# A Model for Increasing the Number of Undergraduates Acquiring Skills in Computational Science

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**Abstract**

This paper presents a model that we have successfully used to increase the number of undergraduates that are acquiring skills in computational science. This model involves the exploration of computational science by freshmen, involvement of undergraduates in interdisciplinary computational science research, preparation of students for summer internships in computational science and related areas, and mentoring of students. The program has shown increase in the number of students that apply computational science skills in their major disciplines. It has led to increase in the number of students that are doing joint and double majors in Computer Science and other fields. Specific successes include the publications of several papers that involved undergraduate students, and participation of students in internships at National Laboratories (Oak Ridge National Lab, Sandia National Lab, and Office of Naval Research Lab in Washington, DC) and high-tech industries (including Oracle Corporation).

## 1. Introduction

Computational Science plays an immense role in research and development in almost all disciplines, especially in mathematics, science, engineering and biomedical disciplines. However, most undergraduate curricula do not have adequate computational science programs that cut across disciplines. While computational skills are incorporated in several science and engineering courses, there is not enough emphasis on real-life applications and research. The major opportunities for the development and applications of computational science by undergraduates are summer research programs and senior projects. Except for discipline closely related to computer science, undergraduate students do not acquire enough computational science skills. In this paper, we present the steps we have taken to increase the number of undergraduates who acquire skills in computational science in a small historically black college, Fisk University. The motivation and objectives for the development of the computational science activities are:

1. Increase students' understanding of computational science and how it could be applied to solve problems in their various disciplines.
2. Promote students' enthusiasm and interest in computational science and encourage them to acquire and use computational science skills in their fields of studies and future career.
3. Train more undergraduates that are capable of proceeding to acquire professional and graduate degrees, as well as take a career, in computational science related fields.

## 2. The Model

The overview of our model for increasing the number of undergraduates that are acquiring skills in computational science is schematically shown in Fig. 1. There are two base infrastructures that provide resources and support for the program. These are *curriculum/teaching* and *undergraduate research activities*.

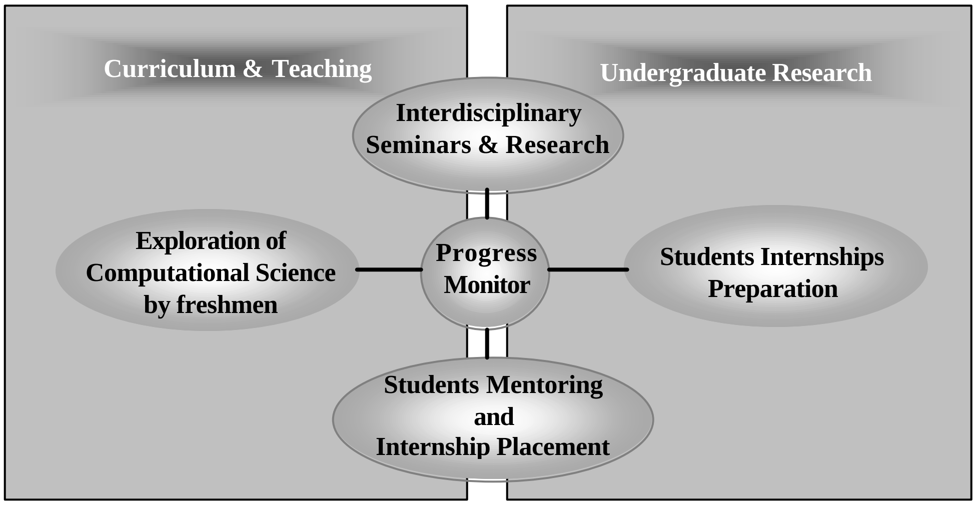



Fig. 1: Schematic of the model.

### *2.1. Curriculum and Teaching Infrastructure*

The curriculum and teaching infrastructure supports the development of a course that serves as both an orientation as well as introductory course in computational science for freshmen. It also provides support for interdisciplinary seminars, students mentoring and internship placement activities. Curriculum development programs give us opportunities to encourage various departments to incorporate strong computational science component/topics in their courses.

### *2.2. Undergraduate research infrastructure*

The undergraduate research infrastructure mainly supports interdisciplinary research activities and students internship preparation for summer work at national laboratories and high-tech industries. It partially supports students mentoring and internship placement activities. The undergraduate research activities are part of high-quality research projects of faculty members. From the faculty projects, we develop smaller components for students, where they could apply computational science skills. Common types of applications include:

1. Evaluation and analysis of experimental data.
2. Modeling and simulation.
3. Visualization.

### *2.3. Management and monitoring of progress*

There is a strong central management component that coordinates all the activities involved in the program. It monitors the progress of the students and all activities, through the use of a well-developed evaluation process. The evaluation of the program is a continuing process. The formal elements of the evaluation process are as follows:

1. Pre-program participation questionnaire is used to record information about the students capabilities and their expected achievements at the end of their undergraduate studies and thereafter.
2. The program management has oral individual interviews with participating students and their staff mentors to determine if their expectations, and the expectations of the program, are being realized. Any problems that arise are addressed at periodic meetings.
3. Periodically, students and their mentors complete several questionnaires and documents that include i) evaluation of the student by their mentors and research supervisors, ii) evaluation of various activities by the students, and iii) evaluation of the activities by mentors and research supervisors.
4. Periodic communication with students after graduation, to monitor how their experiences affect their professional and career goals.

### *2.4. Exploration of computational science by freshmen*

Students are exposed at the freshman level, to computational science, through a strong computational science component that has been incorporated into our *exploring computer science* course.[1] The course was originally designed to give computer science (CS) majors and non-majors an overview of the discipline – content, career opportunities and some foundational skills. Thus, it serves as both an orientation and a gentle preparatory course as described by Cook's paper on CS freshman orientation course.[2] In addition to contributing to the retention of CS majors the course has attracted new majors to the CS Program at Fisk University.[3] The exploratory course is organized as follows:

1. *Regular taught class sessions*. The regular taught class sessions take about 60% of the entire course.
2. *Seminars and workshops*. These cover about 10% of the course. The seminars are given by faculty members, upper class students, outside professionals, and Fisk CS graduates with computational science related jobs in industries or who are in graduate schools.
3. *Laboratory sessions*. The laboratory session is about 10% of the course. The students are introduced to the CS laboratory and are given lab assignments. Some of the lab assignments cover topics from the regular class sessions. The use of the CS laboratory and introduction to one or more programming languages are also included in the laboratory work.
4. *Group projects*. Students are assigned group projects to encourage and introduce them into working in groups. The group work takes about 15% of the course. Students from different disciplines are assigned to one group to foster interdisciplinary experience.
5. *Field Trips*. Students go on one or more field trips, depending on availability of funds. This accounts for about 5% of the course. Before the trip, students are shown videos that describe the industrial sector for the planned visit and the applications of computational science in that area. Students are encouraged to interact with the host industry as much as they can. A short paper describing the experience is required from the students after returning from the field trip.

## 3. Examples of Undergraduate Research Projects

The computational science research activities for undergraduates currently cut across several disciplines – computer science, mathematics, physics, materials science, biological/medical sciences, and chemistry. Some of the outstanding research works by undergraduates are described in the following subsections. Their research results have been included in several scientific publications.[4-6] The example projects described here are selected from the three types of computational science applications (evaluation and analysis of experimental data; modeling and simulation; and visualization) covered in our research group.

### *3.1. Computational evaluation of radiative transitions in fiber laser materials*

In this project, students used computational evaluations to process spectroscopy data obtained from experiments that were designed to study multiphonon relaxation and the effects of temperature changes on laser transitions in Erbium doped materials. Figure 2 shows the results obtained for the green laser line in Erbium doped Lead-Tellurium-Germanate Glass that has applications in fiber lasers. It shows that the green laser line separates into two distinct lines as the temperature of the source falls to very low values.[4]

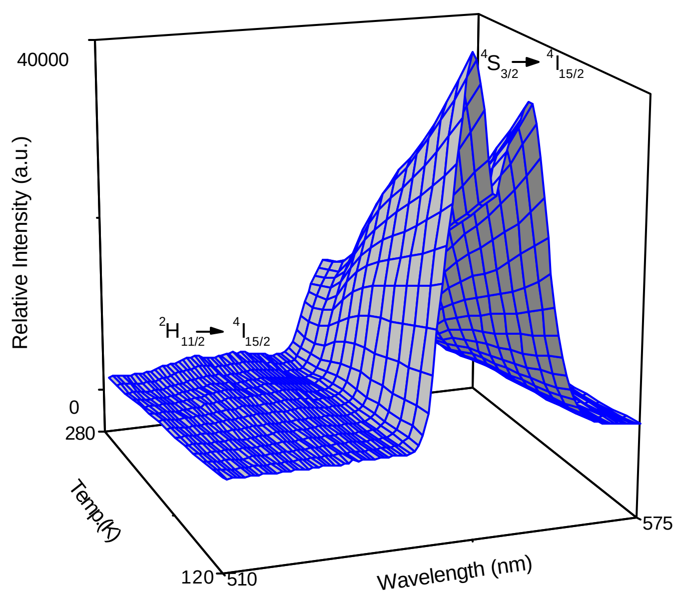



Fig. 2: Effects of temperature on some radiative transitions of $Er^{3+}$ in lead-tellurium-germanate glass.[4]

The computational evaluations enable us to observe the differences in the effects of temperature on the intensities of the $^4S_{3/2} \rightarrow {}^4I_{15/2}$ and $^4F_{9/2} \rightarrow {}^4I_{15/2}$ transitions. The intensity of the $^4S_{3/2} \rightarrow {}^4I_{15/2}$ transition decrease with increasing temperature, and could be explained with increase in depopulation of upper levels of the transition via multiphonon relaxation. On the contrary, the $^2H_{11/2} \rightarrow {}^4I_{15/2}$ transition starts at ~130 K and its intensity increases with increasing temperature, because its intensity depends mainly on 1) the thermally populated $^2H_{11/2}$ energy level according to the Boltzmann distribution, and 2) depopulation via multiphonon relaxation which has increasingly detrimental effect with increasing temperature - the first effect is however dominant. The computational evaluations used the experimentally measured spectroscopic data to map out the behavior of the materials and derive information that is useful in improving the fiber laser source.

### *3.2. Computer modeling of arterial pressure based on medical conditions*

This project involves computer modeling and simulation of arterial pressure based on medical conditions. The medical conditions include blood pressure, stroke, arteriosclerosis, and salt retention. An advanced version of the simulation will be a useful and effective visualization tool for doctors, patients, and for teaching students. Figure 3 shows the visualization results from students' research in this biomedical-computing project.[5] The model is based on the function of the heart and the mechanism of blood circulation. Using the concepts of blood flow rate, stroke volume, flow resistance, and arterial compliance, we obtained a first order linear non-homogenous differential equation that was used in the modeling:

$$dP_a(t)/dt + (3/4R_sC_a)P_a(t) = -15/\, R_sC_a$$

where $P_a$ is arterial pressure, $R_s$ is systemic resistance, $C_a$ is arterial compliance, and $t$ is time. The following solution is obtained using the integrating factor method and the initial condition $P_a(0) = P_{sys}$.

$$P_a(t) = (P_{sys} + 20)\exp(-3t/4R_sC_a) - 20$$

where $P_{sys}$ is systolic pressure. The final mathematical model is

$$P_a(t) = \{[(V/C_a) - 20 + 20f)]/[1 - f] + 20\}f - 20$$

where $V$ is stroke volume and $f$ is an exponential factor defined as $f = \exp(-3t/4R_sC_a)$. Students use this model to develop the mathematical relations between the various medical conditions, which they use in implementing a visualization system to display patients medical data needed to assist physicians in their decisions.

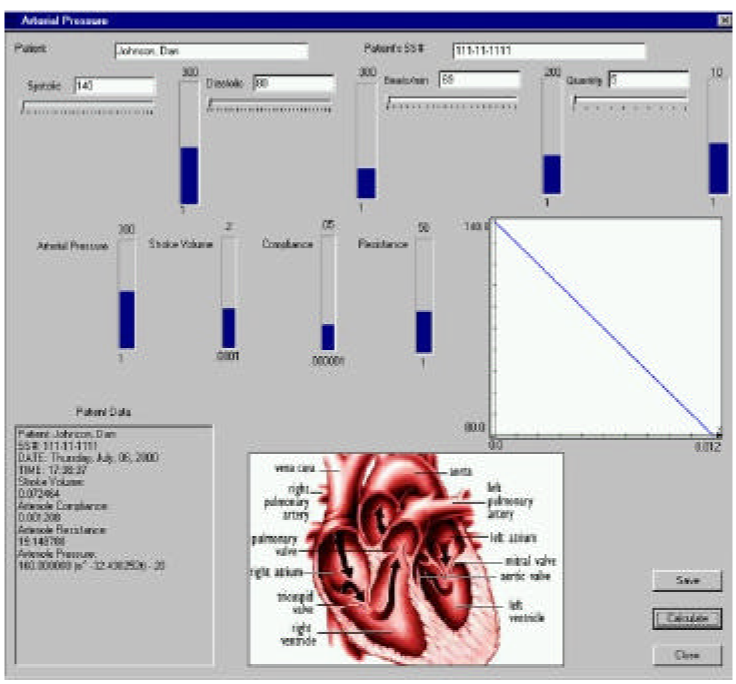



Fig. 3: A demo of phase-I of an arterial pressure visualization system.[5]

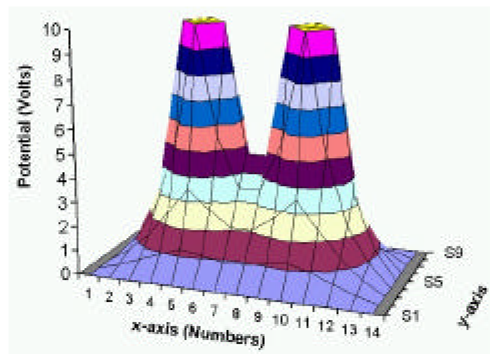
### *3.3. Modeling and visualization of E-field Distribution in Multiwire Nuclear Detectors*

This project is a component of a bigger project in the modeling and simulation of physical and biological systems. Specific interests include nuclear detectors, medical laser systems, and biomedical systems in which we are currently involved. Initial computational activities were in the simulation and visualization of electrostatic field distribution in gas-filled nuclear detectors.[6]

This project is ideal for training students on how to develop computation/simulation models from first principles based on the application, accomplish the modeling, and develop a visualization system that best represent the situation. A simplified example is shown in Fig. 4a, where the boundary conditions of the problem were applied to reduce Poisson's equation to Laplace's equation, and through the use of numerical analysis and matrices we obtained the values shown. The final phase of visualization is shown in Fig. 4b.

| | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0 | 0.26 | 0.58 | 0.94 | 1.22 | 1.09 | 0.93 | 0.93 | 1.09 | 1.22 | 0.94 | 0.58 | 0.26 | 0 |
| 0 | 0.57 | 1.33 | 2.4 | 3.48 | 2.68 | 2.07 | 2.07 | 2.68 | 3.48 | 2.4 | 1.33 | 0.57 | 0 |
| 0 | 0.92 | 2.37 | 5.21 | 10 | 5.52 | 3.47 | 3.47 | 5.52 | 10 | 5.21 | 2.37 | 0.92 | 0 |
| 0 | 1.16 | 3.39 | 10 | 10 | 10 | 4.66 | 4.66 | 10 | 10 | 10 | 3.39 | 1.16 | 0 |
| 0 | 0.92 | 2.37 | 5.21 | 10 | 5.52 | 3.47 | 3.47 | 5.52 | 10 | 5.21 | 2.37 | 0.92 | 0 |
| 0 | 0.57 | 1.33 | 2.4 | 3.48 | 2.68 | 2.07 | 2.07 | 2.68 | 3.48 | 2.4 | 1.33 | 0.57 | 0 |
| 0 | 0.26 | 0.58 | 0.94 | 1.22 | 1.09 | 0.93 | 0.93 | 1.09 | 1.22 | 0.94 | 0.58 | 0.26 | 0 |
| 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |

(a) Computed E-potential values in volts.




(b) Visualization of equipotential regions.

Fig. 4: Computation and visualization of electrostatic field distribution in a gas-filled nuclear detector.[6]

In a gas-filled nuclear detector the electrostatic field distribution is an important factor in its application for tracking the motion of charged particles. The field distribution depends on the shape of the electrodes and the applied potential difference. A good understanding of the field created is useful in accurate designs of a detector and the calculation of the path of the detected charged particle. The simulation and visualization system the students are developing should be capable of digital display of the potential (in volts) at a point defined in 3-D Cartesian coordinates, and a visualization of the field showing the equipotential and electric-field lines.

This is a boundary-value problem with the boundary values defined by the applied potential difference $P$ and the shape of the electrodes. Starting from Poisson's equation the problem results in Laplace's equation where charge density is zero:

$$d^2P/dt^2 = 0$$

where $P$ is potential and $t$ is time. Considering a lattice of squares of unit sides the numerical solution of Laplace's equation, by difference method, gives the potential $P_{i,j,k}$ at a point (i,j,k) as

$$P_{i,j,k} = (1/6)[ P_{i+1,j,k} + P_{i,j+1,k} + P_{i,j,k+1} + P_{i-1,j,k} + P_{i,j-1,k} + P_{i,j,k-1} ]$$

where i, j and k are positive integers in the x-, y- and z-axes respectively.

The above solution is used to set up any number $n$ of potential equations in $n$ unknowns. The resulting equations could be solved using several methods such as Gaussian elimination and Gauss-Siedel iteration methods. The difficult part of the entire process is the manual generation of the potential equations. Using the properties of the shape of the electrodes one could substantially reduce the number of equations to be manually generated. Students' works also include developing simulation equations to generate the required number of potential equations.

## 4. Success and Setbacks

The model succeeded in increasing the number of undergraduates acquiring skills in computational science. There are however some setbacks.

### *4.1. Setbacks*

There are two major setbacks encountered while implementing the model. These are:

1. High teaching and advising/mentoring loads as a result of shortage of instructors with expertise in computational science.
2. Inadequate financial support for students limited the number of hours students participated in research activities.

### *4.2. Success*

The successful outcomes of the implementation of the model are summarized below:

1. We successfully operated a 10-week undergraduate summer institute for research in computational science for 8 students with partial funding from NSF-MII grant, DOE-RAM grant, and NASA through the Fisk-NASA center. Students worked in pairs in 4 projects supervised by 4 faculty members, each serving as mentor in each project group.
2. The program provided unique research experiences to undergraduates who would not otherwise have such opportunities.
3. The 8 undergraduates that participated in the summer institute co-authored 4 publications from their research work.[5-8]
4. Six of the students later qualified for and participated in internships in National Laboratories (Oak Ridge National Lab, Sandia National Lab, and Office of Naval Research Lab in Washington, DC) and high-tech industries (including Oracle).
5. Four students have entered graduates schools.
6. Three students got full scholarships for graduate studies (2 for Ph.D. degree and 1 for M.S. degree).

We got a 3-year $0.3 million DOE RAM grant on September 15, 2002 to support faculty and undergraduate research in computational science. The undergraduates that will be trained in the DOE supported project will proceed to Oak Ridge National Lab during the summer months.

## 5. Conclusions

We have successfully developed and implemented a model based on curriculum, teaching and research for increasing the number of undergraduates who acquire skills in computational science. The major components include an exploratory course that introduces freshmen to computational science, interdisciplinary seminars and research activities, students internship preparation program, students mentoring and internship placement, and evaluation and progress monitoring. Major success include an increase in the number of undergraduates who coauthored scientific publications in computational sciences, an increase in the number of students qualifying and participating in summer research/internship at national laboratories and high-tech industries, an increase in number of students proceeding to pursue computational science related graduate degrees, and increased funding of research proposals. In the future, we plan to expand our activities to include a full-fledged summer institute for computational science research and activities.

## Acknowledgement

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## Biography

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