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Enhancing computational problem-solving skills in materials science and engineering through a molecular dynamics laboratory experience

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Abstract

Computational tools such as modeling and simulation have become essential skills in modern materials science and engineering (MSE) practice. However, undergraduate students in MSE programs often have limited exposure to computational modeling in contrast to their more extensive training in experimental methods. As such, students often undervalue computation as a viable method for solving materials problems, viewing it as secondary or supplementary to laboratory experimentation.

To address this gap, we developed and implemented a hands-on Molecular Dynamics (MD) laboratory module which is integrated into the junior-level laboratory course sequence. This module is designed to build upon and extend the fundamental materials modeling concepts covered in the required computational materials science class, allowing students to apply computation in parallel with experimental practices. Students execute and interpret the results of MD simulations on gold nanoparticles and are introduced to the fundamentals of high-performance computing and materials visualization tools.

We aim to investigate the impact of this intervention on students' perceptions of computation as a powerful problem-solving tool that is commensurate with experiments. Specifically, we will use pre- and post-activity surveys to measure changes in student attitudes regarding the role of computation in MSE relative to experimental methods. Our goal is to evaluate how hands-on computational experiences integrated in existing undergraduate courses influence students' perceived value of computational modeling in their broader engineering education. Longer term, our goal is to ultimately integrate computational modules into multiple MSE undergraduate courses, thereby establishing a computational throughline in the existing curriculum that reinforces the experimental training students already receive.

Introduction and Background

Computational modeling and simulation play an increasingly central role in modern materials science and engineering (MSE) practice. By complementing theoretical and experimental methods, computation supports materials design, characterization, and understanding of complex materials behavior across length scales [1] [2]. There is a broad consensus among faculty and industry employers that computational competencies are now a core form of literacy for modern

engineers, regarded as essential as mathematics and the engineering sciences [1] [2] [3]. However, a significant gap remains between academic preparation and industrial requirements [4]. Foundational surveys by Thornton et al. revealed that while employers desire approximately 50% of new hires to have computational training, only 37% of recent graduates possess these skills [5].

Meeting this demand for computational fluency is challenging, as undergraduate curricula are already densely packed with traditional material, leaving little space for additional standalone courses [3] [4] [5]. As a result, integration of computational content into existing core coursework has emerged as a practical strategy for developing computational proficiency without extending degree timelines or exceeding credit limits. Several studies have documented institutional efforts to integrate computation into undergraduate MSE curricula using this approach [1] [2] [3] [4] [6]. In particular, Mansbach et al. proposed a "computational throughline" in which computational competencies are embedded across multiple required courses without adding new credit hours [2] [3]. This model emphasizes the reinforcement of core disciplinary content rather than isolated skill development, ensuring that computational training is aligned with traditional instruction.

Despite these efforts, students often perceive computational labs as inherently different and less practical than traditional physical experiments [1]. Prior studies consistently report a disconnect between faculty intentions and students' perceptions on the value of computation [7] [8] [9] [10] [11]. Students often exhibit mixed motivation toward programming and computational assignments and have even ranked required computational sequencies as the "least valuable" component of their education [7] [8]. These perceptions often arise from a lack of clear connection between computational activities and real-world materials science problems. Additionally, students in majors perceived as "less computation-focused", such as Materials Science and Engineering, often enter the university with lower computational self-efficacy and a belief that they are fundamentally "not programmers" compared to their peers in other engineering disciplines [9].

To address these challenges, recent pedagogical efforts have focused on scenario-based simulations that are built upon real-world engineering context [6]. Research in both materials science and physics education indicates that computational activities are most effective when embedded within meaningful, discipline-specific contexts [6][7] [12] [13]. Specifically, integrating computational and physical laboratory sequences, such as using data students have personally gathered in a physical experiment as the direct input for a computational exercise, has been shown to make simulation results feel more tangible and relevant to students [1]. Studies of computer-based visualization tools such as OVITO have shown that short, scaffolded computational interventions—combined with reflection and group work—can improve conceptual understanding [13]. Similarly, scenario-based simulations in MSE, such as kinetics modeling activities, have been shown to improve engagement and conceptual understanding by

requiring students to make decisions based on simulation outputs and to interpret physical behavior in realistic materials scenarios [6]. Importantly, these activities emphasize interpretation of the results and physical understanding rather than technical mastery of programming itself.

Building on this prior work, the present study focuses on embedding a Molecular Dynamics (MD) laboratory module within an existing experimental MSE lab course. This approach is designed to operate within the existing curriculum, pairing computational modeling with experimental practice. The module uses a software package, LAMMPS, commonly used in materials research and industry along with on-campus high performance computing (HPC) resources, and it is scaffolded in a way to emphasize interpretation of results, and comparison with experimental concepts rather than details of simulation setup [14]. Through a planned mixed-methods assessment, this work seeks to address the following questions: (1) How does the participation in a hands-on MD laboratory module influence students' perceptions of computation as a problem-solving tool in materials science and engineering, and (2) to what extent does integrating computational modeling within an experimental laboratory context support students' recognition of computation as complementary to experimentation.

In the following sections, we describe the hands-on laboratory activity and the pre- and post-surveys and rubrics that will be used in this study.

Methods

Part 1: Computational module design and integration within the junior-level MSE undergraduate lab

The Molecular Dynamics (MD) laboratory module is implemented within the junior-level materials science and engineering laboratory course. The module is intentionally positioned one semester after students complete a required computational material science course, ensuring prior exposure to atomistic modeling concepts, MD fundamentals, and atomic structure visualization tools. The module is designed to run in parallel with an experimental nanoparticle synthesis laboratory to reinforce the idea that computational modeling serves as a complementary and equally valid approach to materials characterization and analysis.

The MD laboratory module is developed with the following learning objectives:

1. Reinforce students' understanding of atomic-scale structure–property relationships in materials.
2. Develop practical competency in setting up, executing, and interpreting molecular dynamics simulations.
3. Introduce students to high-performance computing (HPC) environments and remote job submission workflows.

4. Provide experience with post-processing and visualization tools commonly used in computational materials research.
5. Encourage students to view computation as a powerful problem-solving tool alongside experimental methods.

The laboratory activity is based on molecular dynamics (MD) simulations of gold nanoparticles, adapted from prior published work on nanoparticle melting behavior [15]. Gold nanoparticles are selected due to their well-documented size-dependent melting behavior and relevance to applications in catalysis, medicine, and nanotechnology. In addition, the experimental exercise involving the synthesis of gold nanoparticles was already integrated into the laboratory curriculum prior to the introduction of the computational module, enabling alignment between experimental and computational content.

Simulations are performed using LAMMPS, an open-source molecular dynamics package widely used in materials modeling [14]. As most students have no prior experience with LAMMPS, the module is structured to scaffold simulation setup and execution. Interatomic interactions are described using an embedded-atom method (EAM) potential for Au–Au interactions [16]. Students explore gold nanoparticles spanning sizes from tens to several thousand atoms, enabling direct comparison of size-dependent thermodynamic stability and phase behavior.

The laboratory module begins with a classroom presentation outlining the activity goals and providing a refresher on MD concepts. During this introductory lecture, students are introduced to LAMMPS, including an overview of the simulation workflow and a guided explanation of the input and submission scripts used throughout the module. Students are then split into small groups, with nanoparticle sizes assigned, such that each group investigates a range of sizes from small to large. This structure enables within-group comparison of size-dependent behavior while promoting collaborative analysis. The hands-on component of the module consists of a structured sequence of computational tasks completed over two or three laboratory periods.

A. Initial Energy Minimization
   Students begin by performing an energy minimization at 0 K for their assigned gold nanoparticle. This step allows students to:
   - Relax the atomic structure
   - Determine the potential energy per atom
   - Identify minimum-energy configurations
   - Visualize atomic geometry using OVITO

   This activity reinforces the relationship between atomic arrangement and thermodynamic stability.
B. Finite-Temperature Molecular Dynamics Simulations
   Students then conduct MD simulations in the canonical (NVT) ensemble at a minimum of five different temperatures. For each temperature:

- Separate simulations are run
- Radial distribution functions (RDF) are computed
- Structural changes are analyzed to distinguish solid and liquid states

Students plot RDFs on a single graph for each nanoparticle size to observe the progressive loss of crystalline order with increasing temperature. Based on these data, students estimate the melting temperature of their assigned nanoparticle and compare it to bulk gold behavior.

C. Annealing Simulations
To further explore phase behavior, students perform annealing simulations using a controlled temperature ramp. By plotting the potential energy per atom as a function of temperature, students examine energetic signatures associated with phase transitions and compare results with the RDF-based estimates.

D. Data Analysis and Reporting
Each student contributes simulation results for a specific nanoparticle size to a group report. Required deliverables include:
- Potential energy per atom (pre- and post- annealing)
- RDF plots across temperature
- Potential energy versus temperature plots
- Visual snapshots of nanoparticle geometry before and after annealing
- Analysis of the relationship between melting temperature and inverse nanoparticle diameter

The reporting structure takes the form of a short, itemized group report and emphasizes interpretation and synthesis rather than procedural description, intentionally shifting student focus from the mechanics of running simulations to the use of computational modeling as an analytical tool for materials science problem-solving.

All simulations are executed on a university HPC cluster. To support students with limited prior experience in remote computing environments, scaffolded instructional materials are provided, including:
- Unix/Linux command references
- File management workflows
- Job submission scripts
- Queue management guidance

Students create separate directories for each simulation by editing the instructor-provided scripts, transfer files to the HPC system, submit jobs, and retrieve output files for local post-processing. This approach exposes students to authentic computational research practices while minimizing technical barriers.

The following section describes a mixed-methods assessment methodology that will be used to evaluate the impact of the MD laboratory module on students' perceptions of computational modeling.

Part 2: Study design and data collection

A mixed-methods assessment approach will be employed to evaluate the impact of the MD laboratory module on students' perceptions of computational modeling in materials science and engineering. The study uses a pre- and post-activity survey design to capture changes in student attitudes, confidence, and problem-solving approaches related to computation and experimentation.

The study was reviewed by the Institutional Review Board (IRB) and was determined to be exempt (IRB Protocol 2386275-1). Participation will be voluntary, responses will be anonymized, and survey participation has no impact on course grades.

Each survey requires approximately 10-15 minutes to complete.

I. Participants and Course Enrollment

The initial data collection will involve students enrolled in the Spring 2026 offering of the junior-level materials science laboratory course, with an expected enrollment of 11 students. Typical course enrollment ranges from approximately 15 to 20 students in future offerings. While the initial sample size is small, the study is designed as a longitudinal effort, with repeated data collection planned across subsequent academic years. This approach is intended to build a larger dataset over time and support more robust interpretation of trends in students' perceptions and reasoning.

II. Survey Instruments

The pre- and post-surveys are designed to examine multiple aspects of students' engagement with computation and modeling and problem-solving perspectives. Both instruments include a combination of Likert-scale items, multiple-choice questions, and open-ended responses. Survey instruments are summarized below (A-D) and included in the Appendix.

A. Prior Familiarity and Exposure

Students self-report their prior familiarity with computational and experimental methods using a 0–4 scale ranging from "no familiarity" to "comfortable using independently." Items include molecular dynamics, Monte Carlo methods, visualization tools, high-performance computing basics, and common experimental characterization techniques. Post-survey responses are compared to pre-survey results to examine changes in exposure and comfort.

B. Problem-Solving Scenarios

Both surveys include open-ended problem-solving scenarios that ask students to describe how they would approach materials science problems using computational methods, experimental methods, or a combination of both. Scenarios are designed to assess students' ability to:

- Select appropriate methodologies
- Identify relevant measurable quantities
- Articulate coherent workflows
- Integrate computational and experimental approaches

The post-survey additionally includes a lab-specific scenario focused on analyzing MD simulations of gold nanoparticles, allowing direct alignment between survey responses and the laboratory experience.

C. Attitudes, Confidence, and Perceptions

Likert-scale items measure students' perceptions of the value of computation relative to experimentation, confidence in selecting appropriate tools, ability to interpret simulation outputs, and intent to use computational methods in future coursework or projects. Items are grouped into constructs such as perceived value of computation, computational judgment, skill confidence, and future intent.

D. Reflection

Open-ended post-survey questions prompt students to reflect on:

- The strengths and limitations of molecular dynamics
- Challenges encountered during the MD workflow
- Concepts about materials behavior that became clearer through the lab
- Potential changes they would make if repeating the activity

These items are designed to capture conceptual shifts that are not readily accessible through closed-form questions.

III. Data Analysis Approach

Qualitative data from Likert scale and multiple-choice items will be summarized via descriptive statistics, with pre- and post-survey results compared to identify changes in student perceptions. Qualitative responses will be analyzed using analytic rubrics developed specifically for this study. Responses will be coded to characterize levels of reasoning,

integration of methods, workflow coherence, and awareness of computational strengths and limitations. Coding will include both ordinal rubric scores and binary thematic tags.

IV. Anticipated Outcomes

Our hypothesis is that participation in the MD laboratory module will lead to positive shifts in students' perceptions of computational modeling as a valuable problem-solving tool in materials science and engineering. Specifically, post-survey responses are expected to show increased confidence in interpreting simulation outputs, greater recognition of the complementary roles of computation and experimentation, and improved ability to articulate integrated computational–experimental workflows. These anticipated outcomes are consistent with prior studies showing that authentic, hands-on computational experiences can improve students' confidence and perceived value of computation in engineering education [1] [6] [13].

Conclusions

The anticipated outcomes of this study will inform broader efforts to integrate computation more intentionally throughout the undergraduate materials science and engineering curriculum. By embedding a hands-on molecular dynamics module within an existing laboratory course, this work demonstrates how computational modeling can be positioned as a parallel and complementary approach to experimentation rather than as a standalone skill. Insights gained from the planned assessment are expected to guide the development of similar computational modules in other core MSE courses, supporting the establishment of a coherent computational throughline that reinforces problem-solving and content retention across the curriculum.

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Appendix A: Pre-Survey Instrument

Introductory survey parts, including student consent to participate, are omitted in this document.

Prior familiarity (0-4 scale)

Topic	**0 1 2 3 4**
Molecular Dynamics (MD)	○ ○ ○ ○ ○
Monte Carlo (MC)	○ ○ ○ ○ ○
Visualization tools (e.g., OVITO)	○ ○ ○ ○ ○
HPC basics (job schedulers, queues)	○ ○ ○ ○ ○
Electron Microscopy	○ ○ ○ ○ ○
UV-Vis	○ ○ ○ ○ ○
FTIR	○ ○ ○ ○ ○
AFM	○ ○ ○ ○ ○
Other experimental methods	○ ○ ○ ○ ○
Other computational methods	○ ○ ○ ○ ○

If “other experimental methods”, please list:

If “other computational methods”, please list:

Problem-solving scenarios (Pre-survey)

Scenario 1: A *thin copper film is deposited on an aluminum substrate and then annealed at 500 °C. Over time, the two elements begin to mix.*

Question 1: How would you investigate this process to determine how fast copper atoms diffuse into aluminum?

Long answer question

Question 2: Which overall approach would you take?

Computational, Experimental, Both

Question 3: Rate your confidence in executing methods (0-4 scale)

0, 1, 2, 3, 4

Question 4: Estimate the split of effort (if applicable)

mostly computational, balanced, mostly experimental

Question 5: Describe the sequence of methods you would use

Open response

Question 6: What insights would your method yield? Check all that apply

Structure, Thermodynamics, Kinetics/Transport, Mechanical Properties, Surface chemistry, Electrical Properties

Scenario 2: *A perovskite solar cell shows decreasing efficiency after several thermal cycles. How could you investigate the degradation mechanisms?*

Question 1: How would you investigate the degradation mechanisms and measure or predict the performance loss?

Long answer question

Question 2: Which overall approach would you take?

Computational, Experimental, Both

Question 3: Rate your confidence in executing methods (0-4 scale)

0, 1, 2, 3, 4

Question 4: Estimate the split of effort (if applicable)

mostly computational, balanced, mostly experimental

Question 5: Describe the sequence of methods you would use

Open response

Question 6: Specify at least one technique and a key parameter (measurable quantity)

Open response

Question 7: What insights would your method yield? Check all that apply

Structure, Thermodynamics, Kinetics, Mechanical Properties, Transport, Surface chemistry

Attitudes and Perceptions (Pre-Survey)

Statement	1 Strongly Disagree	2 3 4 Neutral	5 6 7 Strongly Agree
Computation is as powerful as experimentation for solving Materials Science problems.	○	○○○	○○○
I can decide when computation is the right tool for a problem.	○	○○○	○○○
Combining computation and experiment leads to stronger conclusions.	○	○○○	○○○
I can interpret MD/MC outputs and connect them to measurable properties.	○	○○○	○○○
Experiments are the only trustworthy path to answers in MSE.	○	○○○	○○○
I expect to use experimental methods in a future project or course	○	○○○	○○○
I expect to use computational methods in a future project or course	○	○○○	○○○

Question 1: What makes experiments feel harder or easier than running simulations to study materials behavior?

Open question

Question 2: What is the primary reason you would choose computation for a materials problem? (Select one)

☐ Too expensive or slow to experiment

☐ Need atomic-scale insight

☐ Want to explore many conditions quickly

☐ Complement or interpret experiments

☐ Instructor requirement

☐ Not sure

Appendix B: Post-Survey Instrument

Prior familiarity (0-4 scale)

Topic	**0 1 2 3 4**
Molecular Dynamics (MD)	○ ○ ○ ○ ○
Monte Carlo (MC)	○ ○ ○ ○ ○
Visualization tools (e.g., OVITO)	○ ○ ○ ○ ○
HPC basics (job schedulers, queues)	○ ○ ○ ○ ○
Electron Microscopy	○ ○ ○ ○ ○
UV-Vis	○ ○ ○ ○ ○
FTIR	○ ○ ○ ○ ○
AFM	○ ○ ○ ○ ○
Other experimental methods	○ ○ ○ ○ ○
Other computational methods	○ ○ ○ ○ ○

If “other experimental methods”, please list:

If “other computational methods”, please list:

Problem-solving scenarios (post-survey)

Scenario 1: *A drug delivery system involves a small-molecule drug in a polymer matrix diffusing across a nanoscale lipid membrane. The delivery rate and concentrations of the drug will dictate the efficacy, efficiency, and safety of the drug.*

Question 1: How would you analyze the dynamics of the drug and polymer to determine a delivery rate for the drug?

Long answer question

Question 2: Which overall approach would you take?

Computational, Experimental, Both

Question 3: Rate your confidence in executing methods (0-4 scale)

0, 1, 2, 3, 4

Question 4: Estimate the split of effort (if applicable)

mostly computational, balanced, mostly experimental

Question 5: Describe the sequence of methods that will be used

Open Response

Question 6: What insights would your method yield? Check all that apply

Structure, Thermodynamics, Kinetics, Mechanical Properties, Transport, Surface chemistry

Lab-specific Scenario: *In the lab, you performed molecular dynamics simulations to study the melting of gold nanoparticles of different sizes.*

Question 1: How would you analyze the simulation results to determine the melting point and compare it to bulk gold? What other measurements or experiments could you use to confirm melting?

Long answer question

Question 2: Which overall approach would you take?

Computational, Experimental, Both

Question 3: Rate your confidence in executing methods (0-4 scale)

0, 1, 2, 3, 4

Question 4: Estimate the split of effort (if applicable)

mostly computational, balanced, mostly experimental

Question 5: Describe the sequence of methods that will be used

Open response

Question 6: What insights would your method yield?

Structure, Thermodynamics, Kinetics, Mechanical Properties, Transport, Surface chemistry

Post Survey Check

Question 1: Which of the following did you do in the lab? Select all that apply

Ran an MD simulation
Modified input files or parameters
Visualized atomic structure
Computed a property (e.g., MSD, RDF)
Compared results to theory / experiment

Attitudes and Perceptions (Post-Survey)

Statement	**1 Strongly Disagree**	**2 3 4 Neutral**	**5 6 7 Strongly Agree**
Computation is as powerful as experimentation for solving Materials Science problems.	○	○ ○ ○	○ ○ ○
I can decide when computation is the right tool for a problem.	○	○ ○ ○	○ ○ ○
Combining computation and experiment leads to stronger conclusions.	○	○ ○ ○	○ ○ ○
I can interpret MD/MC outputs and connect them to measurable properties.	○	○ ○ ○	○ ○ ○
Experiments are the only trustworthy path to answers in MSE.	○	○ ○ ○	○ ○ ○
I feel more confident planning a study that integrates simulation and experiment	○	○ ○ ○	○ ○ ○
I expect to use computational methods in a future project or course	○	○ ○ ○	○ ○ ○

Question 1: What did you learn about the strengths/limits of MD from this lab?

Open question

Question 2: If you repeated this lab, what would you change?

Open question

Question 3: Describe one concept about materials behavior that became clearer after completing this lab exercise

Open question

Statement	1 Strongly Disagree	2 3 4 Neutral	5 6 7 Strongly Agree
I understand how atomic-scale dynamics connect to bulk materials properties	○	○ ○ ○	○ ○ ○
I can explain how diffusion or melting can be modeled using MD	○	○ ○ ○	○ ○ ○
I can interpret output quantities from an MD simulation	○	○ ○ ○	○ ○ ○
I feel confident modifying MD input files and parameters	○	○ ○ ○	○ ○ ○
I can set up and run a basic MD simulation independently	○	○ ○ ○	○ ○ ○
I can use visualization software to analyze atomic trajectories	○	○ ○ ○	○ ○ ○
I understand how to identify melting or diffusion phenomena from simulation outputs	○	○ ○ ○	○ ○ ○
I can propose an experiment to validate a simulation result	○	○ ○ ○	○ ○ ○
I can relate computational predictions to measurable quantities	○	○ ○ ○	○ ○ ○

Question 4: Which of the following limitations of MD did you encounter or consider? (Select all that apply)

☐ Time scale limitations

☐ System size limitations

☐ Accuracy of interatomic potentials

☐ Computational cost

☐ Difficulty connecting to experiments

☐ Visualization/analysis challenges

☐ I did not encounter significant limitations

Question 5: Which of the following MD outputs is most appropriate for estimating diffusion? (Select one)

☐ Radial distribution function (RDF)

☐ Mean squared displacement (MSD)

☐ Potential energy vs time

☐ Coordination number

☐ Not sure

Question 6: What part of the MD workflow was most challenging for you? (Select one)

☐ Understanding the physical model

☐ Setting up input files

☐ Running jobs (HPC)

☐ Analyzing outputs

☐ Interpreting results physically

☐ Nothing felt especially challenging

Question 7: What is the primary reason you would choose computation for a materials problem? (Select one)

☐ Too expensive or slow to experiment

☐ Need atomic-scale insight

☐ Want to explore many conditions quickly

☐ Complement or interpret experiments

☐ Instructor requirement

☐ Not sure