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Implementation of a Course in Computational Modeling of Biological Systems in an Undergraduate Engineering Program*

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In this work we present the implementation of a course titled Computational Modeling in Biological Systems that integrates three broad topics of programming, numerical methods, and their application to biological systems. The course was offered in a lab setting with significant components of active learning focused on integrating the key principles of behaviorism, cognitive and constructivist theories of learning. The course was offered to two sections, one of which had a mandatory attendance policy. Student learning was measured using weekly lab assignments, a midterm exam and a comprehensive final exam. It was found that the section with mandatory attendance policy fared much better in the exams, meeting majority of the learning outcomes. This is attributed to the fact that there was more participation from this cohort in the classroom session where: (1) the instructor routinely set the context and defined the targeted learning outcomes, (2) conducted the active learning sessions to enhance the students' cognitive learning and (3) focused on defining meaningful contexts for applying the concepts to real-world biotechnology problems, encouraging collaboration and thoughtful reflection, thereby imbibing the constructivist principles of learning.

Keywords: biotechnology; computational modeling; numerical methods

1. Introduction

Biotechnology is a fairly broad field that deals with the use of living systems to manipulate natural processes for developing new products or systems. Thus, it can be viewed as an amalgamation of science and technology that can have a critical impact in several sectors of our society such as energy sources, food, health and environment. With an increasing demand for qualified professionals in these sectors, there is a growing demand from students to learn and master the foundational principles of this discipline. More precisely, students are keen to master the biological aspects as well as the engineering techniques that can be combined to design and develop new living systems.

One of the important aspects of a biotechnology degree is computational modeling. Computational modeling can be a very crucial tool that can enable the biotechnologist to engineer new and novel solutions. For instance, the expert can use modeling techniques to develop nanoscale views of biomolecules and devices not available through experimental imaging methods [1]. Another application is to used engineering approaches to increase the metabolic fluxes to describe a microorganism's phenotype [2]. Genome-scale metabolic models are used to understand and test hypotheses about these complex networks [2]. Understanding the significance of computational and mathematical modeling for a biotechnology program, at the School of Engineering Practice and Technology, we have introduced a course titled *Computational Modeling in Biological Systems* which is aimed at interweaving the discipline specific skills with mathematical and computational techniques, numerical methods in particular. To this end, an attempt has been made to combine three broad topics of programming language, numerical methods, and biological systems, as part of a single course. The main motivation behind combining the three topics, each of which is a course in itself, into a single course is to minimize the number of courses, keeping in mind the constraints on the number of courses that we can introduce into the overall curriculum in an undergraduate program at our university. From the pedagogical point of view, the combination of science and technology into a single course can be quite overwhelming and challenging for the students. Hence, it is critical to adopt appropriate pedagogical approaches in introducing the various concepts of the course.

A literature review of the possible choices of pedagogical techniques that can be employed for

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this course brings up several options: problem based learning [3–10], small group and co-operative learning [11–16], active learning [17–26], undergraduate research-based learning [27], challenge-based learning [28] and inquiry-based learning [8, 29, 30]. These different techniques of delivering the concepts to the students is a result of pedagogical research on a variety of subjects in a variety of classroom settings and demographics. It is clear that the optimal pedagogical style for a course depends upon the content of the course as well as the program and audience taking the course.

In this work, in a preliminary attempt, we have employed an active learning approach, to teach the concepts of biotechnology in a lab setting. The choice of this pedagogical approach is in line with our school's expertise and experience in this learning environment that has provided rich dividends in the other courses. In delivering the concepts to the students, the instructor defines the targeted learning outcomes and the activities the students will be undertaking during the classroom sessions as well as outside the classroom sessions. The active learning strategy inside the classroom is primarily aimed at enhancing the cognitive learning of the students. In these activities the students are strongly encouraged to interact with their peers as well as the instructor in solving problems that are in the realm of biotechnology. By engaging with their peers to discuss the problems and solutions to propose meaningful solutions, and participating in thoughtful reflections, the students are expected to be able to adapt the cognitive structure in their minds to a physical meaning [31–33].

The rest of this study is structured as follows: Section 2 describes the materials and methods employed in this study. This includes details of the course design as well as the procedure followed to deliver the concepts to the students. Section 3 presents the outcome of the assessments of student learning and a discussion surrounding the learning mechanism. The findings are summarized and pertinent conclusions are drawn in Section 4.

2. Materials and Methods

The course titled *Computational Modeling in Biological Systems* was developed for a third year undergraduate program in Biotechnology. The course has been offered in two terms with a total enrollment of 36 students in the first section and 31 students in the second section. To understand the impact of the course delivery methodology on student learning, periodic assessments were made. The details of the course content, the pedagogical methodology applied and the outcomes are described in detail in the ensuing sections.

2.1 Course Design

As mentioned earlier, course mainly focuses on three broad topics of programming language, numerical methods, and biological systems. Specifically, the objective of the course was to learn and apply computational approaches to study biological systems.

The key learning outcomes that were expected out of this course are:

1. Apply fundamentals of Java programming such as variables, decisions structure and loops for solving application problems.
2. Construct and use java methods for solving application problems.
3. Declare, initialize, and manipulate one-dimensional and two-dimensional arrays.
4. Solve for the zero of a non-linear algebraic function using numerical methods. Develop Java routines for these methods.
5. Identify classes, objects, members of a class and the relationships among them needed for a specific problem.
6. Able to fit a curve for given data set. Use Java code to determine these curves and evaluate values between the given data points.
7. Compute the solution for a first-order ordinary differential equation with initial condition related to biological systems using numerical techniques.
8. Obtain solutions to simultaneous sets of first-order ordinary differential equations related to biological systems using numerical techniques.

For meeting the above objectives, the programming language that was chosen as a computational tool was Java. This tool was taught in the first half of the course. In the latter half, the tool was used to understand numerical methods for curve fitting, ordinary differential equations and a system of ordinary differential equations. All these numerical methods were applied to study biological systems, thereby elucidating the wide applicability of such a course. Both sections were taught the same content and went through the same assessment protocols.

2.2 Procedure

The course was taught for a period of 13 weeks. In each week, there was two 2-hour classes. The class itself was in a computing lab setting that was used to deliver the concepts, demonstrate the concepts with programming examples and also allow students to solve sample problems. The typical characteristic of a classroom session is introduction of the theoretical concepts, demonstration of the concepts through a live coding example and sample practice questions for the students to evaluate their understanding of the concepts. The live coding inside the classroom involves significant active learning and discussion between the students and the instructor.

As part of active learning, within the lectures, Students engage with their peers and the instructor to solve the example problems taken up by the instructor. Through these interactions, the students are informally assessed for their understanding by asking questions during live coding. An example of a typical question that will be taken up for in class discussion is:

The following data define the sea-level concentration of dissolved oxygen for fresh water as a function of temperature (T):

T (°C)	*0*	*8*	*16*	*24*	*32*	*40*
C (mg/L)	*14.621*	*11.843*	*9.87*	*8.418*	*7.305*	*6.413*

Find the concentration of dissolved oxygen at T = 27, using (a) Lagrange Polynomial (b) Natural Cubic Spline

For a formal assessment of the understanding of the concepts, weekly labs are assigned to the students wherein they are required to do a computer implementation of the problem and submit a soft copy of the program and the results to the instructor for evaluation. A typical lab question that a student is required to solve as part of this course is:

Lab: Cell cycle dynamics

The process of cell division is periodic, with repeated growth and division phases as the cell population multiplies. It has been suggested that the division phase is triggered by high concentrations of a molecule called MPF (maturation promoting factor). The production of this factor is stimulated by another molecule called cyclin, and MPF eventually inhibits its own production. Using M and C to denote the concentrations of these two biomolecules (in mg/mL), a simple model for their interaction is

$$\frac{dM}{dt} = \alpha C + \beta C M^2 - \frac{\gamma M}{1+M}, \frac{dC}{dt} = \delta - M$$

Solve the given system of ODEs using RK4 method with h = 0.01 from t = 0 to 10, where

$$\alpha = 3.5,\ \beta = 1,\ \gamma = 10 \text{ and } \delta = 1.2.$$

$$M(0) = 0.4 \text{ and } C(0) = 0.8$$

Store your output data in a file, data.csv. Make sure that data fields (t, M, C) are separated by comma instead of space character. Open this file in excel and plot the graph. Submit your code with graph.

These lab questions test the ability of the students to apply a concept taught in the class to solve a problem. The students are allowed two hours of time inside the computer lab every week to solve these labs. They are encouraged to discuss the implementation details with the peers as well as the instructor. Typically, students self-organize themselves in groups of 2 or 3 to interact with their peers and solve the problem. However, each student is required to make an individual submission. The main objective of this exercise is for them to understand the concepts and have an experience in developing computer based solutions to problems. This enables stimulate students' cognitive learning in which a multitude of mental processes stimulated via such interactions with the peers in combination with their own exploratory efforts will enable them to grasp the concepts better.

In delivering the course through a combination of technology aided demonstration, live coding by students and computer based testing, an attempt has been made to integrate the key benefits of all three influences of learning theory, namely, *behavioral*, *cognitive*, and *constructivist* philosophies.

Behaviorism: With the instructor having control of the class and instructions originating from him, there is considerable stability and a determined course that is pursued by the cohort to meet the learning objective [31, 34]. In other words, the instructor outlines the learning objectives to be accomplished, expectations from the students, activities inside as well as outside the classroom and the associated assessments for evaluating students' learning. With such a significant amount of instructor controlled environment, there is considerable amount of productivity in ensuring that the cohort is steered in the right direction to meet the learning objectives.

Cognition: A potential drawback of running a course that is thoroughly instructor centric will stifle the creativity in student [35]. To ensure that this is not the case, the aspects of behaviorism is only used to set the stage and herd the students in an initial direction. This is immediately followed by introducing problem solving sessions wherein students solve the sample questions in the setting of biotechnology, posed during the classroom sessions, as well as the lab assignments that they are required to solve in the lab sessions as well as outside, the cognitive skills are also fostered [36]. In particular, in designing and developing a program to solve a biotechnology problem, the students' cognitive learning is enabled by engaging them in three processes [37]:

(1) Drawing or inferring new information that is often not explicitly stated in the question.
(2) Manipulating the current knowledge to enable solving the current biotechnology problem in hand.

(3) Evaluating the performance of the solution by running test cases.

Thus, with the problem-solving sessions, the students can acquire, infer, develop and evaluate new knowledge by investigating the problem and the applicable solution strategies themselves. By engaging with the peers in doing these activities the multitude of mental processes will enable cement the concepts in the minds [38].

Constructivism: The problem solving sessions also enable a continuous active learning setup in which the students collaborate with peers and produce meaningful solutions. This exercise involves discussions, sharing problems and solutions, and participation in self-reflection. Collective these acts foster construction of personal interpretations and helps students assign meaning to the knowledge they have gained from this experience [38].

A formal assessment of the understanding and progress of the students was made every week via weekly lab assignments that required the students to apply the recently taught concepts to solve an applied biotechnology problem. In administering these quizzes, the key objective was to ensure that the students are able to apply a recently taught concept to a simple example to gain confidence in implementing the computational solutions as well as develop a good understanding of the underlying principles. In addition to this, there was a mid-term exam and a final exam that the students took to enable us to evaluate their learning. The midterm exam was a computer based exam in which the students are required to write programs for two biotechnology-based application questions. The students were graded for the structure of the program and its functionality. Similarly, the final exam was also computer based in which the students developed programs for 3 application questions.

3. Results and Discussion

There were a total of 67 students involved in this study. The 36 students in the first section and the 31 students in the second section were both taught by the same instructor. The content was identical in the two sections. The number of assessments were the same. The question in the midterm exam and the final exam were slightly different since the two sections did not take the exam in the same term.

The performance of the students in the two sections are as shown in Fig. 1. As seen in this figure, the students in both sections perform exceedingly well in the lab component of the course. This is expected because of the following:

(1) The problems that the students solve vary in the levels of difficulty, ranging from a very simple problem to more difficult ones.
(2) The students are permitted to discuss the solutions with each other and with the instructor who can help them arrive at the appropriate solution.
(3) They are given a week to submit a complete solution to the assigned problems.

The performance of the students in either section decreases progressively as we move to the midterm and the final exam. This is not surprising because of the following:

(1) An exam environment induces significant amount of mental stress and duress among the students. This in itself results in a lower limit of their performance.
(2) The exams involve higher level application problems that are significantly more complex than the lab questions that the students solved.
(3) The exams are taken along with other courses and students often tend to distribute their time between different courses to ensure that they perform equally well in all the subjects.

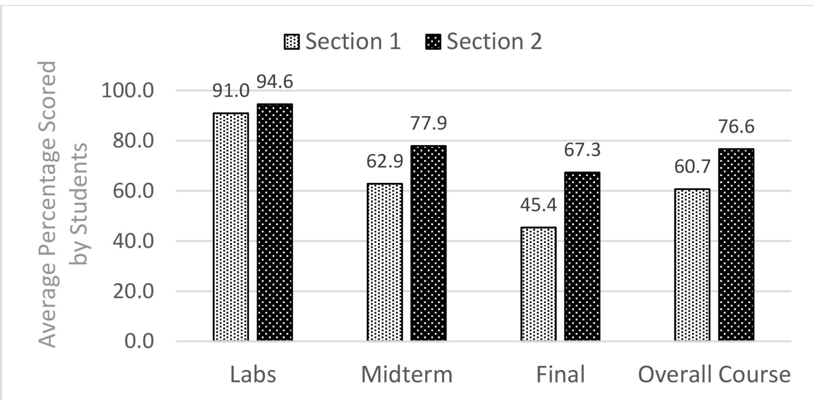

Fig. 1. Performance of the students in the two sections.

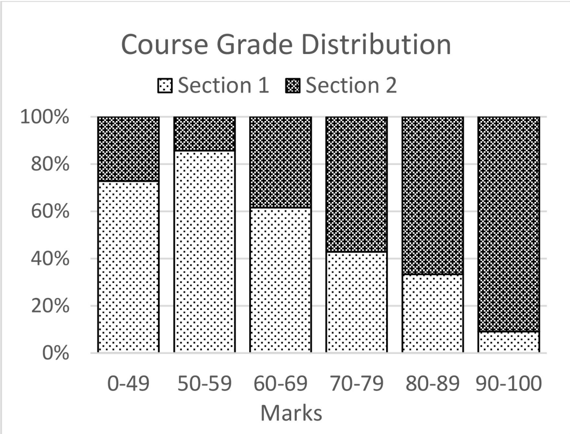

Fig. 2. Stacked grade distribution of the two sections. The graph represents the percentage of students in each section scoring in the respective range specified along the horizontal axis.

An important observation that can be made in Fig. 1 is that the performance of the students in Section 1 is significantly poor compared to the performance of the students in Section 2. In Section 2, attendance was enforced which results in some key behavioral and attitude changes in students, as described in the ensuing section, leading to a better performance. This better performance of the students is also reflected in the stacked grade distribution shown in Fig. 2. While the students in Section 1 have grades that are skewed in the 50–70 range, in Section 2 the grades are on the higher end of the spectrum with several students scoring an A grade or better in the course.

3.1 *Effect of Mandatory Attendance*

By introducing a mandatory attendance policy in the course for the second section, there was a significantly better attendance and participation in the classroom discussion sessions. The performance of the students from the two sections in the midterm and final exam are summarized in Fig. 3. In this figure, for each section, the performance of the students in four questions (2 from the midterm exam and 2 from the final exam) are shown. Together, they assess more than 90% of the learning objectives listed Section 2. Further, each bar represents the percentage of students gaining the different letter grades for that particular question. It is clear from this graph that once attendance is made mandatory, the percentage of students getting the highest grade (A) increases while the percentage of students getting a fail grade (F) on the question significantly decreases.

From the pedagogical perspectives, with regular attendance, the students in the second section received more consistent and timely interventions via the discussion with the peers and the instructor. By participating in routine active learning exercises inside the classroom, the students regularly recall the concepts taught and learn how to apply them to different problems in the area of biotechnology. Such regular active learning sessions not only entrench the concepts but also make students comfortable and confident of applying the concepts to various real-world problems. In these active learning sessions, their minds are stimulated to explore, rearrange and transform the information that they gather in a way so that new insights are gained, thereby significantly affecting the internal cognitive structure of the student. Thus, the classroom environment that promotes discussions, problem solving, investigation and discovery, directly contributes to cognitive structuring. This has been

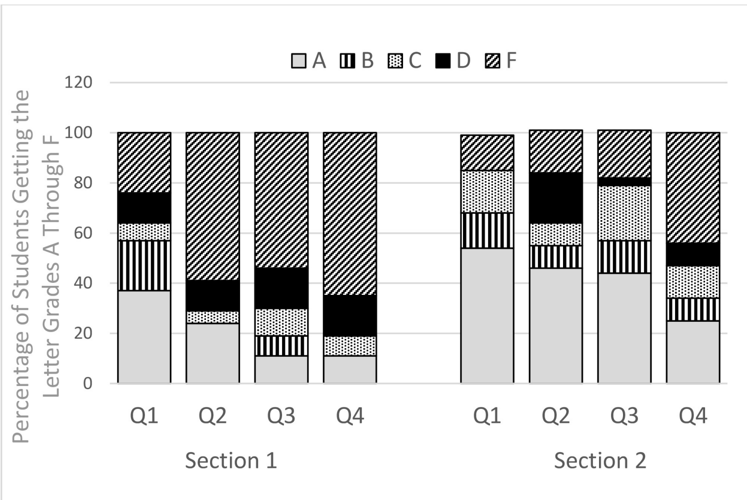

Fig. 3. Performance of students in each section on 4 different exam questions. Two questions (Q1 and Q2) are from the midterm exam and 2 questions (Q3 and Q4) are from the final exam. The letter grades correspond to the numerical grades as: A – >80%, B – 70–79%, C – 60–69%, D – 50–59%, F – < 50%.

critical in fostering confidence in students, ensuring that the concepts are well received and avoiding students from trailing in the class.

It must be noted that the performance in labs is nearly the same in either section because students are often helped by their peers and the instructor in arriving at an acceptable solution. However, with a lack of participation in the classroom and irregular attendance, several students are unable to solve the questions in the midterm and the final exams, where they have to develop solutions to the questions independently without any assistance. The poor performance of the students from Section 1 in these exams exposes the lack of their ability to employ the concepts so design and develop programs for higher level biotechnology related scenarios.

3.2 Integration of Principles of Learning Theories

As discussed in Section 2, the positive influences of the three theories of learning, namely, behavioral, cognitive and constructivist, have been employed in this course. As part of the behavioral instructional strategy, the instructor defines the weekly learning objectives, the activities to be undertaken inside the classroom, and the assessments to be administered to the students. With this, the instructor maintains a significant control of the course to primarily ensure that all the learning objectives are met and that the course contents are covered in a timely manner. However, to ensure that he is not simply running an information transferring session, the interdisciplinary nature of the course is exploited to create opportunities for the student to do some investigations, discovery and thereby some self-learning by working with peers in the problem solving activities inside the classroom.

The engagement of students in such problem solving sessions is primarily aimed at shifting some amount of responsibility of learning on the student. More precisely, after setting the context and guiding the students in an initial direction, in the problem solving sessions, the instructor provides an opportunity for the students to participate in a cycle of thinking, designing, developing and evaluating the computational solutions in the various biotechnology settings. Specifically, students will design a programming logic, implement it as a program, evaluate the test data set to ensure that the program provides the expected results, and interpret the output of the program to determine if any refinement is needed either to correct errors or to improve upon the existing logic. By going through this cyclic process, engaging with peers and the instructor, new insights are gained and the entire experience results in transformation of the internal cognitive structure, ultimately leading to learning. To ensure that this cognitive transformation is a continuous process and happens outside the classroom as well, weekly lab assignments are provided in which the students are to develop computational programs to simple biotechnology problems.

From the constructivist theory point of view, by interlacing the principles of programming with numerical methods and applying them to real-world biotechnology problems, students are able to adapt the cognitive structure in their minds to a physical environment. This is further augmented by engaging in discussions and sharing solutions with peers. It must be noted that in the classroom discussions, the focus of the instructor is in facilitating discussions on meaningful solutions instead of a specific correct answer, thereby generating a meaning for the students and fostering learning. Thus, by defining meaningful contexts for applying the concepts and encouraging collaboration and thoughtful reflection, the constructivist principles of learning are embedded into this course.

4. Conclusions

In this work, we present an approach to introduce a computational course in biotechnology that combines the three key areas of programming, numerical methods and biotechnology. In doing so, we employ the key principles of all three theories of learning to provide an optimal learning environment for the students. From the structure of the course and the offering style it can be concluded that:

1. This style of experiential teaching and learning is conducive to enhance students' participation in the programing activities, engage in discussions with their peers, share problems and solutions, and indulge in thoughtful reflection. All of these are expected to foster a multitude of mental processes that will enable cement the concepts in the minds and aid in transforming their internal cognitive structure.
2. A combination of assessments, some of which allow for collaboration while the others are individual assessments, encourage an environment of constructive thinking that is critical for the formation of concepts in the minds of the students.
3. By progressively enhancing the level of difficulty in the assessments, we can ensure that the learning of the basic concepts becomes much easier with simpler examples, and the more complex examples are used to evaluate the ability of the student to apply multiple concepts in more complicated and real-world situations.
4. Mandatory attendance drive student participation to higher levels. This has a direct positive impact on student engagement levels in the

active learning sessions, collaboration with their peers and instructor, all of which contribute to an improved learning of the material.

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