Enhancing Materials Science & Engineering Curricula through Computation

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Introduction

Objective: To help students gain a better fundamental understanding of materials science concepts and principles, and to advance their algorithmic thinking and computational proficiency.

Approach: Incorporating computation in the introductory Thermodynamics of Materials course, using three types of modules:

1. **Video podcast lectures** or computer-aided instruction i.e., course material captured on digital media for self-paced viewing
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. **Numerical problem solving** i.e., science and engineering problems requiring numerical methods to solve

The Need for a Shift of Paradigm

A survey conducted at the end of the first "traditional" offering of the Thermodynamics of Materials course revealed 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.

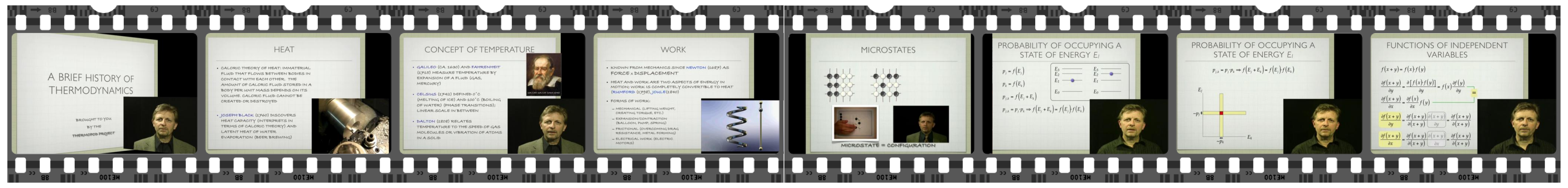
Approach

- **Development**: Instructor and the assistants jointly identify concepts for computer-enhanced instruction in 2007. For every major topic we produce three modules,
  - an electronically recorded lecture (e.g., in Podcast format) that can be easily archived and disseminated,
  - simulation based virtual experiments, and
  - computer-based homework problems.
- **Refinement**: Computer-based instructional modules developed in 2008-2009, implemented in 2010, and refined for 2011.
- **Assessment:** The impact on student learning is assessed based on student performance and survey feedback.

Video Podcast Lectures

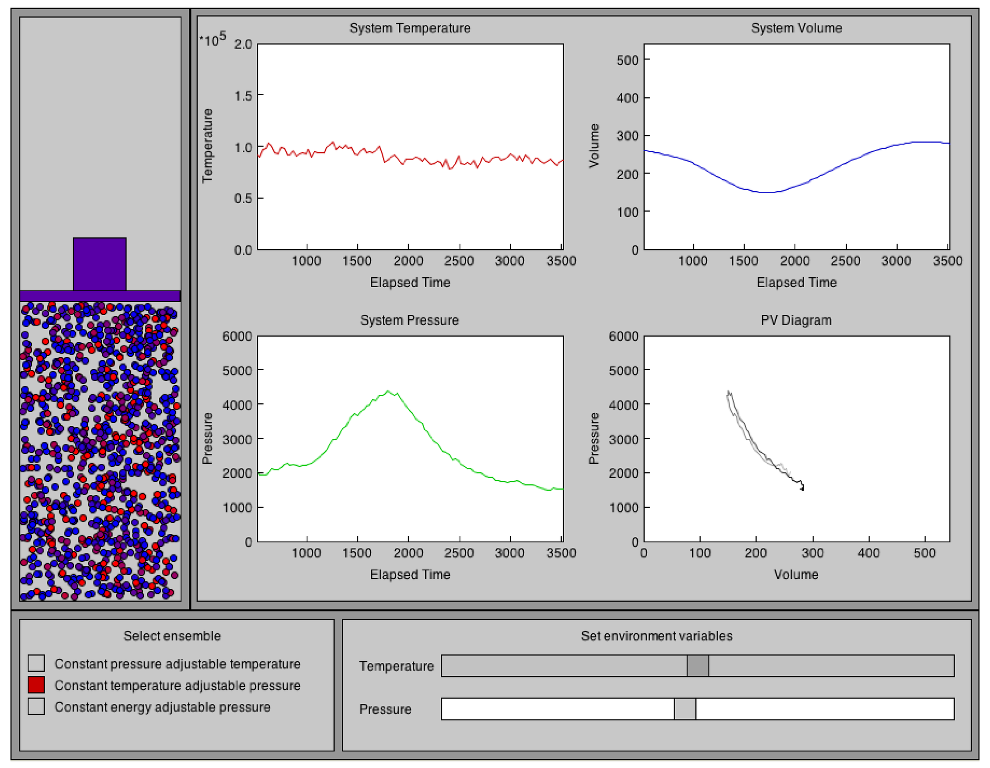
Video podcast lectures are carefully produced using Screenflow (Vara Software) to record Powerpoint presentations of the lecture material. This software records the screen activity, as well as video and voice of the presenter. Individual scenes are subsequently edited and additional audio-visual material are added. Advantages of podcast lectures include:

- they can be easily disseminated,
- can be (re)viewed by students asynchronously and at their own pace,
- free up time in the class room for interactive learning, and
- presentations can be perfected for pedagogic efficiency.

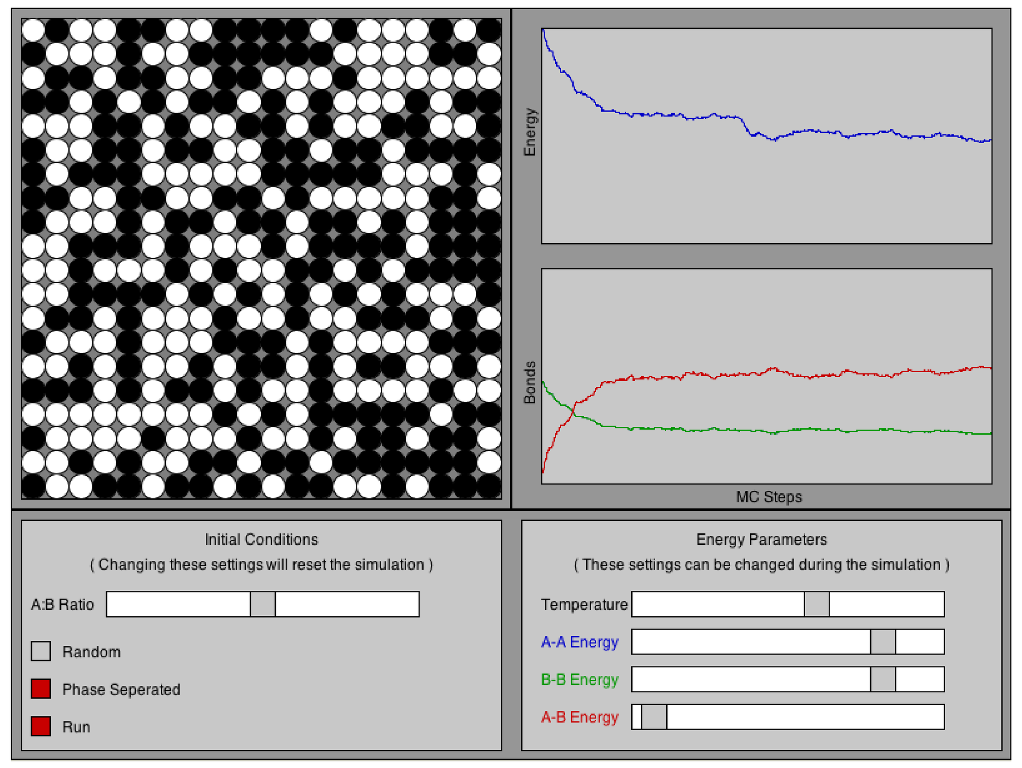


Simulations & Virtual Experiments

Simulations are developed in JAVA using the Processing platform. For virtual experiments and simulations, Processing provides an easy-to-use graphical user interface, and modules can be compiled into standalone applications. 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. Students can vary parameters, e.g., composition, ensemble size, temperature, initial states, pressure, interaction energies, etc. Students can observe and quantify the behavior of the system in real time by based on graphical and numerical simulation output.



Simulation of an ideal gas: control pressure and temperature; observe equation of state and thermodynamic processes.



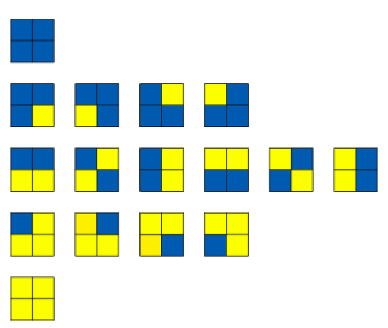
Simulation of binary mixture: control temperature and pair interactions; observe phase behavior.

Numerical Problem Solving

Problems are created that require students to develop algorithmic ways of thinking about a physical phenomenon using the Matlab platform.

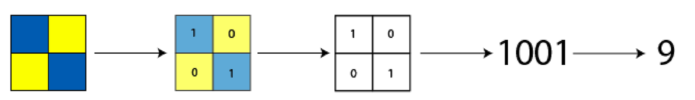
Example problem: *Configurational entropy, S, is defined as $S = k_B \ln \Omega$ where k_B is Boltzmann's constant and Ω is the number of microstates available in the macrostate of interest. Ω is shown, for an ensemble of A + B = N particles, to be $\Omega = N!/(A!B!)$. Verify that this is true for an ensemble 10 atoms and a 50:50 composition by generating a list of unique compositions.*

This problem quickly becomes intractable. A method to generate unique microstate configurations is necessary to ensure that it fits our ensemble's requirements and that is unique.



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

One possible way to think about the problem is to describe configurations using a pattern-based binary representation, which can be translated into MatLab code.

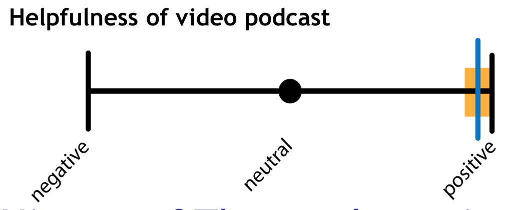


Results

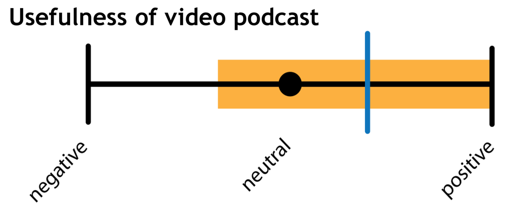
Students were surveyed to assess their comprehension of the content and to provide feedback on the strengths and areas of improves for each module. Student comments were identified as either positive (correct), neutral, or negative (incorrect).

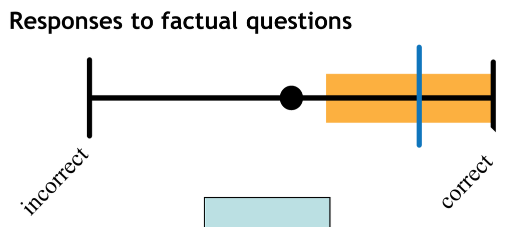
Video Podcast Lectures

Configurational Entropy



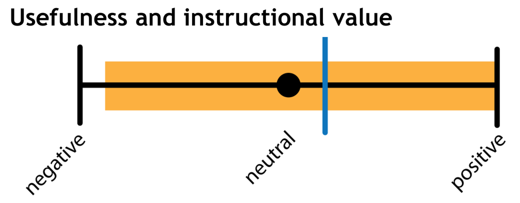
History of Thermodynamics



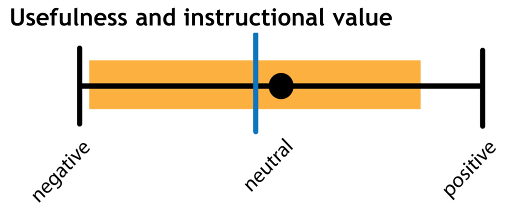


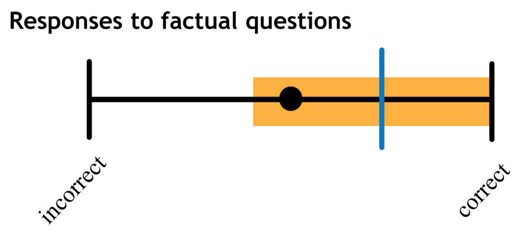
Virtual Experiments

Ideal Gas Simulation



Regular Solution Simulation





Conclusions

- ❑ Student survey identifies the importance of enhancing computation in the MSE curriculum
- ❑ Video podcasts are preferred over virtual experiments and computational problem solving
- ❑ Students expect high-quality modules
- ❑ Phase-I project allowed for establishing necessary production infrastructure
- ❑ 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.