A Model for Guiding Undergraduates to Success in Computational Science

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ABSTRACT

This paper presents a model for guiding undergraduates to success in computational science. A set of integrated, interdisciplinary training and research activities is outlined for use as a vehicle to increase and produce graduates with research experiences in computational and mathematical sciences. The model is responsive to the development of new interdisciplinary curricula in computational biology, chemistry, mathematics and physics.

Categories and Subject Descriptors

K.3.2 [**Computer and Information Science Education**]: Curriculum and Computational Science Education.

General Terms

Design, Management

Keywords

Computational science; mathematical science; interdisciplinary research

1. INTRODUCTION

Over the years, academic institutions have developed initiatives and programs to support single discipline and multidisciplinary research, in which fairly divergent disciplines focused on a demarcated problem or issue. Biology, Computer Science, Chemistry, Physics, Mathematics, and Statistics (BCCPMS) each has its own intellectual history, theoretical framework, and experimental and analytical methods for uniquely investigating problems. However, perspectives from these distinct academic disciplines significantly contribute disciplinary strengths to increasingly sophisticated research activities such as the discovery of functionalities of gene structures. Unlike a multidisciplinary approach, this paper advocates the engagement of undergraduates in interdisciplinary research and training activities that amalgamate concepts and techniques from BCCPMS in ways that will generate new theoretical frameworks. This paper presents a framework for forging collaborations among interdisciplinary faculty members and undergraduates in computational research activities.

2. THEORETICAL FRAMEWORK AND GOALS

The number of institutions incorporating computational science (CS) at alternative levels into undergraduate curricula is progressively rising [6]. Early undergraduate CS (UCS) programs evolved mainly at large research institutions. Today, several institutions offer formal degree programs, minors, certificates or courses in CS. Unfortunately, the majority of UCS initiatives are only supplementing traditional

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programming, data structures, graphics, linear algebra, numerical analysis, ordinary and partial differential equations courses with interdisciplinary computational Biology, Chemistry, and Physics (CBCP) courses. Questions remain unanswered about the curriculum and training in UCS. What is the intellectual core of an UCS? What competencies should students in UCS exhibit? What constitutes an interdisciplinary UCS program? What learning and training models should be used in UCS?

The Society of Industrial and Applied Mathematics (SIAM) distinguishes CS and Engineering (CSE) as a distinct field of study, but it offers no UCS curriculum guidelines [5]. SIAM recognizes CSE as a multidisciplinary subject that combines knowledge and methodologies from computer science, applied mathematics, engineering and science. SIAM offers comprehensive roles of CSE in research areas such as worldwide climate modeling and combustion simulation.

A pioneering virtual laboratory model for engaging faculty and computer science undergraduates in collaborative research exists [7]. The National Computational Science Institute (NCSI) offers practical computational science, numerical models, and data visualization tools for interdisciplinary curriculum development at different locations in United States [4]. NCSI offers rigorous interdisciplinary use of modeling and visualization tools for collaborative discovery of existing courses, creation of new CS courses and promotion of novel modes of undergraduate research in CS. NCSI sponsors discipline specific and interdisciplinary web-based CS courses and interactive learning resources for undergraduates and faculty. In alignment with the initiatives of SIAM and NCSI, we propose a model, Guidance of Undergraduates to Success in Computational Science (GUSCS), for implementing interdisciplinary curricula and research in computational BCCPMS with the following specific goals:

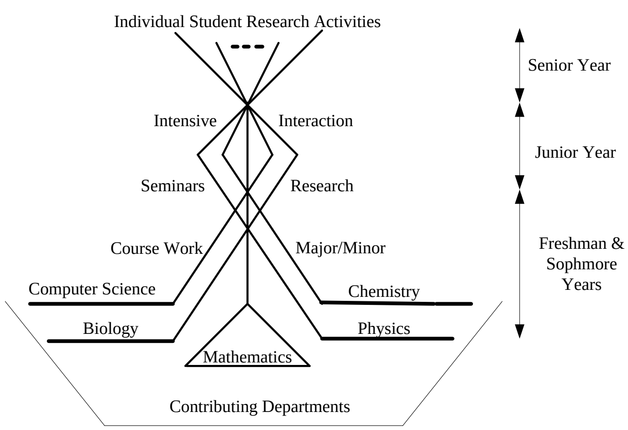
a. Use interdisciplinary courses and seminars to improve the independent learning of students in computational and mathematical sciences.
b. Provide opportunities for students to build research and mathematics competencies in CBCP.
c. Provide opportunities for students to collaborate, share responsibilities and resources, manage professional relationships, and participate in long-term research experiences with faculty members in computational and mathematical sciences.
d. Use interdisciplinary courses, research and seminars to increase skills, knowledge and enhance opportunities for students to pursue industry careers and graduate programs.

3. STUDENT LEARNING AND TRAINING

The schematic view of the interwoven organizational and administrative structure of the model is shown below. The structure portrays the intermingling that occurs in seminars between students and faculty designed to promote exposure to interdisciplinary initiatives.

The organizational structure requires collaboration among the BCCPMS departments. The administrative structure provides opportunities for students to intermix with faculty and students from different academic disciplines. Students participating in the GUSCS activities are teamed amid mathematics majors with computational science options, and then progress to become fellows in this model. Freshmen and sophomore fellows are guided by experienced faculty to fill their fundamental course requirements. Fellows complete courses in data analysis, applied mathematics, computing, biology, chemistry and physics prior to engaging in advanced research. Junior fellows participate in required interdisciplinary CS seminars. During the junior year, the GUSCS fellows select projects in consultation with the active research faculty. At the end of the junior year, the fellows begin the research process and complete twelve hours of electives and capstone research courses during the senior year. In the senior year, the individual research faculty mentors meet with their assigned students at least twice each week; each student work ten hours per week on a research project under supervision; and the culmination is the production of a research paper for submission and presentation at a conference.

The model includes biweekly seminars on topics of interest to BCCPMS fellows. Junior fellows undergo instructional and research enrichment activities for two weeks in the summer prior to their senior matriculation. The goal of the instruction is to assist junior fellows to discover the use of SAS, MAPLE and MATLAB programming environments, and selected principles of BCCPMS in scientific research. Teams of faculty members from BCCPMS departments create and deliver the interdisciplinary instructional and research materials.



4. COLLABORATIVE RESEARCH ACTIVITIES IN BCCPMS

The GUSCS model offers fellows the opportunity to participate in research projects that provide experience with actual discovery and development of research techniques and skills. Here is a sample set of collaborative interdisciplinary projects for the faculty and fellows.

Gene networks genetically determine and control all cellular processes: cell metabolism, cell division and differentiation, and the functioning of different organs [1]. Today, there are algorithms for identifying and classifying gene sequences. However, genes exhibit convergence, parallel, interaction and split motions in the presence of metabolism, making it difficult to identify the functionalities of gene structures. This project is focused on the gene network functioning using data accumulation and a generalized chemical kinetic method for mathematical simulation of gene network functional dynamics in selected gene network databases.

The field of differential equations varies from the highly abstract end to the highly computational mission-critical fluid dynamics relevant to NASA, Boeing, etc. Nonlinear differential equations arising from varying dynamical systems lack closed form solutions [3]. They can be solved using numerical approximation methods. This project is focused on the monotone iterative method that produces sequences of approximating solutions from above and below and convergence. Numerical computation and visualization of approximating sequences might also be explored.

Luminance in pattern recognition of faces or other objects is one of the most difficult aspects of pattern recognition. This project is concerned with examining the impact of various light compensations schemes on the stability and repeatability of the wavelet coefficients when multiple copies of the same image are processed under different lighting schemes impacting the luminance coefficients. The second objective is to consider representations of the face that allow transition to an expressive alphabet for describing the individual face independent of some of the luminance characteristics and the individual movement of the face through its various manifestations. Existing techniques lend themselves to fast recognition using alphabetic expressions of unknown strings of symbols [2]. The existing image processing system is far too sensitive to slight alterations in the image luminance introduced by the process of digitizing the image and needs to provide a texture for a realistic image. This project is focused on eliminating this very low level of texture, adjusting the luminance to present standards and processing the conditioned image according to a set of pixels or expressions that characterize the actual image in a parameter space.

5. CONCLUSION

This paper outlined a structured, concrete set of interdisciplinary training and research initiatives for guiding undergraduates in mathematical sciences to success in computational science. However, numerous questions linger on the implementation of the advocated model. Who will manage the project? How will faculty be selected? How will students be connected to computational research opportunities in industry and at government agencies? How reliable is this model? Where is the validity evidence for the model? Where is the fund for this project? The response to these kinds of questions will vary depending on the level of commitment to this model by an academic institution. For example, a principal investigator might be appointed to implement the administrative structure for the smooth running of the GUSCS activities, and work with project faculty to schedule and supervise the training, mentoring, and research activities. With an available pool of faculty strength in BCCPMS, the number and category of faculty members who participate in the GUSCS activities might change due to circumstances such as faculty attrition. Thus, faculty members might be rotated based on research productivity, and research interests of students. Faculty members should actively explore and pursue federal, industrial, and private sources of funding for undergraduates in mathematical and computational sciences. In spite of the lack of an exhaustive answers to all questions surrounding the bided model, we feel positive that the explicit project activities outlined in this paper are useful for reshaping the training of undergraduates in mathematical sciences, and for constructing interdisciplinary computational research and curricula.

6. REFERENCES

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