Enhancing Materials Science & Engineering Curricula through Computation

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Team Members: John Kieffer (PI), Michael Aldridge, Jessica Bickel, Arthur Feldman, Michael Katz, Michael Warren, Changgua Zhen (Graduate Assistants), Tershia Pinder-Grover (Evaluator)

Introduction

The objective of this project is to devise a more effective instructional process by incorporating computation and cyber infrastructure (CI) into materials science core courses. We expect students to gain a better fundamental understanding of materials science concepts and principles, and to advance their algorithmic thinking and computational proficiency. To this end we develop instructional modules that (i) visually present fundamental concepts in materials science, thereby increase student comprehension; (ii) actively engage students in computer-based experimentation; and (iii) concentrate student attention on algorithmic thinking and concepts in scientific computation. The modules we develop can be categorized into three types:

1. Computer-aided instruction (CAI), i.e., course material captured on digital media for self-paced viewing, compiled into an interlinked library

2. Virtual experiments that students can interactively control, i.e., computer simulations of processes, phenomena, or concepts that are difficult to create or visualize in the classroom or laboratory

3. Science and engineering problems of a level of sophistication that requires numerical methods to solve

This phase-I CCLI project is intended to provide a proof of concept. We selected the undergraduate course on the Thermodynamics of Materials, an introductory undergraduate level course in thermodynamics required for all students in MSE, as the test bed for this purpose.

The Need for a Shift of Paradigm

A survey conducted at the conclusion of the first "traditional" offering of the Thermodynamics of Materials course, was used to give insight into how students viewed the course and to gauge their level of comfort with computer based numerical methods. Beyond the general agreement that thermodynamics is "abstract" the survey reveals the following:

1. Knowledge gap - 42% of students were unfamiliar with computer-based numerical problem methods prior to taking the course.

2. Utility gap - Though 63% of students think that computational methods are very important for their careers, only 28% thought they were useful for other courses and a mere 11% found them useful in the course they had just completed.

3. Learning gap - At the conclusion of the course 77% students still found it somewhat, very, or extremely difficult to connect formulas to the physical phenomenon they describe and the same percentage found that visualizing physical phenomena was key to understanding.

Approach

The project team consists of the course instructor, graduate research assistants, and a professional evaluator from the Center for Research on Learning and Teaching (CRLT) at the University of Michigan.

The project period covers two consecutive offerings of the course. In a first round graduate assistants observe and the course is analyzed for content to be transformed for computer-enhanced instruction. Instructor and the assistants jointly identify the concepts for a series of modules; ideas are discussed and perfected. The teaching and learning efficiency of this first traditional offering is evaluated, including mission-specific questionnaires, to establish a baseline against which we will later compare the impact of the computer-based modules.

Computer-based instructional modules are developed in the time between the first and second offering. This is done as a team effort, involving regular meetings and frequent discussions.

Modules are implemented and evaluated during the second course offering. The impact on student learning is critically evaluated. Student feedback is collected and modules are improved accordingly before they are disseminated.

Podcast Video Lectures

For every major topic we produce three elements, (i) an electronically recorded lecture (e.g., in Podcast format) that can be easily archived and disseminated, (ii) simulation based virtual experiments, and (iii) computer-based homework problems. Adjacent are some screenshots of the lecture on configurational entropy.

We use Screenflow (Vara Software) to record Powerpoint presentations of the lecture material. This software records the screen activity, as well as video and voice of the presenter. Individual scenes can subsequently be edited, assembled into longer segments, and exported to a variety of formats (e.g., quicktime, wirecasts, podcasts, etc.) The raw footage requires about 2 Mb per sec. of presentation, but compresses by a factor of 20 or more upon export.

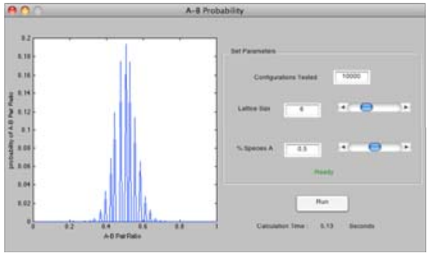
Advantages of podcast lectures are that they (i) they can be easily disseminated, (ii) can be (re)viewed by students asynchronously and at their own pace, (iii) free up time in the class room for interactive learning, and (iv) presentations can be perfected for pedagogic efficiency.

Simulations & Virtual Experiments

The ubiquity of relatively powerful computers on college campuses make incorporating simulations into coursework possible. Students report that visualizing physical phenomena is a major key to understanding the equations describing these phenomena. More so than reading diagrams or watching movies, interacting with simulations allow students to explore physical phenomena via virtual experiments. Simulations covering a gamut of thermodynamic phenomena that reflect fundamental areas of thermodynamics are at the students' disposal throughout the course.

Simulations and computational homework problems are developed on the MatLab platform. For virtual experiments and simulations, MatLab provides an easy-to-use graphical user interface, and modules can be compiled into standalone applications. The MatLab platform is ideally suited for homework problems, as it is part of the repertoire of most engineering students (it is taught in our freshmen computer programming class) and it is supported on all major computing platforms.

Below are two simulation modules that illustrate the possibilities of using virtual experiments to aid students in visualizing thermodynamic principles while simultaneously introducing concepts in numerical problem solving.

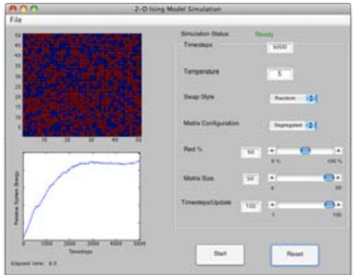


A-B Probability

This module demonstrates the concept of configurational entropy of an ensemble A two-species, A and B, ensemble of a certain size and composition is specified. The A-B bond percentage is used as an order parameter to characterize microstates. The frequency of occurrence of microstates is computed using a Monte Carlo scheme. Energy and temperature are specifically ignored here to underscore their irrelevance to configurationally entropy. This simulation reinforces the concept that though all microstates of a specific ensemble are equally likely, but there is a larger number of microstates that maximize disorder in the sample.

2-D Ising Model Simulation

The Ising model is used as an introduction to Monte Carlo experiments and to illustrate the concept of the energy of mixing, a more sophisticated simulation than the bond probability experiment above. Students here are provided with more parameters to vary, e.g., composition, ensemble size, temperature, initial states, and data output options are presented. Students can verify the behavior of the free energy of the system in real time by varying these parameters.



The Monte Carlo method itself provides an instructive look at how numerical methods can be used to approximate physical processes. In the Ising Model two elements from the ensemble are selected at random and their positions swapped and this change is accepted or rejected based on a conditional test. Additionally, students can explore questions of computer simulations from the important "how many time steps are required to stabilize a system?" and "what is this temperature unit?" to the mundane, "how many time steps per update do I really need?" to the extreme, "what if the temperature is 10^{10}?"

Numerical Problem Solving

Problem sets in thermodynamics texts often lack problems that require substantial computing. In an effort to increase the percentage of students who recognize the value of using numerical methods in thermodynamics, problems are created that are with certainty beyond the reach of pen and paper, and thus require students to develop algorithmic ways of thinking about a physical phenomenon.

These problems encourage students to think about how computers can be used to solve problems, how to devise effective algorithms to solve these problems, as well as to understand the limitations of computers.

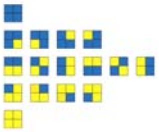
Verify the number of microstates in a macrostate

Problem:

Configurational entropy, S, is defined as $S = k_B \ln \Omega$ where k_B is Boltzmann's constant and Ω is the number of microstates available in the macrostate of interest. Ω is shown, for an ensemble of A + B = N particles, to be $\Omega = \frac{N!}{A!B!}$.

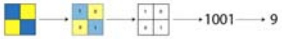
Verify that this is true for an ensemble 10 atoms and a 50:50 composition by generating a list of unique compositions.

Setting up the solution:
For a small system this a simple problem to visualize and solve by hand, but it quickly becomes intractable at large systems. This is an ideal numerical problem for a computer to solve.



$$\Omega = \frac{4!}{4!0!} = 1$$
$$\Omega = \frac{4!}{3!1!} = 4$$
$$\Omega = \frac{4!}{2!2!} = 6$$
$$\Omega = \frac{4!}{3!1!} = 4$$
$$\Omega = \frac{4!}{4!0!} = 1$$

Students must learn to analyze problems in ways that the computer can approach them. In this problem a method is required to generate a microstate configuration and to ensure that it fits our ensemble's requirements and that is unique. Here is one possible way to think about the problem:
In order to verify the above equation a random number is generated and broken into a binary representation that is tantamount to our ensemble. The MatLab code required to do this is shown below.



This program outputs a list of acceptable configurations of a macrostate, so long as it is allowed to run for a sufficient time. Creative thinking from the students combined with guidance from instructors allows students to explore a variety of numerical methods, and to find solutions and methods that are even more efficient.

Conclusions

- Student survey identifies the importance of enhancing computation in the MSE curriculum
- Students need to be challenged to use numerical methods to solve problems of greater complexity
- Students need to learn algorithm thinking to digest the concepts underlying physical phenomena, and understand the magnitudes of numerical problems
- Project approach requires significant resources in terms of person time, but the experience thus far indicates that is well worth it
- Software resources and computational power making it feasible to creatr the modules now exist
- Graduate students involved with the project are engaged and consider the project to be a valuable learning experience in terms of their own understanding of the subject and as preparation for careers as educators.