# Integrating computational activities into the upper-level Paradigms in Physics curriculum at Oregon State University

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(Received 14 September 2007; accepted 21 December 2007)

The Paradigms in Physics project at Oregon State University has reformed the entire upper-level physics curriculum. The reform has involved a rearrangement of content to better reflect the way physicists think about the field and the use of several new pedagogies that place responsibility for learning more firmly in the hands of the students. In particular, we employ a wide variety of computational examples and problems throughout the courses. Students use MAPLE, MATHEMATICA, JAVA, and other software packages to do calculations, visualizations, and simulations that develop their intuition and physical reasoning. These computational activities are indispensable to the success of the curriculum. © 2008 American Association of Physics Teachers. [DOI: 10.1119/1.2835052]

# I. INTRODUCTION

For practicing scientists and engineers, the computer has become a ubiquitous problem-solving tool. Unfortunately, the education students receive often does not represent this advance. Students use, and sometimes overuse, their calculators and are web-savvy computer users, but they do not use computers with the ease and regularity of practicing scientists, nor for the purposes that professionals do. We would be remiss if we did not use computers to the fullest extent possible to teach the advanced curriculum and to educate students to use the same problem solving tools and techniques used by physicists.

Computers are used in a variety of ways to teach science in general and physics in particular. Lectures have been enhanced with computer-based demonstrations<sup>1</sup> and computational simulations,<sup>2</sup> recitations have been augmented with computer-based tutorials,<sup>3</sup> and laboratories now routinely use computers for data acquisition and detection and for virtual experiments.<sup>2</sup> Such computer-based activities are a way to get students more actively engaged in their learning, which has been shown by physics education research (PER) to be critical to students' success.<sup>4</sup> Studies have shown that computer-based instruction can be as or more effective than traditional methods.<sup>5,6</sup> In some activities the computational aspects are largely hidden from the students, and the computer may be used primarily as a tool to deliver curricular content. Alternatively, students may be taught explicitly to use the computer in the same way as the developer of the activity.

There are a number of examples of curricula that have added separate computational physics courses to their programs.<sup>7</sup> The Matter & Interactions text is an example of a pedagogical strategy that integrates student-authored computational activities using VPYTHON as a central focus of the introductory physics sequence.<sup>8–10</sup>

At Oregon State University we have developed an upperlevel undergraduate curriculum designed to help students learn to work and think like professional physicists.<sup>11,12</sup> We deliberately embrace many approaches to incorporating computation into the curriculum, from using computers to deliver new curricular materials, to activities where students explore new physics by controlling parts of the code, to activities where the students have the opportunity to learn computational skills. In this paper, we describe our curriculum, the rationale and various approaches to integrating computational activities, and give concrete examples. We will illustrate how the use of computation impacts learning and ties into our pedagogical approach. Many of our activities are available on the web sites of the individual courses, <sup>13</sup> and on a developing portfolio site that also has instructor's guides, video clips of classroom practice, and other supporting materials.<sup>14</sup>

## **II. CURRICULUM**

The restructuring of our upper-level curriculum comprised changes in content, pedagogy, and delivery. The content was regrouped around particular model examples more akin to the way physicists structure their knowledge; we call the curriculum "Paradigms in Physics." The pedagogy incorporates results from PER on how to improve student learning, primarily with active engagement.<sup>15</sup> The delivery involves intensive three-week modules that students take in sequence.

An overview of the Paradigms curriculum is shown in Table I; more complete details are available in Refs. 11 and 12. The junior year consists of short case studies of paradigmatic physical situations that span two or more traditional subdisciplines of physics and are designed to help students gradually develop problem-solving skills. These junior-year courses are intensive courses that meet seven hours per week for three weeks and are taken serially. The senior year consists of more conventional three-hour-per-week, singlequarter lecture classes in the traditional subdisciplines of physics. Two or three such classes are taken in parallel. The format of these Capstone courses is more condensed than in the traditional curriculum because the content builds on the examples of the Paradigms courses in the junior year. The restructuring of the junior-year courses around common themes or paradigms exposes students to the four major subdisciplines in their junior year, especially quantum mechanics, and provides for a more gradual transition from the introductory lower level to the advanced upper level. The new curriculum provides a synthesis of ideas that was lacking in the previous curriculum. For example, the One-Dimensional Waves course discusses mechanical waves on a string, electrical waves in a coaxial cable, and quantum mechanical waves, and stresses the similarities and differences. In our traditional curriculum, students saw these topics in different courses over their junior and senior years, and few were able

Table I. Paradigms in Physics curriculum.

Paradigms courses (junior year)	Capstone courses (senior year)
Symmetries and Idealizations	Classical Mechanics
Static Vector Fields	Electromagnetism
Oscillations	Quantum Mechanics
Spin and Quantum Measurements	Mathematical Methods
One-Dimensional Waves	Thermal Physics
Central Forces	
Energy & Entropy	
Periodic Systems	
Rigid Bodies	
Reference Frames	

to synthesize their understanding to the extent that most students report being able to do in the new program.<sup>12</sup>

We have taken advantage of results from PER which indicate that students learn better when they are actively engaged in the learning process.<sup>15</sup> Our revised schedule has two-hour class sessions twice a week, which we use for extended group activities, computer activities, and laboratory experiments. This hands-on approach is one of the major successes of our new curriculum. We also employ a spiral approach to learning so that students are exposed to critical ideas several times throughout the curriculum and in different contexts, with an increasing level of sophistication each time. To deliver this new curriculum effectively, it is important that the faculty teaching the many courses work coherently. We meet regularly to discuss the curriculum and the cohort of students. However, we do not employ a strictly unified approach to the courses, and have found that the students benefit from the diversity of voices and viewpoints that they experience throughout their two years in the upper-level curriculum.

In parallel with the development of the Paradigms curriculum, our department has developed a new undergraduate degree program in computational physics.<sup>16</sup> This degree program is one of five such programs in the United States and is supported by five computational physics courses in the department, including an introductory course for first-year students. This introductory course serves as the gateway to the computational physics degree program and is required of all our physics majors. Such an early introduction provides a solid basis for the computational aspects of the Paradigms curriculum. In this introductory, one-quarter course the students learn how to use computers to solve simple physics problems. Although many of these students have not yet had college-level physics, their high school physics training and the additional material provided in the course is sufficient. During the course, students learn to use MAPLE and JAVA. The MAPLE part of the course focuses on using the computer as a powerful calculator, doing algebra and calculus, graphing and visualization, and understanding the limitations of computers for doing numerical calculations. The JAVA material is oriented toward procedural programming, numerical calculations, visualization, and floating point and integer format limitations.

# III. COMPUTATIONAL ACTIVITIES: RATIONALE AND IMPLEMENTATION

We use computation for in-class activities, classroom demonstrations, homework, laboratory projects, and senior theses. Each physics major is required to write a senior thesis, and because our department has a research program in computational physics, many of our students choose thesis projects with computational aspects. The use of computation in the curriculum supports our pedagogical approaches of active learning, spiral learning, and first studying examples before learning general theory. Continuous and frequent use of computation helps to breed familiarity and build student confidence. Our goal is for students to go beyond the notion of computer-as-calculator, and to embrace the full problemsolving power of graphics, fast data manipulation, simulation, and of course, calculation. In combination with effective active-engagement and group-learning activities, these computational activities make the computer in the physics classroom a meeting place where people gather to brainstorm.

#### A. Physical environment

Incorporating active engagement into the curriculum, particularly the computational aspects, required redesign of our classroom facilities. The tables are arranged so that three or four students can easily roll their chairs to form small groups, and each table has one computer that serves two to three students. The students' computers and the instructor's computer, whose display can be projected onto a large screen, have identical suites of software packages. The most important elements, after the choice of the software, are that students are able to work comfortably and effectively in groups and that the computers are well managed. An adjacent room for the laboratory component of the courses has identical computers and software suites for data acquisition and analysis. In addition to its important communitybuilding advantages, the room offers students full-time access to the computational facilities. This ready availability is very important if students are to embrace computation in all aspects of their work.

# **B.** Software tools

Unlike many other curricula with integrated computational aspects, ours is not a unified approach. We develop some of our own software, but more commonly adapt and adopt software for particular parts of our curriculum. Different software tools have different strengths, and providing students with a broad array of tools and viewpoints speeds their development. We have made extensive use of MAPLE worksheets for visualizations and calculations. We have recently also obtained site licenses for MATHEMATICA and MATLAB, and our students now use these interchangeably with MAPLE. These widely used problem-solving environments offer a broad range of functionality for visual, numerical, and algebraic approaches to understanding. We do not make extensive use of the algebraic power of these tools, choosing to focus on developing students' paper-and-pencil skills in these areas. We also use MAPLE for simulations, and several problem-specific simulation packages are a part of our curriculum.

Many students have made superficial use of spreadsheets, but have not typically been exposed to their powerful data analysis capabilities.<sup>17</sup> We use Excel to analyze data in several Paradigms courses that have integrated laboratory experiments. We are presently incorporating LabVIEW to acquire and analyze data in some of them. Students also use LabVIEW in a computer interfacing laboratory course. Our students are exposed to such a variety of computational environments that we have been able to use an advanced software package, WIEN2K,<sup>18</sup> in a senior level solid-state course where the students do a project on band structure calculations of crystal structures.

#### C. Pedagogical design

We have experimented with many types and styles of computational activities and have identified several key issues that are important in designing and evaluating effective activities. For each issue we pose questions about the activity whose answers provide insight into why the activity may or may not be successful. There is no one correct way to design an activity, but addressing these issues has helped us understand what works, what does not, and how to improve our activities. There are so many computational activities available online and elsewhere that it can be difficult to distinguish which are most effective. Active engagement activities (including computational ones) require significant class time investment, and should be used for the most important concepts, where mastery accelerates subsequent learning. We have found it useful to consider these following issues and questions when we are looking for new activities.

#### 1. Pedagogy

What is the pedagogical goal of the activity? Does the activity have the proper framework to give students the highest probability of achieving the goal as envisioned by the instructor? This issue is the most critical to ensure effective educational results. The instructor must have a clear goal for the activity and structure the activity in a way that students are guided toward that goal. It is easy to produce impressive graphics to illustrate physical phenomena, yet lose sight of how much understanding the students are actually taking away from the experience.

Integration of the computational activities with other activities, class discussion, and/or mini lectures may be needed to achieve the intended outcome. The group structure used in active engagement small groups (cynic, taskmaster, scribe) works well for these computer activities also.<sup>19,20</sup> The questions that we give to students to focus their attention on the computational experience are often open ended to encourage exploration; in this case, the faculty member must be very proactive to keep the activity on track. We have found it useful to write instructor guides that make it clear what the goals are, and how the activity is intended to guide the students toward that goal. These instructor guides are typically much more detailed than the student materials.

#### 2. Scope

Does the activity address one issue or many? Does it bring up unintended questions or issues? Can the activity be completed in a timely fashion? We favor short activities over long activities to keep the students focused on one or a few key issues. Early in our curriculum development we had some long activities that were not as effective as we had hoped, and we shortened them or divided them into smaller pieces, with much greater success. It is important to have instructor oversight, otherwise an activity loses focus, which results in frustrated students. Such oversight also helps identify questions or topics that the students encounter that the instructor did not intend.

#### 3. Control

Who controls the direction of the activity, the student or the instructor? Some activities are very directed and some are more open ended. We favor open-ended activities to encourage exploration, but take care to ensure that the point of the activity is clear to all and that most students can achieve the intended goal. We try to design activities with direction in the beginning stages, but with open-ended options. Another successful strategy is to have several almost-equivalent tracks within an activity—one for each group—which are then all discussed by the class as a whole. The faster students can then do more examples in class and remain engaged, while the slower students can take the remaining examples home to pursue at their own pace.<sup>21</sup>

## 4. Coding

How much of the coding is given to the students, and how much is hidden? In some cases, we hide the code so as not to obscure the physics, while at other times, the coding is included to build skills in that area. The Paradigms curriculum is not focused on coding (that skill is addressed in our upperlevel computational physics courses), but we strive to develop students' coding skills within the confines of the goals of the program. Highly complex code is hidden, as is code that is too long and does not contribute to the learning goals. We try to have students write very simple code, with the sophistication increasing as the junior year progresses. By the senior year, many students independently use the computer to produce useful graphics and calculations in assigned projects.

#### **IV. EXAMPLES**

The following examples of computational activities illustrate the principles and issues discussed in Sec. III. We have chosen examples that illustrate the use of simulations of experiments, that showcase the power of visualization, and that stress the importance of integrating other active engagement activities with the computational activities for effective pedagogy. Other examples from our curriculum can be found online.<sup>13,14</sup>

#### A. Simulation of Stern–Gerlach experiments

The rearrangement of content in our curriculum allows students to begin their exploration of quantum mechanics in the middle of the junior year. Our course on Spin and Quantum Measurement uses the simple two-level spin-1/2 system to introduce students to quantum mechanics. This approach is often considered too abstract, but we use a computer simulation of Stern-Gerlach experiments to make the problem concrete.<sup>22,7</sup> <sup>23</sup> Although it is generally preferable to do real experiments, time, money, and accessibility factors make computer simulations very attractive for giving students a tangible view of how nature works and developing their physical intuition. We have ported the original Stern-Gerlach simulation software<sup>22</sup> to JAVA to make it usable on multiple platforms and have added new features to increase its pedagogical utility. The new SPINS software can run as a stand-



Fig. 1. Components of the SPINS software that simulates the Stern–Gerlach experiment. The oven is the source of particles in spin quantum states, either random or pure states. The analyzer measures or separates particles according to their spin projection along the indicated axis. The magnet causes spin precession around the indicated axis. The counter detects particles.

alone application or as an applet within a web browser and is available online.<sup>23</sup> The software has been adopted by several institutions and has been incorporated into the Open Source Physics framework to allow for additional instructor control.<sup>24</sup>

The SPINS software is a full-featured, menu-driven application that allows students to simulate successive Stern-Gerlach measurements and explore incompatible observables, eigenstate expansions, interference, and quantum dynamics. A SPINS simulation consists of a few simple components (shown in Fig. 1) which are controlled with menu and/or mouse commands. The students do no coding in this simulation, but are in full control of building experiments from the available components and running them to obtain data. Figure 2 shows a variety of possible experiments, including spin projection measurement [Fig. 2(a)], successive spin measurement [Fig. 2(b)], and an interferometer [Fig. 2(c)]. Students learn that a beam prepared in a pure "z-up" state by passing it through a z analyzer will have an x-up component after analysis by an x analyzer, and has a z-down component after a subsequent z analyzer-all highly non-



Fig. 2. Examples of experiments using the SPINS simulation software. (a) Measurement of the spin projection along the z axis. (b) Successive measurements of spin projection. (c) An interferometer with spin-1/2 particles. (d) Analysis of spin precession of spin-1 particles in a uniform magnetic field.

classical results. One of the central activities of the course calls for students to use spin projection measurements to determine unknown quantum states that are coded into the program. This approach is similar to a real experiment, but the opposite approach is taken in traditional curricula where students are asked to predict the results of an experiment from an initial known quantum state. The mathematics of spin-1/2 matrices is easy—sometimes too simple—so complexity and depth can be introduced in the form of spin-1 experiments [see, for example, Fig. 2(d)].

The use of the SPINS software enables us to take this unique approach to the introduction of quantum mechanics. The beauty of the simulation is that students steeped in classical physics perform the ultimate quantum experiment and learn the most fascinating and counterintuitive aspects of quantum mechanics at the earliest stage. In this instance, the computation facilitates an early introduction to quantum mechanics which is mathematically simple and intellectually stimulating, and one that gets to the heart of quantum measurement.

#### B. Visualization of quantum mechanical states

Visualizations of physical phenomena and mathematical relations are an important part of higher-level physics and are becoming more so as visualizations become more commonplace. Zollman, Rebello, and Hogg recount a long history of using visualization to teach quantum mechanics.<sup>25</sup> Recent GRE exams also demonstrate an increasing reliance on visual thinking.<sup>26</sup> Students typically have a good understanding of classical mechanics based on their everyday experiences, but as they venture into electromagnetism, statistical physics, and quantum mechanics, they must rely less on their mechanical intuition, and more on their ability for abstract reasoning. Visualization is key to developing this ability; a graph or animation triggers connections with what they already know more easily than equations or words.

Student difficulties and misconceptions regarding quantum mechanics are well documented and visualizations are widely accepted as useful in addressing these problems.<sup>27–29</sup> The power of computer calculations also opens up a broad range of new problems that can enhance understanding. The asymmetric quantum well is an example that has received recent attention as a system that provides insight into some basic features of quantum wave functions.

We have placed particular emphasis on using computation to aid student understanding of wave functions and probability densities. The representation of three-dimensional densities is especially problematic, and we take the traditional building-block approach by proceeding from one to two to three dimensions. We first study the quantum mechanics of a particle confined to a ring and then to a sphere, before studying a particle confined in a central three-dimensional potential. This approach also develops the ideas of angular momentum eigenstates. The plots in Fig. 3 show multiple graphical representations of the probability density of a particle confined to a one-dimensional ring in a superposition state. Students work with a short MAPLE worksheet to make these plots for a variety of states. The standard plot in Fig. 3(a) conveys the idea of a varying density, but the single dimension fails to make it clear that the left and right ends are connected and must have the same density. This connection becomes obvious to the students when they plot the density using color as a parameter along a ring as shown in



Fig. 3. Probability distribution of a particle in a superposition of angular momentum states confined to a ring represented by (a) height of a curve, (b) shading around the ring, (c) shading and height above the ring. The animation is available online (see Ref. 33).

Fig. 3(b). The plot in Fig. 3(c) combines the ideas of the previous two plots by using both the vertical scale and color to represent the density. This representation is redundant, but it provides an extra level of sophistication that helps students think about how they might represent several quantities in a single graph in an analogous fashion. Being able to use all three representations and understand their equivalence is a landmark on the students' path to becoming professional physicists.

This example is illustrative of the emphasis we place on the use of multiple representations. Physicists routinely use pictorial, graphical, algebraic, and verbal representations of physical quantities and often are not conscious of switching from one to another. For example, a student's question about an equation, say  $x^2 + y^2 = r^2$ , almost always prompts an instructor to respond with a graph, a circle in this case. Students' facility to switch between representations is much more limited, and they need specific training to develop this skill.<sup>32</sup> We have found that consistent and frequent use of multiple representations can be effective in guiding students' development, and computation integrated with other activities that encourage students to really engage with the visualization is particularly helpful with the graphical aspect, especially with different types of graphs and with connecting algebra to graphs.

At the conclusion of the particle-on-a-ring example students are asked to animate the probability density plots as a function of time to address the important issues associated with stationary states and time-dependent states. The animation of Fig. 3 is available online.<sup>33</sup> We have found that when students animate a plot to show time or other parameter dependence, new understanding follows. We use MAPLE and MATHEMATICA extensively to create animations of waves, fields, orbits, and quantum states, for example.

For a particle confined to a sphere, the eigenstates are the spherical harmonics for which there are many common graphical representations. Rather than focus on a preferred method, we present multiple representations and have students work to understand each. The polar plot shown in Fig. 4(a) is the traditional way of representing spherical harmonics. As such, it is simple for physicists to interpret and use, but is difficult for students when they first encounter it. The polar plot is not analogous to the rectangular plot of Fig. 3(a), and it is often not explained that the radial distance in Fig. 4(a) represents the probability density (or wave function, if not squared) in that angular direction. This angular distribution is often confused with the three-dimensional distribution. To connect this example to the ring example, we use the plot of Fig. 4(b), where the density is represented by



Fig. 4. Probability distribution of a particle confined to a sphere represented by a (a) polar plot, (b) shading on a sphere, (c) shading and polar plot. This example is the p, eigenstate.

color on the sphere. This representation is not common, but we have found it helpful for students. The combination of the two representations is shown in Fig. 4(c).

When we consider the full three-dimensional hydrogen atom problem, the choice of representation becomes especially problematic. There is not an extra dimension to use for displaying the probability density as in the ring and sphere problems. It is common to show a two-dimensional slice of the full three-dimensional distribution, and then use color or height as the probability density. We have found it useful to use the computer to show many slices in an animation with each frame being a different slice. Figure 5 shows single frames of two such animations with slices perpendicular to the *x* and *z* axes, respectively. The animations allow students to explore the extent of the solutions in more depth than traditional representations. This exploration is especially im-



Fig. 5. Probability density of an electron in the  $2p_z$  state of the hydrogen atom represented by shading a planar slice at a given value of (a) x and (b) z. Animations vary the x or z positions to illustrate the complete three-dimensional charge density (see Ref. 33).



Fig. 6. Two representations of particle motion in a central potential. (a) The solid line shows the effective potential energy for a particle with angular momentum and the dashed line shows the total energy. (b) The solid line shows the elliptical orbit and the circles show the particle position at equal time intervals.

portant in order to understand that there are shell structures of many of the distributions that are not always evident.

# C. Integration of activities on effective potentials and classical orbits

A valuable sequence of activities arises in our discussion of classical orbits and illustrates how computation must be integrated with other activities to achieve the pedagogical goal. We would like our students to understand how the shape of an orbit depends on various parameters such as reduced mass and the z component of angular momentum, and how this shape can be predicted by an effective-potential diagram. We start with a fairly traditional mini lecture that introduces the effective potential. Students are then asked to explore in small groups how the shape of the effective potential diagram in Fig. 6(a) depends on the various parameters. In this case it is valuable to use a (prewritten) worksheet in a computer algebra package such as MAPLE or MATHEMATICA, rather than a prettier, but "black box" simulation such as a JAVA applet, so that students can actually see the mathematical expressions that are being plotted. Next, the students perform an activity that integrates the equations of motion and plots both the effective potential and the corresponding orbits for various values of the parameters, as in Fig. 6(b). Here, a black box simulation is fine; the details of the numerical solution of the differential equations are a significant enough departure from the main flow of this course that we choose not to address them. Originally, we had a single, long MAPLE worksheet which first showed the effective potential, and then showed the orbit for any set of physical parameters. However, without intervention, many students did not immediately see how these two different graphical representations were related to each other. We now address this issue by interposing the following kinesthetic activity. A single student, carefully chosen to be someone who will be comfortable with being put on the spot, is asked to come to the front of the room to act out the part of the orbiting planet while the teacher plays the part of the Sun.

Most students, on their first attempt, will walk around the teacher—after all, this is what planets do. When directed to refer to the effective potential diagram, with its classical turning points, most students, on their second attempt, will move toward and away from the teacher in a straight line, with an embarrassed laugh for the obvious absurdity of their motion—this is not what planets do! It takes a significant class discussion to bring out the role of the angular momentum in reconciling the two representations of the motion. After this experience, most students are more effective at using the simulation to explore the shape of the orbits in depth. For example, a common question that arises is how we know where the minimum and maximum radii of the orbit occur.

#### V. SUMMARY

Paradigms in Physics is a new upper-level curriculum that tightly integrates research-based instruction and computation into the curriculum. Computational and other activeengagement activities help deliver a curriculum that unifies the traditional subdisciplines and provides a more gradual transition to the advanced course content. The computational components are designed to encourage students to use the vast simulation, visualization, calculational, and data analysis capabilities of computers to approach physics problem solving as would experienced physicists.

## ACKNOWLEDGMENTS

The authors acknowledge fruitful discussions with the entire Paradigms group and with Rubin Landau. We thank Kerry Browne, Tevian Dray, Jason Janesky, Lichun Jia, and Shannon Mayer for their contributions to authorship of the computational activities referred to in this article. This material is based on work supported by the National Science Foundation under Grant Nos. 9653250, 0231194, and 0618877.

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