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Alliance for Computational Science Collaboration
HBCU Partnership at Fisk University
Final Report
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1. Introduction

Computational Science plays a big role in research and development in mathematics, science, engineering and biomedical disciplines. The Alliance for Computational Science Collaboration (ACSC) has the goal of training African-American and other minority scientists in the computational science field for eventual employment with the Department of Energy (DOE). The involvements of Historically Black Colleges and Universities (HBCU) in the Alliance provide avenues for producing future DOE African-American scientists. Fisk University has been participating in this program through grants from the DOE.

The DOE grant supported computational science activities at Fisk University. The research areas included energy related projects, distributed computing, visualization of scientific systems and biomedical computing. Students' involvement in computational science research included undergraduate summer research at Oak Ridge National Lab, on-campus research involving the participation of undergraduates, participation of undergraduate and faculty members in workshops, and mentoring of students. These activities enhanced research and education in computational science, thereby adding to Fisk University's spectrum of research and educational capabilities.

Among the successes of the computational science activities are the acceptance of three undergraduate students to graduate schools with full scholarships beginning fall 2002 (one for master degree program and two for Doctoral degree program).

2. Accomplishments

2.1 Developing Distributed Computing Laboratory for Internet Embedded Systems and Applications

The laboratory for distributed computing is being developed to support research activities involving Internet based virtual computation centers. There are several target capabilities, including:

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1. Several researchers in different geographical locations working on the same computational problem at a virtual computing center via the Internet.
2. Virtual laboratories that provides virtual experiments for teaching and training applications.
3. Internet embedded real-time experiments in remote laboratories
4. Hybrid computational, database and real-time experimental activities.

An example project for real-time experiment and computational activities with a common database is schematically shown in Fig. 1. The system demonstrates shared computing problems for experimental analysis and theoretical simulations at different hosts with common data resources.

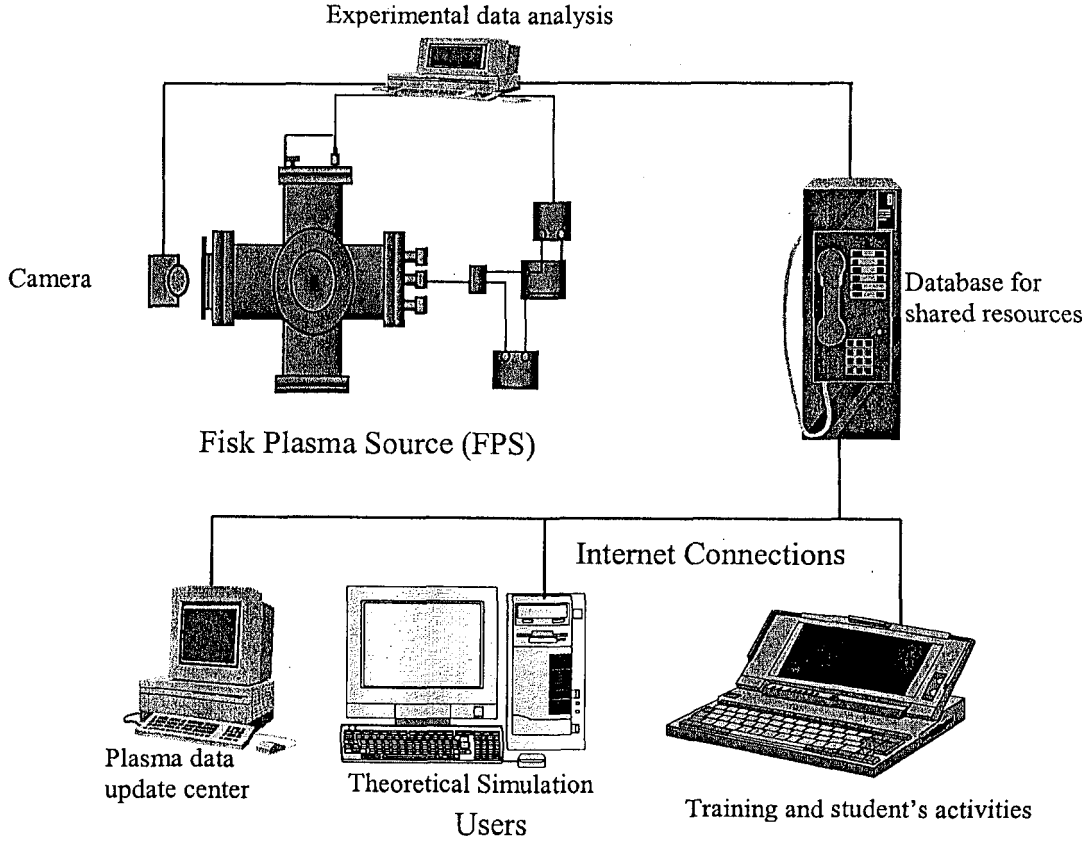


Fig. 1: Distributing computing structure that supports experimental and theoretical work.

The work done in this project involved the participation of four minority undergraduate students, and led to the development of virtual experiments for web-based electricity learning and tutoring systems [1].

2.2 Biomedical Computing

There are two major target research projects in this area:

1. Computer modeling and simulation of arterial pressure based on medical conditions – The medical conditions include blood pressure, stroke, arteriosclerosis, and salt retention. The simulation will be a useful and effective visualization tool for doctors, patients, and for teaching students.
2. Optimization of decision mechanism in spectroscopic detection and monitoring of cancer cells – our focus would be on breast cancer and prostrate cancer.

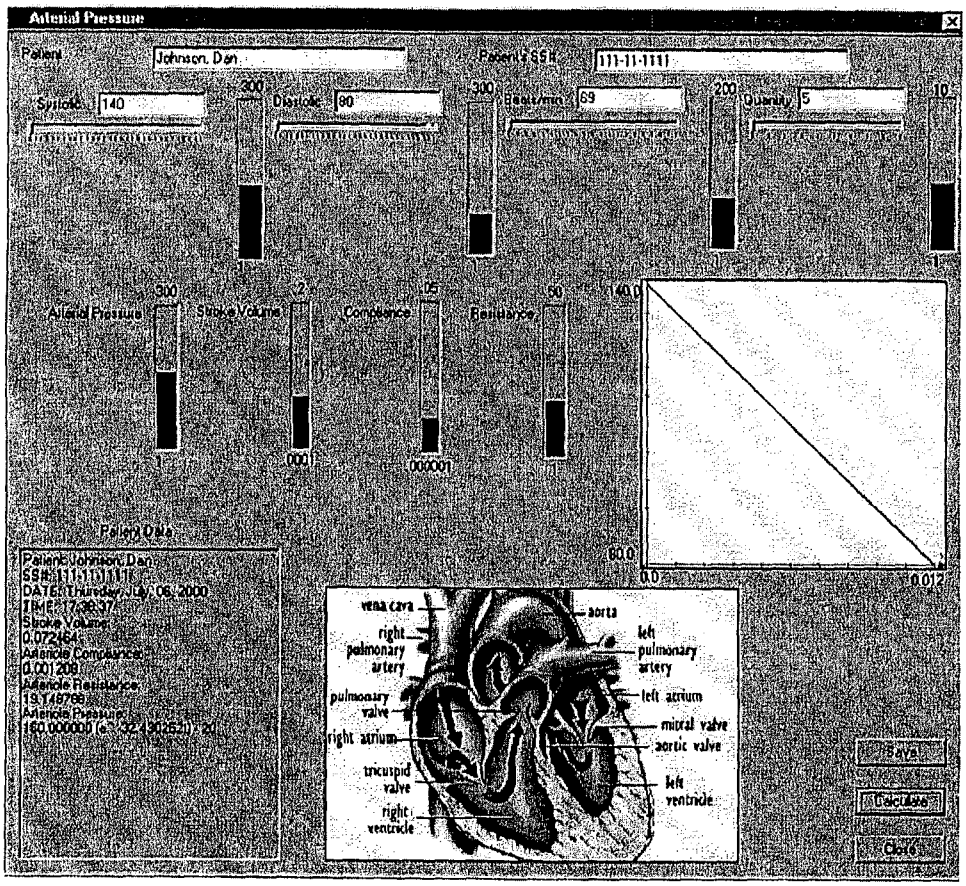


Fig. 2: A demo of phase-I of an arterial pressure visualization system. From Egarievwe *et. al.* [2].

Our research in biomedical computing involved the modeling and simulation of arterial blood pressure, with the end result of a visualization tool (phase I) for medical applications [2]. Three minority students were involved in this project. 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

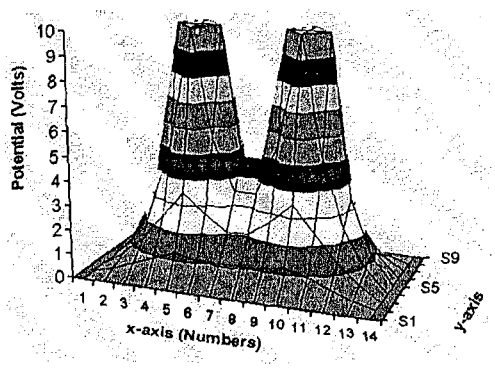
resistance, and arterial compliance, we obtained a first order linear non-homogenous differential equation that was used in the modeling. The demo of the first phase is shown in Fig. 2.

2.3 Modeling and Simulation

We are currently involved in the modeling and simulation of physical and biological systems. Specific interests include nuclear detectors, medical laser systems, and biomedical systems. Initial computational activities were in the simulation and visualization of electrostatic field distribution in gas-filled nuclear detectors [3]. This project served more in training the three minority students participants, how to develop computation/simulation models from first principles based on the application, accomplish the modeling, and developing a visualization system that best represent the situation. A simplified example is shown in Fig. 3a, 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. 3b.

0	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



(b) Visualization of equipotential regions.

Fig. 3: Computation and visualization of electrostatic field distribution in a gas-filled nuclear detector. From Egarievwe *et. al.* [3].

2.4 Students Participation in RAM Summer Internship at ORNL

Fisk University undergraduate students have participated in the Research Alliance for Minorities (RAM) summer internship program at Oak Ridge National Lab (ORNL) for the past three years. Each student was paid a total amount of $4,750 for a ten-week stay at ORNL in the summer. These students expressed strong interests in pursuing career goals in the field of computational science. A

very successful case is that of Miss Charita Brent who will be continuing her education at Howard University graduate school next fall. This program had a major influence on her decision to do graduate studies in computer science.

2.5 Students Mentoring and Participation of Students in Research

The computational science activities at Fisk University also include students mentoring through their involvement in workgroups and research. Students participated in research projects under the supervision of the faculty members in charge of the projects. Specific students project topics include:

1. Computer Based Instrumentation of a Plasma Generation and Studies Laboratory.
2. Web-Based Function and Graph Tutor.
3. Computer Simulation of Arterial Pressure Based on Medical Conditions.
4. Internet Based Remote Experiment – Data Acquisition and Analysis.

A total of ten minority students consisting of eight computer science (CS) majors, two physics majors with minors in CS, and one biological science major, have participated in computational science research since 1999.

2.5 Publications and other Success Outcomes

With additional funding from NSF and NASA, the success of the computational science activities at Fisk University include

1. The publications of six papers [1-6] in journals and conference proceedings.
2. Three undergraduate students got admitted to graduate schools with full scholarships beginning fall 2002 – one for master degree program and two for Doctoral degree program.
3. Participation of undergraduates in summer research at national labs and in internship programs.
4. Several poster presentations by undergraduate students at conferences.

Four of the six publications involved eight undergraduate students participants [1-4]. An award winning student poster presentation is that by Miss Charita Brent at ADMI 2001, Hampton VA, May 31 – June 3, 2001. Her poster titled "Web-Based Geography Tutor for Elementary Schools" won second position prize [7].

The computational science activities fostered internal collaborations within Mathematics, Computer Science, and Physics disciplines. There were also external collaborations with other universities and research centers. Dr. H. Mann

had collaborations with Tennessee State University, and Dr. S. U. Egarievwe had collaboration with Vanderbilt University.

References (Undergraduate students underlined)

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[3] S. U. Egarievwe, O. K. Okobiah, A. O. Ajiboye, L. A. Fowler, S. K. Thorne, W. E. Collins. "Internet Application of LabVIEW in Computer Based Learning." *European Journal of Open and Distance Learning*. 2000.

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