Embedding computation with experimentation in the sophomore and upper-level Physics curriculum

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Embedding computation with experimentation in the sophomore and upper-level Physics curriculum

In the University of St. Thomas physics department, we have begun an ambitious, collaborative project to embed computation and experimentation in five required physics courses that span our sophomore and upper-level offerings. The laboratory for our sophomore Applications of Modern Physics course, which is a required course for all physics and electrical engineering majors, is being redeveloped to serve as an introduction to computer simulation. All of our students are now expected to be proficient in a common computational language—MATLAB—which can then be used as a tool in upper-level courses. We are embedding MATLAB in large and small ways throughout the curriculum, from simple tasks such as plotting functions, to sophisticated tasks such as simulating the dynamics of a complex system. We are also connecting the theory of idealized physical systems with real systems through the combination of computer simulations and validation experiments. Through continued exposure, we anticipate that our students will embrace computation as a useful tool in their arsenal. This paper describes our project, which involves five physics faculty and an advisor from the School of Engineering who has expertise in education.

Introduction

Most physics research these days involves the use of computers for data collection and analysis, simulations, symbolic manipulation, and numerical analysis. As the American Association of Physics Teacher's "Statement on Computational Physics" says, "Computational physics has become a third way of doing physics and complements traditional modes of theoretical and experimental physics." [1] Computation should be an important component in the physics undergraduate curriculum, and ideally it should merge seamlessly with the rest of the curriculum.

Throughout the past 15 years, the University of St. Thomas physics department has been implementing an integrated physics curriculum where students gain the theoretical, experimental, computational, and communication skills they will need to succeed in their careers. The computational work in our department began with an NSF-sponsored effort (DUE-0311432) to develop computational modules in several upper-division physics classes.[2] Our current efforts seek to strengthen the connection between a variety of physical systems and the theory and computational models that describe them: experiment grounds the theory while computation allows us to study more complex, less idealized systems. In this paper, we describe these curricular projects that use computation as a link between theory and experiment in our sophomore and upper-level courses. Our hope is that students will show a clear benefit from this continued and systematic exposure in a multitude of settings, both in their embrace of computation and in their ability to communicate results in an organized and professional manner.

We are currently developing curricula that embed computation and experimentation in five required[3] physics courses that span our sophomore and upper-level offerings: PHYS 225: Applications of Modern Physics, PHYS 341: Electricity and Magnetism, PHYS 331: Theoretical Mechanics, PHYS 347: Optics, and PHYS 431: Quantum Mechanics.

PHYS 225: Applications of Modern Physics

This sophomore-level course covers modern physics from a materials science perspective, building from the properties of single atoms to collections of atoms (quantum dots and other nano-scale systems), and then to solids, with applications interwoven throughout. The course has a separate laboratory that meets for 3.5 hours once a week. Time in the laboratory is used to reinforce concepts learned in class through the use of simulations and tutorials, while also introducing students to computational modeling using MATLAB. Descriptions of all laboratories developed for this course can be found in the course's curriculum development webpage.[4]

We have extended two tutorials adapted from materials from the University of Colorado-Boulder PhET[5] simulations to include a computational component along with short validation experiments:

> Laboratory: The Wave Equation
> *Conceptual goal:* Become comfortable with the mathematical formalism of differential equations with boundary conditions. Understand how applying boundary conditions leads to quantization.
> *Experimental goal:* Use the pattern of standing waves in a microwave oven to estimate the speed of light.
> *Computational goal:* Learn how to plot surfaces using MATLAB.

In the wave equation tutorial, students solve the wave equation for electromagnetic radiation inside a microwave oven and find that the boundary conditions lead to only certain allowed wavelengths (a first glimpse of quantization). The tutorial developed at UC-Boulder was extended to include visualization of the stationary waves in two dimensions by plotting in MATLAB. Students use paper moistened with a $CoCl_2$ solution to reveal the pattern of microwaves in an oven.[6] They then estimate the speed of light from the distance between nodes on the paper and the known operating frequency of the microwave.

> Laboratory: Lasers
> *Conceptual goal:* Develop a basic understanding of the relationship between energy levels in an atom and how lasers work.
> *Experimental goal:* Use of a spectrometer to record intensity vs. wavelength. Relate results to an energy level diagram.
> *Computational goal:* Learn how to open and read a data file using MATLAB; practice array manipulation and basic plotting.

Students discover the requirements for building a laser while following a tutorial and exploring the associated PhET[5] simulation. We have extended this laboratory by having students develop expected emission spectra for a He-Ne laser from energy level diagrams for helium and neon. Students are given NIST Atomic Spectra Database[7] files with a large number of energy levels for helium and neon along with relative intensities for transitions between levels. Students manipulate the data in MATLAB in order to find energy differences and compute the corresponding wavelengths of emitted photons. They then use the computed wavelengths along with relative intensities to plot the expected emission spectra. Students use spectrometers to record the spectra of the transversely emitted (non-lasing) light of a clear-case HeNe laser, and compare these results with their previously-calculated spectra.

PHYS 331: Theoretical Mechanics

Theoretical Mechanics is an upper level course focusing on the study of physical systems through the application of classical mechanics. During the semester, the ideas of Newton, Lagrange, and Hamilton are developed and applied to a wide spectrum of problems ranging from the motion of charged particles to coupled oscillators. Mathematical techniques are infused throughout the course; vector calculus, differential equations, matrix algebra, complex variables, and variational calculus all find their way into the discussion.

<u>Homework Module: Large Angle Pendulum Motion</u>
Conceptual goals: Use energy techniques to develop the equation of motion for a physical pendulum.
Experimental goal: Measure the period and compare with predictions from the numerical model.
Computational goals: Demonstrate the ability to numerically integrate differential equations using MUPAD.

The behavior of a physical pendulum swinging through large angles provides an excellent example where traditional analytical tools breakdown. Students quickly recognize that the system is not a simple harmonic oscillator. Predicting the period requires numerical integration and introduces students to the power of MUPAD, which is included in the Symbolic Math Toolbox add-on for MATLAB. The experimental system consists of a large metal pendulum supported by a ball bearing shaft. The large mass is necessary to reduce dampening by air resistance.[8]

<u>Homework Module: Catenary Curves</u>
Conceptual goals: Implement variational calculus techniques to model how the shape of a hanging chain depends on the chain density, length, and the separation of the supports.
Experimental goal: Verify that the model predicts the correct shape.
Computational goals: Develop a facility with MATLAB fitting tools by comparing the actual catenary shape with the predicted shape.

Variational calculus techniques are rather abstract and difficult for students to apply the first time they are introduced to the topic. Having a concrete example helps to remove some of the abstraction from the problem. Determining the overall shape of a catenary is a fairly standard problem in variational calculus; however, understanding how the shape depends on specific boundary conditions is a bit more difficult. To help guide their study, the students are given an expanded reference to the problem.[9] Because the catenary is stationary, it lends itself nicely to simple measurements demonstrating how its shape depends on chain length, separation, and mass. Using segments of ball-chain, different configurations can be rapidly set up and characterized.

Homework Module: Chain Falling From a Heap (g/3 -vs- g/2)
Conceptual goals: Use Lagrangian and Hamiltonian techniques to investigate the behavior of a falling chain.
Experimental goal: Experimentally resolve the conflicting theoretical results that arise from different starting assumptions about the system. *Computational goals:* Refine curve fitting skills in MATLAB.

Variable mass problems often have subtle effects that are easy to get wrong. A chain falling from a stationary heap is a classic variable mass problem that is frequently solved incorrectly. Students are introduced to the problem and develop models of the system dynamics. After grappling with the problem, they are presented with a paper[10] which leads them to a theoretical understanding of the system using Lagrangian and Hamiltonian techniques. After deciding on the proper approach, students test their theory by recording a video of a falling chain and extract the time-position data using video analysis software. The time series is fit using MATLAB to determine the acceleration of the chain.

Homework Module: Coupled Mechanical Oscillators
Conceptual goals: Use Lagrangian techniques to set up the differential equations describing a coupled mechanical oscillator. Solve the resulting eigenvalue problem and describe the normal modes for the system as well as the general behavior.
Experimental goal: Verify that the model predicts the expected behavior for a variety of initial conditions using actual mass-spring-pendulum systems
Computational goals: Develop linear algebra and plotting skills in MUPAD.

Modeling the behavior of coupled systems is a complicated topic where symbolic linear algebra tools are particularly useful. By solving the eigenvalue problem and plotting the expected system behavior for different initial conditions and then comparing the predicted behavior with an actual system, students solidify their conceptual understanding as they develop modeling skills.

PHYS 341: Electricity and Magnetism

The first half of a two-semester sequence, this junior/senior level course covers electro- and magneto-statics and Maxwell's equations, while the second semester covers wave propagation and applications such as antennas and transmission lines. This course does not have a lab component, and many students find the abstract material difficult to grasp. Since the course deals with fields that are invisible and remote from daily experience, the material is typically presented mathematically, and analytical methods are used to solve problems. However, only the simplest of cases can be solved analytically, and most real-world applications of electromagnetics use finite element methods to find numerical solutions. We believe that the use of experimental and computational elements in this course will improve student understanding of the material and provide them useful professional tools. Our goal in this class is to use MATLAB to perform calculations of electric potentials to introduce finite difference methods to the students. Coupled with in-class validation experiments, the calculations help students visualize the meaning of the mathematical formalisms used throughout the semester.

In-class Exercise: Electric Potential of Two-dimensional Systems
Conceptual goals: Understand how finite difference methods can be used to solve Laplace's equation to determine electric potentials. Visualize electric fields for non-trivial geometries, such as microstrip transmission lines.
Experimental goal: Use electrodes in a water tank to map the electric potential for two-dimensional systems.
Computational goal: Learn how to use finite difference methods in MATLAB.

Prior to this unit, students have learned to find the electric potential analytically for several simple geometries such as infinitely long concentric cylinders. However, these analytical approaches do not yield solutions for more complex geometries that lack symmetry. In this unit, students see through in-class demonstrations that potentials in a water tank can be used to map electric potentials and that these experimental results match analytical results calculated in class for a case where an analytical result is available (e.g., the electric field and potential in a coaxial cable). Although this method provides a way to measure potentials for more complex geometries, the approach is labor intensive and tedious.

We then introduce finite difference methods for solving Laplace's equations. Previously, this method was discussed in class, but the students did not have the opportunity to use the technique in homework assignments. Thus, we have developed a MATLAB assignment in which students use finite difference methods to find a potential, allowing them to test their understanding and practice this useful skill. In the case of a coaxial cable, the calculation is done in a one-dimensional or two-dimensional approach, and the results are compared to both experiment and theory for verification.

Once students are comfortable with their ability to model two-dimensional problems, we ask them to model a practical configuration like a microstrip transmission line that lacks the symmetry needed for analytical solution, but is commonly used in circuit boards. This geometry is also modeled via electrodes in a water tank so that students can validate their simulation results with experimental data.

PHYS 347: Optics

This junior/senior level course focuses on "physical" optics: wave theory, polarization, interference, diffraction, and light-matter interactions. The first half of the course's laboratory component deals with practical optical techniques, while the second half comprises a series of advanced, modern applications of those techniques. The laboratory is closely tied to lecture material, but missing from this course was a significant computational component that provides a more sophisticated link between theory and experiment. As a first step, we developed additions to the two-part laboratory unit on polarized light, in which students simulate and analyze optical systems using MATLAB. In the future, we will add similar modules to the interference and diffraction units.

Laboratory: Creation and Manipulation of Polarized Light (Part 1: Imaging)
Conceptual goals: Understand the nature of polarized light, how polarization changes upon reflection and transmission, and how insects use polarized light for navigation and communication.
Experimental goals: Learn how to operate CCD cameras in conjunction with linear polarizers. Quantify how various materials either polarize or depolarize scattered light.
Computational goals: Use MATLAB's Image Acquisition Toolbox to acquire images from CCD cameras. Learn basic image processing in MATLAB to create polarization maps of optical targets.

This first experiment in the polarized light lab introduces students to polarimetric imaging, a method that is widely used in science, engineering, and medicine. Using a CCD camera followed by a rotatable linear polarizer, they acquire two images of an optical target with the Image Acquisition Toolbox. The first image is taken through the polarizer when its axis is horizontal, and the second image uses a vertical polarization axis. Students process their images in MATLAB by taking the difference-over-sum of the two images to produce a map that quantifies how the target influences polarized light. Pixels on the map have values between zero and one, and they equal the scene's "degree of polarization." By applying an appropriate color palette to this map, students optimize their visual sensitivity to small changes in polarization. Optical targets include dielectrics, metals, diffusers, commercial optical films, objects buried in turbid media, butterfly wings, and scarab beetle elytra. In this laboratory, special emphasis is placed on its application to insect vision. Many insects are very sensitive to polarized light and use it to identify mates as well as navigate during migration. The polarization maps that students create are meant to approximate what insects might see. The experimental portion of this project was previously developed and was largely based on our publication in the *Physics Teacher*.[11]

Laboratory :Creation and Manipulation of Polarized Light (Part 2: Electro-optics)
Conceptual goals: Understand the nature of polarized light, how polarization changes upon reflection and transmission, and how it can be precisely manipulated and measured with modern instruments.
Experimental goals: Learn how to operate an electro-optic modulator and use it to control polarized light for a variety of polarimetry experiments.
Computational goals: Learn how to use various linear algebra, Fourier analysis, and plotting functions in MATLAB. Translate the matrix representation of polarized light into a simulation of an electro-optic modulator in order to understand experimental results and calibrate an optical system.

In this second experiment with polarized light, students use two types of electro-optic modulators—liquid crystal retarders and photoelastic modulators—to precisely quantify the polarization properties of targets such as stretched plastic, compressed gelatin, sugar-water solutions, commercial polarizing elements, calcite crystals, and so on. We have developed a computational component for this laboratory in which students translate the traditional matrix representations of polarized light into a versatile MATLAB simulation that accounts for all possible combinations of static and time-varying polarizing elements, including targets of interest. The program calculates output polarization states, plots intensity curves for reflected and/or transmitted light, and performs Fourier decompositions of those curves. When students later perform their experiments, they validate their program's predictions by analyzing signals displayed on oscilloscopes and lock-in amplifiers. Results from simple, nearly ideal optical targets initially build students' confidence in both the physics and the simulations. Not only does the MATLAB simulation give students deeper understanding of polarized light, it is essential for proper calibration of their optical systems. After calibration is complete, more complex optical targets reveal the true power of the simulation because some materials affect polarized light in complicated ways that are tough to analyze with only paper and pencil. Much of the theoretical and experimental groundwork for this module is highlighted in our *American Journal of Physics* publication.[12]

Physics 431: Quantum Mechanics

This one-semester course studies the fundamentals of quantum mechanics with mathematical rigor. Students are mostly seniors, though a few juniors typically take the class as well. Students in the class have all taken Modern Physics, and most have taken the other 300-level courses listed above. In that sense, Quantum Mechanics is a capstone course and can build on the knowledge and skills gained in the previous courses

We currently incorporate a computational component as a final project in the course, developed through the NSF grant for computation mentioned above (DUE-0311432). In this module, students calculate and plot several electron density functions for a hydrogen atom using the von Neumann accept/reject Monte-Carlo technique.[13] We have developed an additional computational project that builds explicitly on the two-week quantum dots lab that students perform in PHYS 225.

> <u>Homework Module: Modeling Quantum Dots as Infinite Spherical Wells</u>
> *Conceptual goal:* Understand the connection between quantum dots and the infinite spherical well model.
> *Experimental goal:* Revisit the quantum dot system and understand how different wavelengths of light are produced from dots of different radii.
> *Computational goals:* Use MATLAB to numerically model the infinite spherical well for the case that is appropriate for quantum dots. Compare the numerical results to the analytical solutions derived in class.

In PHYS 225, students spend one lab period measuring the spectral characteristics of several CdSe quantum dots, whose differing radii correspond to different emitted colors. They then analyze and plot their results with MATLAB. In the subsequent lab period, students are introduced to the three-dimensional infinite square well as an initial model for the quantum dots, and they use MATLAB to numerically solve the corresponding Schrödinger equation using a finite-difference approximation. However, since quantum dots are roughly spherical, it would be far more appropriate to model them using the infinite spherical well. In PHYS 431, we analytically calculate the lowest order ($l = 0$) wavefunctions and corresponding energies for the infinite spherical well. We have developed a computational exercise in which students use MATLAB to numerically determine the solutions to the infinite spherical well for several values of l using Numerov's method.[14] We anticipate that students will benefit from the additional exposure to numerical methods of solving differential equations, particularly in a system with which they are already familiar.

Impact and Assessment

This project improves five of the eight physics courses offered by our department beyond the introductory level. The curricula we have developed will give students continued exposure to computation and experimentation throughout their undergraduate years. Of particular importance, most curricula described in this paper can be included in traditional lecture-only courses, and the benefits of this work can be easily extended to other institutions.

The materials described in this project were developed over Summer 2012 and continue to be refined. During the 2012-13 academic year they are being phased into the classroom. We will assess results from this project by monitoring proficiency in MATLAB as students work through the physics courses involved. We are in the process of gathering this data and will report results at a future date. We expect to review and revise all materials in the summer of 2013, and will then post descriptions of the materials to the curriculum section of the UST Physics Department website (http://www.stthomas.edu/physics/research/Curriculum). We encourage readers to contact any of the authors if they are interested in trying the materials in their own courses. We expect to continue developing similar computational and experimental exercises in the coming years.

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