Explorations in Integrated Science

By Joceline C. Lega, Sanlyn Buxner, Benjamin Blonder, and Florence Tama

We describe a third-year undergraduate course that focuses on multiscale modeling and protein folding and has as its primary goal the encouragement of students to integrate thinking across and beyond disciplinary boundaries. The ability to perform innovative and successful research work in STEM (science, technology, engineering, and mathematics) fields is often dependent on being aware of the multiple connections between the sciences, but how to develop such an integrated perspective is rarely taught in college classes. Designed for STEM majors, the course combines laboratory sessions and lectures, assessed through student journals and oral presentations. We report on some of the activities we developed for this course and on the associated outcomes. A syllabus, an assessment, and interview questions, as well as examples of student responses, are provided as supplementary materials (available at www.nsta.org/college/connections.aspx). The course topics discussed in this article include an analogy between desiccated corn starch and basaltic columns, a discussion of the size of trees, diffusion at the microscopic and macroscopic levels, and computational aspects of protein folding. Teaching materials, including handouts, experimental methods, and MATLAB codes, as well as student journals, are available from the course website.

College teaching is often highly compartmentalized, with disciplines divided into subjects taught by specific departments and by professors who specialize in particular areas. Although giving access to experts is essential to a good education, this compartmentalization may prevent students from developing an understanding of science that has both depth and breadth. The ability to use ideas from one discipline to understand a phenomenon in another, and the development of critical-thinking skills that can be applied broadly and in unfamiliar contexts, are essential components of the training of future scientists and nonscientists (Association of American Medical Colleges, 2009; Bialek & Botstein, 2004; Handelsman et al., 2004; Labov, Reid, & Yashamoto, 2010; Wood & Gentile, 2009). Integrated science is an approach that emphasizes conceptual aspects common to STEM (science, technology, engineering, and mathematics) fields and is a natural practice of STEM researchers. It is, however, not typically taught to undergraduates because of the compartmentalization discussed above.

This article describes a one-semester, junior-level course entitled Explorations in Integrated Science, which was developed over a period of 3 years with support from the Course, Curriculum, and Laboratory Improvement program of the National Science Foundation. The version presented here was taught in Fall 2010 by four faculty members (two holding appointments in Chemistry and Biochemistry, one in Mathematics, and one in Physics) and a graduate student (in Ecology and Evolutionary Biology). It was cross-listed between Molecular and Cellular Biology, Mathematics, and Physics; prerequisites were two semesters of calculus and satisfaction of a midcareer writing assessment requirement. Particular emphasis was placed on incorporating mathematical modeling and practices into the teaching. Examples that illustrate the integration of physics, chemistry, and biology may be found in the literature (Van Engelen, Suljak, Hall, & Holmes, 2007; Van Hecke, Karukstis, Haskell, McFadden, & Wettack, 2002; Purvis-Roberts et al., 2009). The course was completed by 11 undergraduate students majoring in either science or mathematics. Although the development of this course required a rather high instructor/student ratio, we believe that the teaching materials available online make it possible for two instructors (with respective expertise in applied mathematics/physics and biochemistry) to team-teach a regular offering of this course.

Course contents

The course met 3 hours per day, 2 days a week, for 15 weeks. The syllabus is provided as supplementary material (available at www.nsta.org/college/connections.aspx); the curriculum consisted of a 10-week module on multiscale modeling and biological motion and a 4-week module on protein folding. These topics were chosen as models of current research areas that integrate science and mathematics. Each module mixed formal lectures with hands-on activities designed to encourage students to formulate their own ideas, experiment, and start thinking beyond disciplinary boundaries. Activities were performed in small groups and based on articles published in the scientific research literature (available from the course website), thereby exposing students to the contents and structure of research reports.

Three-day unit on corn starch and lava flows

This 3-day unit, developed and taught by Joceline Lega (Mathematics) and Koen Visscher (Physics), was spread over multiple weeks and followed a discussion of pattern formation in nature. It was based on the analogy (Müller, 1998) between the cooling of lava flows leading to the formation of basalt columns and the desiccation process of corn starch: Water in the latter plays the role of temperature in the former, the two systems being modeled by similar partial differential equations, although with parameters that differ in significance and orders of magnitude. Its purpose was to encourage students to think "beyond space and time scales" (centimeters in corn starch correspond to meters in basalt columns, with "drying" front speeds that change by an order of magnitude), as well as "across disciplines," because a simple classroom experiment could be used to model the formation of geological structures.

We asked groups of three to four students to prepare a mixture made of a two-thirds volume of corn starch and one-third volume of distilled water in a crystallization dish and to let it dry under a lamp for about a week. The apparatus, including a time-lapse camera that was used to record the surface of the dish, was left in the classroom for the duration of the entire experiment. Students could check on the progress of the drying front as they came to class. As the corn starch dries from the top, first-generation cracks that meet at roughly 90 degrees appear together with an irregular network of second-generation cracks. As the drying front propagates toward the bottom of the crystallization dish, the cracks organize themselves into a regular polygonal structure, leading to vertical columns of increasing cross-section size. After a week, the dried corn starch can be removed from the dish to observe the columns that formed during the process. A picture of the result is shown in Figure 1. We shared MATLAB code to create videos from the time-lapse camera images and provided enough information for students to modify the code for this and other experiments.

We then repeated the experiment under different conditions. This way, we successfully encouraged students to make observations, build a conceptual framework to understand what was happening, make hypotheses, and test them through experimentation. For instance, they were free to change the size of the dish, the way they prepared the mixture, and the initial proportions of corn starch and water. Without prodding from the instructors, one group decided to gather information on "best practices" from the other groups and tried to perfect the experiment. One student had noticed that the first big crack never appeared in the middle of the dish and hypothesized it must always be closer to the light source. The latter could not be placed right above the dish because it would have been in the way of the camera. This student's group marked the side of the dish closest to the light, and they redid the experiment to confirm their hypothesis. The best-practice group then decided to use two symmetrically placed light sources and was able to observe a first generation crack that was then roughly in the middle of the dish.

FIGURE 1

Dried corn starch.

Two-day unit on the scaling of tree sizes

This unit was developed and taught by Benjamin Blonder (Ecology and Evolutionary Biology) to illustrate the use of mathematical methods in ecological and environmental sciences. It addressed the following question: How wide must a tree be to grow to a given height, and why? Student interest was generated by estimating how much carbon is stored in forests and making a link to climate change. In the classroom, the instructor spent an hour at the blackboard working through two competing theories: compressive failure (the risk of a tree of radius r and height h being crushed by its own weight) and elastic buckling (the risk of bending and suddenly collapsing, as with a drinking straw). Students could thus see how physical concepts translated into mathematical models, leading to a correct but uninformative maximum tree height of 5,739 meters in the first case and to a scaling relationship $h \propto r^{2/3}$ in the second. Details of the two models and corresponding estimates are given in a handout available on the course website.

Students were provided with measuring tapes and clinometers and spent the remainder of Day 1 in small groups measuring the radius and height of campus trees. Clinometers, which are devices for measuring tree heights, can either be purchased or easily made from paper and straws (see Project WILD; www.projectwild.org) or, in our case, from goniometers weighed by clamps. This section was very popular because students were able to learn and immediately apply forestry surveying techniques to a familiar environment and also were given the chance to perform a hands-on inquiry outside of the classroom. Instructors circulated around the campus with students to help with methods, but no significant management was required—students were very engaged in the data collection process.

On Day 2, we pooled all the small groups' data into a large communal spreadsheet. We then provided a short blackboard introduction to regression models in MATLAB and gave students example code that enabled them to analyze their data and test the second model for tree diameter and tree height. We also provided students a data file containing the diameter and height of hundreds of large trees across the United States. We asked each small group to compare and contrast both data sets. The entire class gathered at the end of the day for a guided discussion of their results and of practical issues pertaining to forest ecology.

Six-day unit on diffusion

The main objective of this unit, developed and taught by Joceline Lega (Mathematics) and Koen Visscher (Physics), was to help students realize that diffusive processes are associated with random walks at the microscopic level and that different types of random walks lead to different forms of diffusion at the macroscopic level. Beyond emphasizing the link between microscopic and macroscopic considerations, our goal was to illustrate how processes that typically occur at different scales, such as heat transfer and the motion of animals, are unified by this approach.

We began with a simulation of Brownian motion (http://www.aip.org/history/einstein/brownian.htm), showing the trajectory that a "big" particle follows as it is "pushed around" by a large number of smaller particles. We then introduced the simplest random walk, in which a walker moves on a straight line, taking steps either to the left or to the right, with equal probability. We used MATLAB to simulate the process and estimate the distance d from the origin after N steps. Once students realized that a large number of random walks as well as averages needed to be taken to establish the square root law $<d> \propto \sqrt{N}$, where $<d>$ represents the average of d over multiple experiments, they also appreciated how easy it is to use computers to explore random processes. We were surprised to see that most students identified the word *random* with a process involving uniformly distributed events, and we were able to correct this misconception by discussing probability distribution functions.

Still using MATLAB, we moved to random walks in two dimensions and introduced a bootstrapping method to establish the square root law in situations, like experiments, where it is not feasible to assemble large data sets. Students then went to the lab, recorded the Brownian motion of micron-size beads in a fluid under the microscope, used tracking software to computerize the trajectories, and then used the above method to estimate the relationship between $<d>$ and N. Most groups had reasonable results, one had excellent ones, and one found a linear relationship between $<d>$ and N. They concluded that there must have been a leak in their apparatus, leading to advection of the beads in the fluid.

Students were further introduced to the idea that bacteria swimming in a fluid also perform a random walk and that their motion can therefore be described as a (possibly biased) diffusive process at the macroscopic level. Although we did not have the time to discuss subdiffusion and superdiffusion in class, the course website (http://math.arizona.edu/~lega/303/) provides links to articles of general scientific interest on these ideas and on how they can be applied to the movement of foraging animals.

A second part of the module consisted of looking at the diffusion of temperature in a metallic rod, inspired by an article on how physicists grappled with the concept of heat in the 18th and 19th centuries (Narasimhan, 2010). We used beeswax to coat metallic rods (bought in a hardware store) of various types and cross sections (square or circular and of different sizes). Each rod was then held with two clamps over a long piece of aluminum foil, and a candle was placed just below the rod, near its middle point. The diffusion of heat along the rod was easy to visualize, because the wax would start melting when the temperature of the rod reached its melting point (see Figure 2). Students were encouraged to redo the experiment with different types of rods, compare the results, and propose explanations for the changes they observed. Videos taken by the students

FIGURE 2

Diffusion of heat in a metallic rod, from http://www.youtube.com/watch?v=LPT_TrbEOrM.

are available online (see, for instance, the YouTube video at http://www.youtube.com/watch?v=LPT_TrbEOrM). The link between this activity and the random walk discussion was provided by a lecture on the derivation of the heat equation.

Four-day unit on protein folding

This unit, developed and taught by Florence Tama (Chemistry and Biochemistry), followed a 4-day introduction to protein folding via the game foldit (http://fold.it/). Its purpose was to present computational aspects of protein folding, with emphasis on how computer science, physics, and chemistry come together to solve a problem relevant to biology. We used a mixture of lectures (atomic interactions in protein structure, molecular dynamics (MD) simulations) and computer laboratory sessions. The former were given in the first hour of each class period to provide necessary background to all students. The rest of the class was dedicated to guided computer tutorials designed to reinforce the concepts introduced in the lectures and emphasize the interdisciplinary nature of biochemistry.

Day 1 concentrated on protein structure and on principles of chemistry that pertain to structure stability. To illustrate these concepts, we visualized the protein Aquaporin and identified some of the chemical/physical interactions that stabilize its tertiary structure. For example, students were asked to look for positions of hydrophobic and hydrophilic residues, hydrogen bonds, and electrostatic interactions. On Day 2, we introduced computer models and algorithms used in MD simulations to sample protein conformational space. Building on the notions of stability introduced on Day 1, we started with the following questions: What would you need to simulate a protein, and how? Our goal was to promote a discussion that would help students identify key ingredients of MD simulations. Students with a strong biology background typically focused on atomic interactions, whereas students with a more physical/mathematical background proposed equations (e.g., Newton's equation) and algorithms that could be used for the simulation.

In the computer lab, students analyzed simulated data sets showing the folding of a small peptide. After visualizing the folding trajectory, students were asked to identify atomic details that appeared to be important for correct folding, including hydrogen bonds and angles. The folded structure was compared with a NMR structure and questions regarding the accuracy of the prediction led to a discussion of the advantages and limitations of MD simulations.

Assessment and evaluation

The overall course goals were to train students to make connections between different disciplines in mathematics and science and to apply knowledge from one topic/discipline to another. Course assessments included surveys, online journals, in-class discussions and presentations, postmodule reports, and student interviews, as described next.

Surveys

Students' understandings of the nature of science were assessed pre- and postcourse by an external evaluator, using the Views of Nature of Science instrument (Lederman, Abd-El-Khalick, Bell, & Schwartz, 2002). Questions as well as examples of responses are provided as supplementary materials (available at www.nsta.org/college/connections.aspx). The course does not appear to have led to an overall shift in the students' views of science (laws vs. theories, tentative and empirical aspects of science, use of creativity and imagination in science), although one student included a reference to the interdisciplinary nature of science in the postsurvey: "Science is the process of thinking and the methods of solving the questions that we face everyday whether it be in science, math, physics or just in life in general."

Journals

We used Google Drive for online journaling, because it made it possible for all four instructors and students to view entries throughout the semester and give feedback. This format also facilitated dynamic journals in which students could directly link to resources, upload images and videos, and easily receive feedback on their work. In addition to writing up activities, students were asked to reflect on how each topic was related to integrated science. This was done through a common assessment, which included questions listed in Table 1. Student journals (examples may be found at https://sites.google.com/a/email.arizona.edu/is303lbk/ and https://sites.google.com/a/email.arizona.edu/is303njdowdy/home/journal) were graded by the instructors as part of the course assessments and also scored by the external eval-

TABLE 1

Common assessment questions.

Question 1	List the disciplines associated with this topic.
Question 2	How would your understanding of the topic have been affected if one of the disciplines mentioned above had not been used in the discussion?
Question 3	Given your current understanding of this topic, what additional scientific discipline could further enrich your understanding of this topic? Explain.

TABLE 2

Scoring rubric.

Score	Description
0	No indication of interdisciplinary thinking
1	Only listing the disciplines involved in a problem/topic with no explanation
2	Either giving a surface explanation showing the underlying relationship between disciplines or a discussion of how multiple disciplines helped students understand a topic/problem
3	A deeper explanation showing the underlying relationship between mathematics and the sciences that was not described during class and showed students applying their understanding to new situations

uator on the basis of the quality of ideas expressed for each of the 12 course topics according to the rubric described in Table 2. A large number of instances of ideas rated "3" indicated a better appreciation for integrated science and correlated positively with higher grades in the class. Instructions on how to complete the journals and other written assignments were left purposely vague to encourage student initiative and creativity. As a consequence, some students reported they would have liked more explicit directions and guidance. Journal scores related to interdisciplinary thinking ranged from 1 to 28 out of a possible total score of 36, with an average score of 13 and mode score of 12. Two students had scores over 20 and consistently demonstrated their understanding of interdisciplinary thinking in their journal entries.

In-class discussions, presentations, and postcourse interviews

Overall, in-class discussions were often animated and creative, and student presentations were of high quality. Most students were able to articulate connections across various disciplines. Postcourse interviews revealed students' appreciation for the insight gained from the course to help them understand the importance of mathematics in scientific investigations and the connections between disciplines, as illustrated in the following student quote:

> What I got from the class, is that a lot of the ways that these are integrated is in the mathematical tools that can be applied to each of them. And I think of math as sort of logic statistics and not as algebra and specific equations. But the way that mathematicians think about problems is useful for a biologist and a chemist and all of that. And this course helped me see that more.

Interview questions and other examples of student responses are included as supplementary material (available at www.nsta.org/college/connections.aspx). Students who did not make integrated science connections had lower grades and journal scores. Fewer students mentioned problem solving in an integrated science context during postcourse interviews. Half struggled demonstrating an appreciation for the role of computers in understanding protein folding beyond a surface descriptive response (e.g., computers help us see proteins).

Conclusion

All of the units described in this article are stand-alone ones, and we hope readers will consider incorporating some of them in their own courses. Materials, including software codes, are available online at http://math.arizona.edu/~lega/303/. Our experience shows that challenges presented by the one-semester time frame and the wide range of student backgrounds can be alleviated by providing a variety of units that mix lectures and inquiry-based activities. For future implementations, more time should be devoted to overviews of the primary literature and to in-depth discussions of mathematical models and data analysis. Examples of successful journals should also be provided to the students and discussed in class. ■

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