CV) lab offered as part of *MASC 110L: Materials Science* at University of Southern California. The CV lab introduces students to a practical use case of ML techniques in MS&E. Using a brass surface image obtained in another lab module, students are exposed to an end-to-end ML workflow designed to achieve automated grain segmentation. The lab consists of three primary steps: 1. selecting a region of interest and removing unnecessary color channels, 2. annotating the image to enable the ML model to learn the grain location and shape as well as differentiate grain boundaries from twin boundaries (Figure 6), and 3. fine-tune a pre-trained CV model (Mask R-CNN) using the image data previously prepared. The lab is designed for students without prior experience of ML nor programming; thus, all hands-on activities maximally utilize graphical user interfaces, online web-based apps and Jupyter Notebooks on Google Colab. In their lab reports, students evaluate the accuracy of model predictions (Figure 7) and assess the effects of several hyperparameters such as model sizes and training epochs to demonstrate their understanding of the subject and procedures they went through in the lab. To date, over 250 students have completed the CV lab. Students' responses are generally positive, acknowledging the importance of integrating modern ML/AI technologies into MS&E education. Having previously performed manual grain size analysis students are primed to appreciate the utility of computational approaches to handle large data sets in a more efficient way.

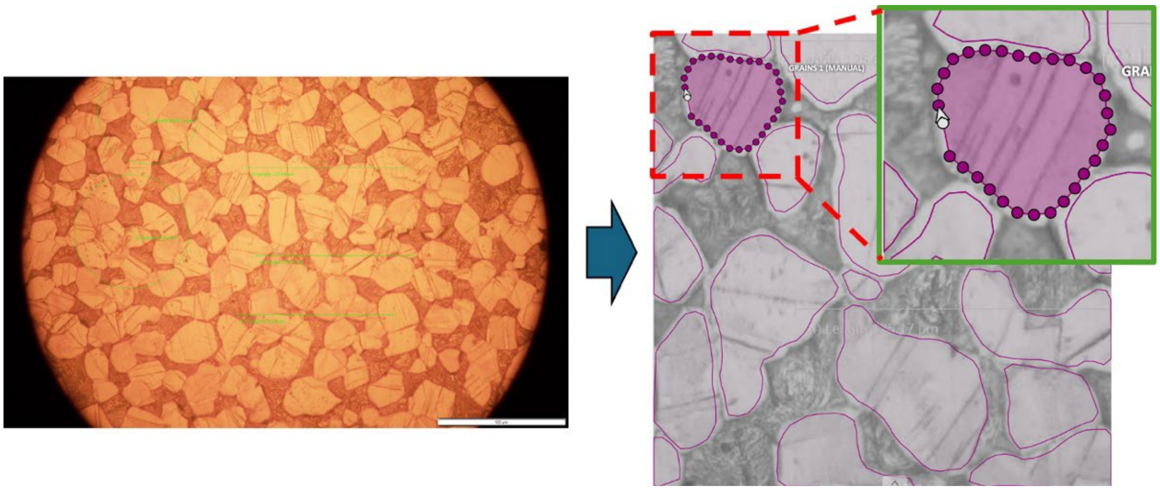

Figure 6: (left): Screenshot of brass surface image obtained in metal microstructure lab. (right): An example of image annotation process. Purple lines are drawn along grain boundaries to capture the shape and location of grains.

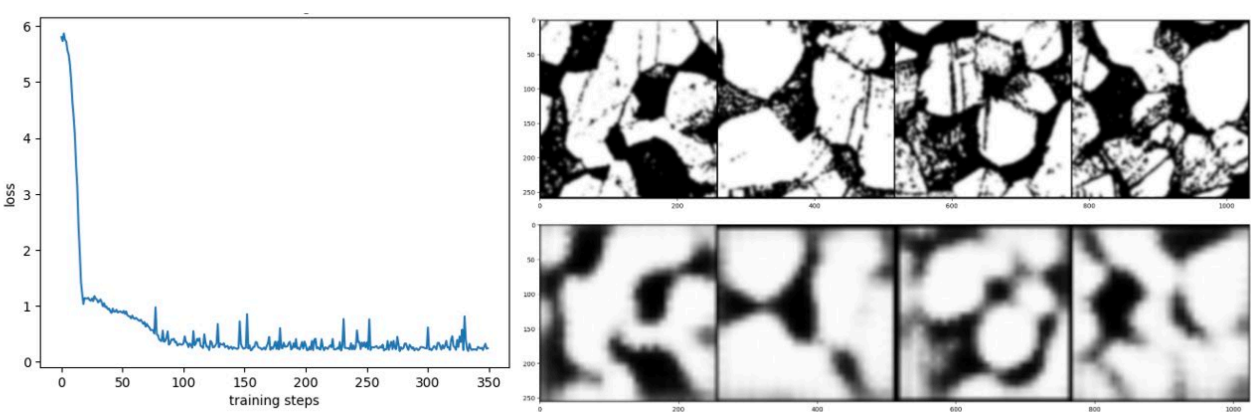

Figure 7: (left) Training performance: the loss vs. number of epochs. (right): test dataset and corresponding model predictions highlighting metal grains in white and other regions in black.

In addition to the published open-source learning exercises summarized in Table 2, educators also have access to an increasing number of AI/ML tools and datasets that have been published alongside materials design and development research studies (e.g., [11, 41-46]). While these resources are frequently beyond the level of an undergraduate classroom, the tools have enabled undergraduate capstone engineering students to gain in-depth experience with AI/ML software tools and by implementing them in novel ways, leading to innovative applied research and valuable research experiences for undergraduates. A recent example of this is undergraduate research published by Beaver et al. [47].

Design-Driven Approaches

The design-driven approach to teaching AI and materials engineering centers on the use of pre-existing software tools employed in industry to solve materials design and discovery problems. This approach is focused on a specific materials design challenge and focuses on the role of the materials engineer in solving the problem with AI tools. In contrast to the computer-science-driven approach, no immediate computer programming knowledge is needed to begin tackling the problem. Instead, the design problem and a ‘no-code’ AI software tool can be used as a ‘launchpad’ for learning about computer science topics. This approach may be advantageous when computer science and programming are not well ingrained in an MS&E curriculum.

The cloud-based, enterprise-level Citrine Platform is one example of a user-friendly “no-code” AI tool with a graphical user interface (GUI) that is accessible via any web browser. The Citrine Platform provides the capability to assess complex materials data, build ML models, and design experiments, all without coding. The software has been successfully applied to a variety of problems in the development of materials and chemicals development including superconductors, thermoelectrics, metal alloys, and organic conductors [48-51].

The workflow of the Citrine Platform GUI is based on a “branch” workflow. The platform allows students to tweak ML parameters and see the effects of these changes in real time, making it an ideal tool for enhancing classroom interactivity and developing an intuition for how the ML “black box” functions, without in-depth programming knowledge. The Citrine Platform’s unique ML-driven DoE capability provides a real-world application of ML to industry, enabling students to understand and identify the characteristics of successful AI-driven product development projects. The ability for students to learn and perform an end-to-end data science workflow without writing a single line of code, all within the context of materials design, has the potential to enhance their educational experience and improve their employability in a rapidly advancing field.

The Citrine Platform has been used to help expose second- and third-year undergraduate MS&E students to AI and ML through an iterative activity that involves development and curation of a material and process property dataset of 3D printed plastics [25]. The process is shown in Figure 8. Students began by collecting and organizing plastic filament data from published literature and from an existing dataset provided by the instructor. The output of this data curation step is a structured data table that has been organized in a predefined format (Table 3). After data structuring and curation, the data can then be ingested to train an ML model. Next, the ML model is used to perform Design of Experiments (DoE), generating new possible experiments (material and 3D printing process combinations) based on a specified design space. Students apply their MS&E domain knowledge when defining the design space of the new possible experiments and when they prioritize candidates for further exploration. The newly generated data can be fed back into the AI model. Survey results indicated that, through this case study, students reported an increased understanding of what ML is and how it can be applied to real-world engineering problems [25].

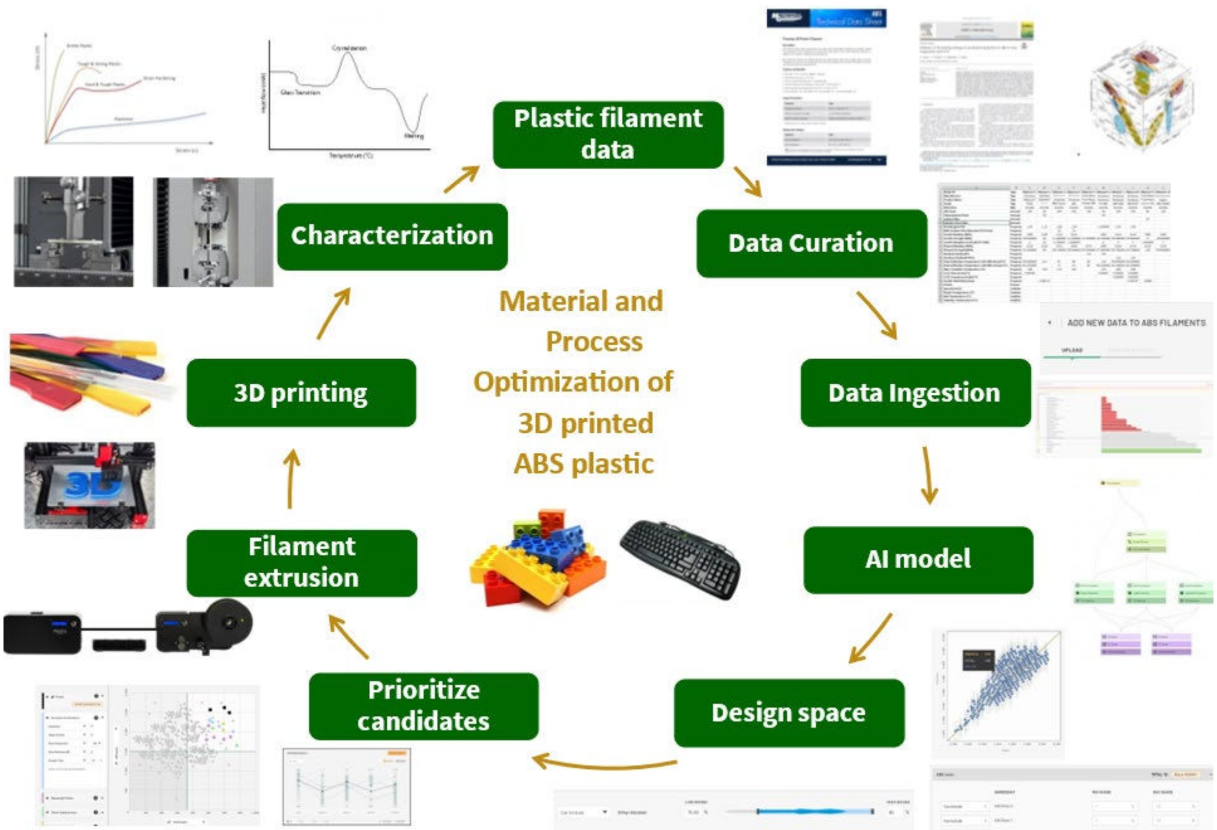

Figure 8: An overview of material and process optimization exercise for 3D printed plastic. The closed-loop nature of the exercise allows students to thoroughly investigate the application of ML to MS&E and its potential benefits and shortcomings [25].

Table 3: Structured data template for use with the Citrine Platform.

Name	Ingredient A	Ingredient B	Ingredient C	Ingredient D	Ingredient E	Process Name	Process Condition A (units)	Process Condition B (units)	Process Condition C (units)	Property A Name (units)	Property B Name (units)	Property C Name (units)	Condition Name 1 for Property C (units)	Condition Name 2 for Property C (units)	Property D	Notes
Type	Amount	Amount	Amount	Amount	Amount	Process	Condition	Condition	Condition	Property	Property	Property	Condition	Condition	Property	Skip
Sample_ID 1																
Sample_ID 2																
Sample_ID 3																
Sample_ID 4																
Sample_ID 5																
Sample_ID 6																

Another commercially available ML tool utilized in materials engineering is the Materials Image Processing and Automated Reconstruction (MIPAR) Image Analysis Software [52]. MIPAR utilizes deep learning, typically via custom algorithm development for the end user by MIPAR engineers, to perform complex image analysis tasks. The user interface is a drag-and-drop format with simple and intuitive navigation and features like side-by-side image viewing. Figure 9 shows a screenshot of the user interface and an example of the analysis and quantification tools available in the MIPAR software. MIPAR has been implemented in academic research and industry for materials applications including microstructure analysis [53, 54], defect analysis [55], and particle size classification. It is also used in fields outside of MS&E e.g., life sciences, drone and surveying, biomedical, environmental engineering [56], and manufacturing applications. At The Ohio State University, MIPAR has been integrated into the undergraduate curriculum via *MSE 2331: Structure and Characterization Lab*. MSE 2331 exposes students to visual characterization techniques like optical and scanning electron microscopy, as well as image analysis methods [57]. In the course, students are first trained to perform manual image segmentation using ImageJ. They are then introduced to MIPAR and shown how to create an algorithm to automate segmentation and improve both the speed and reliability of the process. In the first five years that MIPAR was included in the course, over 400 students used the tool, and faculty indicated that its use led to a more enjoyable and educational experience than manual analysis alone. Specifically, professors cited the benefit of reduced analysis time, which enabled more complex and in-depth laboratory experiments to be performed within the limited class time.

Design-driven approaches to incorporating AI and ML into the curriculum—such as those described above—have the added benefit of training students on tools they may encounter in the workforce, given that the use of the Citrine Platform, MIPAR, and similar tools in industry is only increasing.

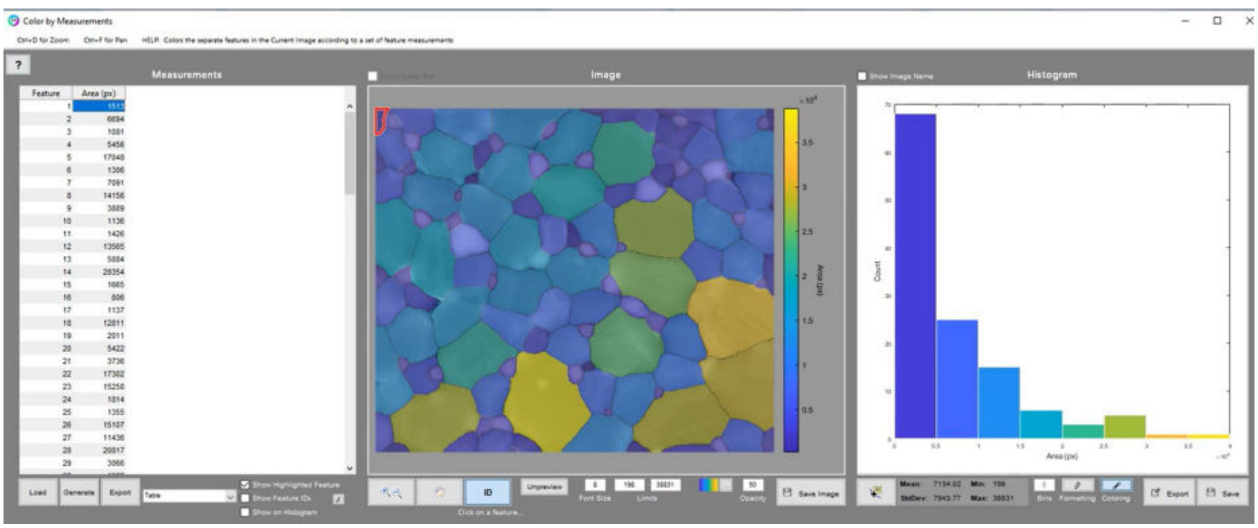

Figure 9. Example of the analysis and quantification tools available in MIPAR, in this case grain size determination with the generation of a color map of grain area and a histogram of grain size distribution [58].

Challenges to teaching AI/ML in MS&E

The multi-disciplinary nature of AI/ML and curriculum integration

Meaningfully integrating AI and ML into MS&E curricula is fundamentally challenging because instructors and students must possess a variety of skills to successfully implement AI/ML tools for solving real-world problems. Strong foundational domain knowledge is necessary to properly frame a problem for an AI tool to solve. This knowledge is critical for establishing the design space and search space for an ML algorithm. In addition, data science expertise is needed to structure data effectively for use with an AI tool and to create compelling data visualizations of ML model results. Programming skills are required to write software in languages such as Python—or at least a basic understanding of programming to interpret how pre-existing code implements an ML algorithm in a Jupyter Notebook. Finally, critical thinking skills are essential across all these steps to ensure a meaningful and useful application of AI/ML to materials engineering problems.

Incorporating all these aspects into an already time-restricted curriculum is a significant challenge for materials engineering educators. It typically entails considerable time commitment from instructors to upskill on these topics. However, regular hands-on workshops on AI and ML topics for MS&E researchers—such as those held at Materials Research Society (MRS) meetings [59], may help educators acquire the necessary skills.

To overcome these issues, it has been suggested that small AI/ML modules be incorporated into existing courses. This approach, however, may pose additional challenges, such as the need for training on specific software tools or programming languages. Adopting no-code cloud computing tools, such as the Citrine Platform or MIPAR, and emphasizing the specific roles of the materials engineer in applying these tools i.e., how their domain-specific knowledge is leveraged, may further alleviate these challenges.

'Black Box' AI tools and algorithm selection

The input/output nature of ML tools makes them susceptible to the "garbage in, garbage out" phenomenon, where the quality of the output is directly related to the quality of the input (Figure 10). This issue is particularly concerning when students apply pre-existing AI and ML tools without understanding the underlying algorithm. The goal of training material scientists and engineers is often not only to predict how a material behaves but also to understand why it behaves that way, that is, to elucidate the underlying physical material phenomena. One challenge with many AI tools is that they frequently do not provide insight into these underlying phenomena. Moreover, "black box" methods in MS&E can produce incorrect answers or predictions. However, these tools may still be useful if [60]:

1. The cost (economic, societal, ethical) of wrong answers is low.
2. The wrong answer inspires some new ideas or approach to the problem.

Thus, black box AI and ML tools can still be valuable in classroom exercises related to materials design and discovery, even though they cannot be used to uncover the underlying physical mechanisms in a material.

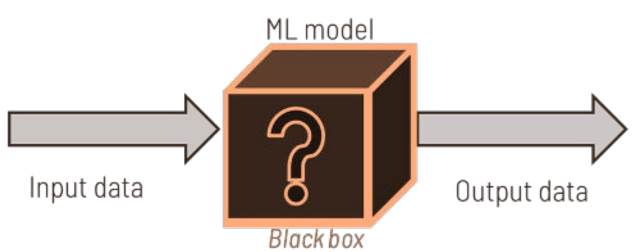

Figure 10: The input/output nature of ML models means that they are susceptible to garbage in garbage out and they do not provide significant insight into underlying physical material phenomena.

Datasets for real-world materials engineering problems

Finding and adapting relevant materials data for classroom use remains a challenge. Data for ML models can come from a variety of sources, including experimental data, external databases, published literature, and physics-based simulations. Both data quality and quantity are crucial for drawing reliable conclusions, which presents several challenges when applying ML tools to materials engineering problems in the classroom. There are several existing materials data repositories (Table 4) that could potentially be used in classroom applications of AI/ML tools. Moreover, an increasing number of materials datasets are being published in AI/ML research related to materials, and these could potentially be adapted for classroom use; however, they are frequently at a level that is beyond the comprehension of undergraduate MS&E students.

Table 4: Comparison of materials data repositories with material property information [34].

Name	Structure information	Mechanical properties	Thermal properties	Electronic properties	Data license
Materials Project	Y	Y	Y	Y	CC BY 4.0
Open Quantum Materials Database	Y	N	Y	Y	CC BY 4.0
AFLOW for Materials Discovery	Y	Y	Y	Y	Unknown
Novel Materials Discovery (NOMAD)	Y	Y	Y	Y	CC BY 4.0
Open Materials Database	Y	N	Y	Y	CC BY 4.0
Citrine Informatics	Y	Y	Y	Y	CC BY
Materials Platform for Data Science	Y	Y	Y	Y	CC BY 4.0
AiiDA/Materials Cloud	Y	Y	Y	Y	Varies
NREL MatDB	Y	N	Y	Y	Own license
NIST TRC Alloy Data	N	N	Y	N	Free
NIST TRC ThermoData	N	N	Y	N	NIST SRD
NIST JARVIS-DFT/-ML Database	Y	Y	Y	Y	Public domain
MatWeb	N	Y	Y	N	Paid
Total Materia	N	Y	Y	N	Paid
Ansys Granta (MaterialUniverse)	N	Y	Y	N	Paid
MATDAT	N	Y	Y	N	Paid

Conclusions and Outlook

The recent surge in AI and ML within MS&E represents a new frontier for many instructors. Teaching these topics to undergraduate students poses several challenges, regardless of the approach taken. Key obstacles include the interdisciplinary nature of AI/ML, the integration of these topics into existing curricula, the “black box” nature of AI tools, and the need for relevant and accessible data sources. However, introducing AI and ML concepts through practical, real-world case studies can help students understand how these tools are applied in MS&E and prepare them for their future careers. Recent research progress in AI and ML within MS&E also provides avenues for open-source data and ML code that could potentially be used in undergraduate education.

For instructors adopting a computer-science–driven approach, numerous high-quality, open-source resources are available to facilitate teaching. Platforms such as Jupyter Notebooks and interactive environments like Google Colab make these resources both accessible and engaging for undergraduates. Additionally, repositories such as GitHub and nanoHUB allow students to experience the power of collaborative, open-source science and engineering. In contrast, the design-driven approach using existing software tools offers an alternative for students to explore AI and ML without a heavy emphasis on programming or computer science. By utilizing “no-code” tools, students with little or no coding experience can still grasp the role of AI and ML in solving engineering problems. Because AI and ML tools are still emerging in the classroom, there is currently a lack of comprehensive data comparing the effectiveness of computer-science–driven versus design-driven approaches.

Regardless of the approach, it is crucial to emphasize the importance of domain knowledge and structured data in addressing real-world MS&E problems. These skills are fundamental for students as they apply AI tools in their careers. Modern pedagogical approaches, such as universal design for learning (UDL) methods [61], may offer new opportunities for integrating AI/ML topics in the classroom. For example, the classroom integration of materials engineering podcasts [62], other modern MS&E software tools [63], and the gamification of materials science [64], may all offer future outlets for incorporating AI and ML into the classroom.

Acknowledgements

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