Alliance for Computational Science Collaboration:
HBCU Partnership at Alabama A&M University

Continuing High Performance Computing Research and Education at AAMU

(DE-FG02-06ER25746)

Final Performance Technical Report

To

Department of Energy, Office of Science
Office of Advanced Scientific Computing Research (ASCR)

Submitted by

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Abstract

This is the final report for the Department of Energy (DOE) project DE-FG02-06ER25746, entitled, "Continuing High Performance Computing Research and Education at AAMU". This three-year project was started in August 15, 2006, and it was ended in August 14, 2009. The objective of this project was to enhance high performance computing research and education capabilities at Alabama A&M University (AAMU), and to train African-American and other minority students and scientists in the computational science field for eventual employment with DOE. AAMU has successfully completed all the proposed research and educational tasks. Through the support of DOE, AAMU was able to provide opportunities to minority students through summer interns and DOE computational science scholarship program. In the past three years, AAMU

(1). Supported three graduate research assistants in image processing for hypersonic shockwave control experiment and in computational science related area;
(2). Recruited and provided full financial support for six AAMU undergraduate summer research interns to participate Research Alliance in Math and Science (RAMS) program at Oak Ridge National Lab (ORNL);
(3). Awarded highly competitive 30 DOE High Performance Computing Scholarships ($1500 each) to qualified top AAMU undergraduate students in science and engineering majors;
(4). Improved high performance computing laboratory at AAMU with the addition of three high performance Linux workstations;
(5). Conducted image analysis for electromagnetic shockwave control experiment and computation of shockwave interactions to verify the design and operation of AAMU-Supersonic wind tunnel.

The high performance computing research and education activities at AAMU created great impact to minority students. As praised by Accreditation Board for Engineering and Technology (ABET) in 2009, "*The work on high performance computing that is funded by the Department of Energy provides scholarships to undergraduate students as computational science scholars. This is a wonderful opportunity to recruit under-represented students.*" Three ASEE papers were published in 2007, 2008 and 2009 proceedings of ASEE Annual Conferences, respectively. Presentations of these papers were also made at the ASEE Annual Conferences. It is very critical to continue the research and education activities.

1. Introduction

The continuation of the high performance computational science research and education at AAMU project was supported through DOE under grant DE-FG02-06ER25746 in August 2006. The objective of this grant was to enhance high performance computing research and education at AAMU, and to train African-American and other minority students and scientists in the computational science field for eventual employment with DOE. As indicated in Figure 1, the key elements of this grant were to encourage minority students to become more involved in computational science activities through computational science research, DOE computational

Science Scholarship program, undergraduate RAMS internship program, graduate research support and improvement of high performance computing laboratory at AAMU.

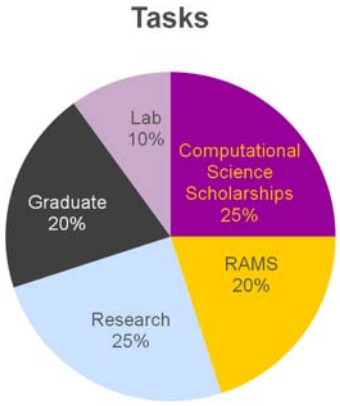


Figure 1. Key elements of DOE-AAMU grant of High Performance Computing Research and Education.

2. Achievement

In the past three years, all proposed tasks in research and education were accomplished. In the following sections, DOE computational Science Scholarship program, improvement of high performance parallel computing laboratory at AAMU, RAMS student summer research internship program at ORNL, graduate research and high performance computing research are discussed. Three papers were published:

(1) An ASEE paper, AC-2007-1103, entitled "Enhancing Minority Engineering Education at AAMU through DOE Sponsored Project," was published in the Proceeding of 2007 ASEE Annual Conference, The presentation was also made at the 2007 ASEE Annual Conference in Honolulu, Hawaii in June 2007;

(2) An ASEE paper, AC-2008-753, entitled, "Lessons Learned from Minority Computational Science Research and Education Project", was published in the proceeding of 2008 ASEE Annual Conference in June 2008. The presentation was made in the 2008 ASEE Annual Conference in Pittsburgh Pennsylvania in June 2008; and

(3) An ASEE paper, AC 2009-1964, entitled, "Research Alliance in Math and Science (RAMS): An Excellent Research Internship Program for Minority Science and Engineering Students," was published in the proceeding of 2009 ASEE Annual Conference in June 2009. The presentation was also made in the 2009 ASEE Annual Conference in Austin, Texas in June 2009.

As a continuation of previous research on particle in cell simulation, a presentation entitled, "Computation of Ion Trajectories in a Pulsed Magnetic Nozzle," was made in Directed Energy Professional Society's Tenth Annual Directed Energy Symposium in November 2007. Appendix A lists the abstracts of these published papers and outline of the presentation. Due to wind-tunnel manufacture restrictions, computational research results on shockwave interaction and verification of supersonic wind tunnel design and operation are not permitted to publish at the present time.

2.1 DOE Computational Science Scholarship Program

The DOE Computational Science Scholarship program at AAMU has been conducted in the past three years. The scholarship application announcement and application form, were posted on the HPC web-site (http://www.aamu.edu/set/me_hpl.aspx) and around the AAMU campus in science and engineering departments. To apply for the scholarship, students need to fill out the application form, write an essay about their understanding and interests towards high performance computing, and two faculty recommendation letters are required. Upon receipt of the application package, careful evaluation was conducted based on the scholarship criteria. Upon receiving preliminary award notifications, students are required to sign a scholarship obligation agreement to accept the scholarship awards. Recipients are required to stay in science and engineering majors, maintain a GPA of 3.25 or above and agree to work in the area of computational science for DOE if a job is offered.

In the past three years, more than 50 scholarship applications were received. 30 competitive undergraduate scholarships were awarded to science and engineering students through this grant. Each award is $1500. Scholarship recipients were from Chemistry, Biology, Mechanical Engineering, Electrical Engineering, Civil Engineering, and Computer Science. Figure 2 shows the picture of scholarship recipients at the award ceremony in 2008 and 2009. Figure 3 shows scholarship recipients GPA distributions from 2007 to 2009 and the averaged GPA in the past three years.

Figure 2. Group picture of 2008 and 2009 Scholarship award ceremony.

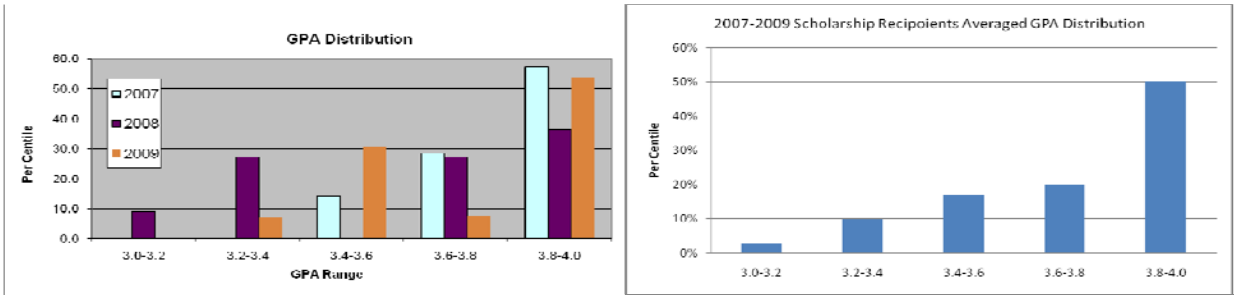


Figure 3. DOE Computational Science Scholarship recipients GPA distribution.

As indicated in Figure 3, the GPA of the majority (more than 85%) of the scholarship recipients was higher than 3.4. About 50% of the recipients have GPA above 3.8. In order to attract more averaged science and engineering students to computational science, we put emphasis on faculty recommendations for students with GPA between 3.0 and 3.2 or lower. Faculty evaluated applicant's academic strength, interest on computational science, programming capability and potential success assessment in the academic field. If a student demonstrated a great potential and interest in working in computational science area, but currently suffered by low GPA (3.0-3.2), we recommend student to apply summer research internship program offered by his DOE project. In the past three years, it was proved that the computational science scholarship program created a huge attraction to top minority engineering students. It is a good recruiting and retention tool and greatly enhanced engineering education to minority students. As praised by Accreditation Board for Engineering and Technology (ABET) in 2009, "*The work on high performance computing that is funded by the Department of Energy provides scholarships to undergraduate students as computational science scholars. This is a wonderful opportunity to recruit under-represented students.*"

2.2 Improvement of High Performance Parallel Computing Laboratory

The high performance computing laboratory at AAMU has 8 Pentium based Linux workstations, two Sun Ultra 10 workstations. With the support of DOE grant, in the past three years, three new Dell-Precision LINUX workstations with fast processor and bigger memory were purchased and configured to run computational fluid dynamics applications. Figure 4 shows the physical setup of the HPC lab.

Computational fluid dynamics research has been established in AAMU through this high performance computing laboratory. The WIND code, (developed by AEDC and Boeing company, a generic aerodynamics computation code), was configured and upgraded on these three new workstations. Pre- and post-processing software to visualize the CFD data were also installed and configured on these LINUX stations.

Figure 4. The improved High Performance Computing Laboratory at AAMU, ETB 148.

With the addition of these three new workstations, we were able to reduce our simulation turn-around time by approximately 50%.

2.3 RAMS Student Summer Internship at ORNL

The RAMS program is a twelve-week summer research internship program at ORNL for undergraduate and graduate minority science, engineering and technology students. Application for the program is posted on the RAMS website January each year. Students who apply for the internship program are required to submit on-line applications, official transcripts, and an essay describing how to handle difficult situations or problems. Students were also required to work with his/her faculty advisor to develop a research proposal for the summer internship project. In addition to student applications, two faculty advisors recommendation letters are required.

All AAMU-RAMS applicants are hand-picked by an AAMU faculty advisor before submitting RAMS applications. The principal investigators of this project introduced the ORNL on-going research activities to students before their application. Student summer research proposals are then generated with the help of a faculty advisor. Applicants are also carefully reviewed by ORNL mentors. Once selected by RAMS, AAMU-RAMS interns were provided support of up to $5800 to participate in 12 weeks of research and study at ORNL. Student performance is closely monitored by the joint effort of an AAMU faculty advisor and RAMS administrators and mentors. In the past three years, AAMU was able to support six RAMS interns through this grant. Sample RAMS report posters are listed in Appendix B.

It was noticed that students with high GPAs are likely to receive summer internships from variety of sources. This is especially true in AAMU where many high-tech research companies are located nearby. In order to attract science and engineering students to computational science, we interviewed potential RAMS applicants prior to their application. Faculty evaluated the applicant's academic strength, the student's interest in computational science and the student's programming capability. If a student demonstrated a great potential and interest in computational science, but currently suffered by low GPA, we still recommend the student to apply for the summer research internship program.

Student commitment to RAMS internship is critical. Sometimes, students changed their minds in the very last minutes before they report to work at ORNL. This created problems for RAMS program execution at ORNL. Realized this, AAMU faculty investigators make sure that students from AAMU are committed to RAMS program when they apply the internship.

Close-monitoring of RAMS interns' progress was also proved to be critical for successful completion. During the 12 weeks stay at ORNL, AAMU-RAMS interns kept closed communication with faculty mentors.

The activity after their RAMS internship have brought positive impact to AAMU science and engineering students in the area of computational science. When RAMS interns return to school in the Fall semester, they bring their research papers and posters back to school. Their research posters are displayed at the school of engineering open house, high school senior day at AAMU, Science, Mathematics, Engineering and Technology (SMET) day competition at AAMU and high performance computing workshops. In 2008 and 2009, AAMU-RAMS interns participated in the STEM day competition at AAMU. One RAMS student research was awarded third-place

in 2009. AAMU-RAMS Interns are also provided a chance to present their research project and experience at ORNL to fellow science and engineering students.

2.4 Graduate Research

In order to maintain the operation of the high performance computing laboratory (tasks including updating software, hardware configuration, image processing), we recruit three graduate research assistants. They are top computer science and electrical engineering graduate students at AAMU. However, most of graduate students, even in computer science program at AAMU, have never been exposed to computational science or parallel computing. Construction of the parallel network computer system using PVM or MPI is a challenge. Additionally, all students were trained in Microsoft Window environment. Students have zero or minimum experience in LINUX/UNIX operating system and programming environment. None of the students can program in FORTRAN or C. Therefore, intensive training of the graduate research assistants in the area of parallel computing, LINUX operating system and scientific programming language was conducted. With the introduction of MatLab, students were able to conduct image processing analysis. In the past three years, graduate students were able to upgrade the previous 8 Linux workstations to run RedHat Linux Enterprise WS 4 with computational applications with PVM package. Students were also participated in research of shockwave interaction image analysis using MatLab and scientific visualization. This laboratory is available for use by project participants and by researchers, faculty and students at AAMU. Students were from Mechanical Engineering, Electrical Engineering, Chemistry, and Computer Science Departments, who involved in high performance computing project and image processing. This parallel computing laboratory is the only computing lab at AAMU that uses LINUX/UNIX operating system.

2.5 High Performance Computing Research

Research on high performance computing was conducted on computational fluid dynamics simulation of supersonic wind tunnel operational test volume Mach numbers and supersonic shockwave interactions. The particle-in-cell simulation was continued from previous research and results were presented in the Directed Energy Professional Society's Tenth Annual Directed Energy Symposium in November 2007, entitled, "Computation of Ion Trajectories in a Pulsed Magnetic Nozzle."

Prediction of Test Volume Mach Number for a Supersonic Wind Tunnel and Shockwave Interactions: The WIND code was installed on the high computing lab at AAMU. Preliminary simulations were conducted to predict test volume Mach number for a supersonic wind tunnel that to be installed at AAMU. We noticed that the prediction of the test volume Mach number depends on specification of downstream conditions if Laminar flow simulation model is used. If simple extrapolation of pressure downstream boundary conditions were used, we observe complete supersonic expansion in the subsonic diffuser causing exit pressure to be near vacuum. This un-realistic condition cannot be achieved in the experiment at room conditions. This suggested that conventional boundary conditions used by CFD simulations for shockwave interactions and simulation of wind tunnel operation may not be accurate. In order to capture shockwave interaction phenomena, one must consider turbulent modeling for shockwave interaction inside the supersonic wind tunnel. Extensive simulation was performed in order to

select a valid turbulent model. The turbulent models used in the prediction play important role in controlling wall boundary layer growth. It was concluded that Spalart turbulent model was good for the wind-tunnel flow simulation. Due to restrictions from wind-tunnel Manufacture, the detailed simulation results of test volume Mach number are not allowed to be published at the present time.

Image Processing of Hypersonic Shockwave Structure Experiment: In order to investigate the electromagnetic control of a hypersonic shockwave, previous experimental image of shockwave locations were investigated to pixel level. The image processing work was done by principal investigators and graduate research assistants. Image of shockwave locations near the leading edge of the test article were obtained from experiments conducted by investigators in 2007 through high speed high resolution video (2000 frames per second high resolution recording, 5 minutes of test duration for each test configuration). These images were processed in order to see effect of the electromagnetic field on the shockwave location. Figure 5 shows the sample comparison of images for test #20, at time frames of 3043, 3781, and 4043. These time frames represent the critical time frames when interaction of electromagnetic field with shockwave is on. The history of Red element of the image was extracted from the original video. The cross hair represents the shockwave location in Figure 5. Notice that slight change of shockwave locations was observed. The data file size of the image data for each test configuration is very large, causing difficulty in analyzing the precise history of shockwave movement. Analysis of these images is still underway.

2.6 Conclusions

This DOE Grant provided unique enhancement to high performance computing research and education capabilities at AAMU. It especially increases minority student's interests in pursuing a career towards computational science fields. This program supported faculty research in high performance computing. It established a model laboratory for high performance computing using clusters of LINUX workstations. Graduate student Research Assistants, undergraduate Summer Interns (RAMS), and the DOE Computational Science Scholarships were proved to be the best ways to attract top quality minority students in computational science. With the support of DOE, AAMU has successfully provided research and educational opportunities to minority students in the field related to computational science.

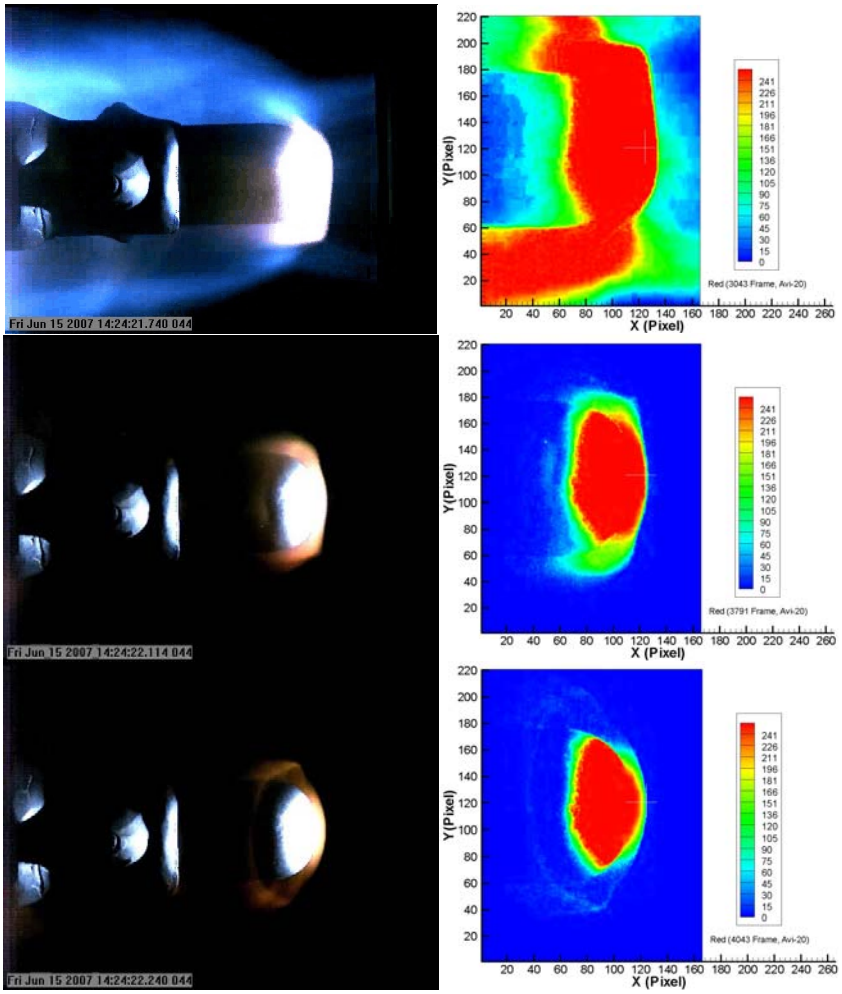


Figure 5. Extraction of RGB-Red from experimental high speed image on shockwave location prediction down to pixel level. Three time frames were plotted. (3043, 3791, 4043) (Results were not published yet)

3. Recommendations

The support provided by DOE-ASCR provided best opportunity for a HBCU like AAMU to prepare themselves in the field of computational science. It is critical to focus on continuation efforts to build overall ability of AAMU to produce best minority scientists through research, summer Interns, and scholarship programs. For AAMU, with the new start of engineering graduate program, computational science education should be extended to graduate engineering program. It is also necessary to continue pursuit of opportunities for research and education collaborations with DoE Labs such as ORNL.

4. Acknowledgement

This project was supported by the Department of Energy Office of Advanced Scientific Computing Research. We greatly appreciate the support of Dr. George Seweryniak.

APPENDIX A
Papers (Abstract) and Presentations

(1). Cathy Qian, Z.T. Deng and George Seweryniak, "Enhancing Minority Engineering Education at AAMU through DOE Sponsored Project," *Proceeding of 2007 ASEE Annual Conference*, ASEE paper # AC 2007-1103. Also Presentation was made at the 2007 ASEE Annual Conference in Honolulu, Hawaii in June 2007.

AC 2007-1103: ENHANCING MINORITY ENGINEERING EDUCATION AT AAMU THROUGH DOE SPONSORED PROJECT

Cathy Qian, Alabama A&M University
Dr. Cathy Qian is an Associate Professor of the Department of Mechanical Engineering at Alabama A&M University in Huntsville, AL. Dr. Qian earned her Ph.D. and M.S. in Mechanical Engineering from the University of Tennessee. Dr. Qian is the principal investigator of the high performance computing research and education project at AAMU.
Zhengtao Deng, Alabama A&M University
Dr. Z.T. Deng is an Associate Professor of the Department of Mechanical Engineering at Alabama A&M University in Huntsville, AL. Dr. Deng has an extensive background and research
experience in Computational Fluid Dynamics numerical simulation in particular high-speed aerodynamics/flows with heat transfer phenomena. He earned his Ph.D., Aerospace Engineering, University of Tennessee, 1991.
George Seweryniak, DoE
U.S. Department of Energy MICS Program Manager.

Abstract
This paper describes our experience in enhancing minority engineering education at Alabama A&M University through a DOE Sponsored project. Strategies, activities and outcome were discussed in the following area: (1) Establishment and enhancement of high performance computing laboratory at AAMU; (2) Training of minority graduate and undergraduate students in computational science and engineering; (3) DOE Computational Science scholarship program at AAMU; and (4) Minority undergraduate summer research interns at the computational science division of Oak Ridge National Lab (ORNL). Outcome assessment was discussed.

(2). Cathy Qian, Z.T. Deng and George Seweryniak, "Lesson Learned from Minority Computational Science Research and Education Project," *Proceeding of 2008 ASEE Annual Conference*, ASEE paper # AC 2008-753. Also Presentation was made at the 2008 ASEE Annual Conference in Pittsburgh, Pennsylvania, June 2008.

AC 2008-753: LESSONS LEARNED FROM MINORITY COMPUTATIONAL SCIENCE RESEARCH AND EDUCATION PROJECT

Xiaoqing Qian, Alabama A&M University
Dr. Xiaoqing (Cathy) Qian is currently an Associate Professor of the Department of Mechanical Engineering at Alabama A&M University. She is also principal Investigator of the DOE High Performance Computing Research and Education project.
Zhengtao Deng, Alabama A&M University
Dr. Z.T. Deng is currently an Associate Professor of the Department of Mechanical Engineering at Alabama A&M University.
George Seweryniak, DoE Computational Science Division
Mr. George Seweryniak is currently the DOE program manager for the research and education project.

Abstract

This paper describes lessons learned from U.S. Department of Energy (DOE) sponsored minority computational science research and education project at Alabama A&M University (AAMU). Project strategies, activities and outcomes were evaluated in the following areas: (1) High Performance Computing Research and training using the high performance computing laboratory at AAMU; (2) DOE Computational Science scholarship program at AAMU; and (3) Minority undergraduate summer research interns at the computational science division of Oak Ridge National Lab (ORNL). The collected data in the past six years were analyzed. Challenges and improvement strategies to get average student involvement in the summer research internship and scholarship programs were presented.

(3). Cathy Qian, Z.T. Deng, George Seweryniak and Debbie McCoy, "RESEARCH ALLIANCE IN MATH AND SCIENCE (RAMS): AN EXCELLENT RESEARCH INTERNSHIP PROGRAM FOR MINORITY SCIENCE AND ENGINEERING STUDENTS" *Proceeding of 2009 ASEE Annual Conference*, ASEE paper # AC 2009-1964. Also Presentation was made at the 2009 ASEE Annual Conference in Austin, Texas, June 2009.

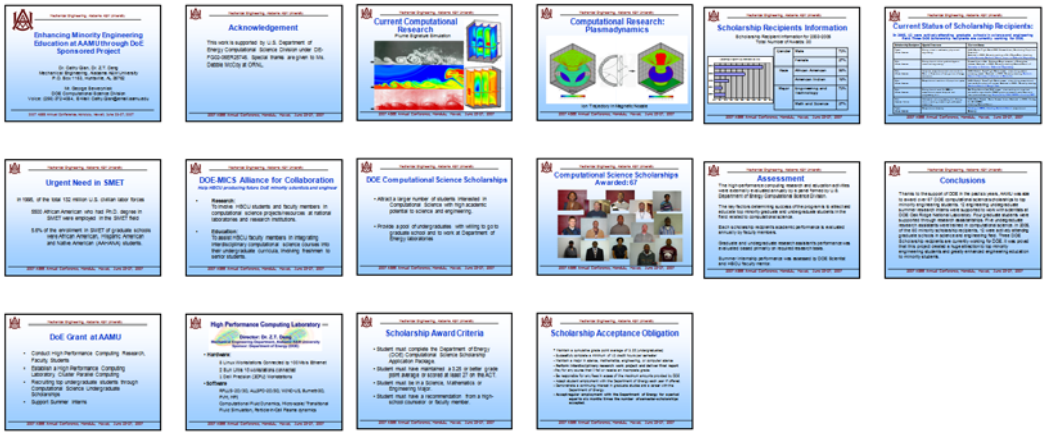
AC 2009-1964: RESEARCH ALLIANCE IN MATH AND SCIENCE (RAMS): AN EXCELLENT RESEARCH INTERNSHIP PROGRAM FOR MINORITY SCIENCE AND ENGINEERING STUDENTS

Xiaoqing Qian, Alabama A&M University
Dr. Xiaoqing (Cathy) Qian is an Associate Professor in the Mechanical Engineering Department of Alabama A&M University. Dr. Qian is also Director of High Performance Computing Research and Education project at Alabama A&M University.
Zhengtao Deng, Alabama A&M University
Dr. Z.T. Deng is a Professor in the Mechanical Engineering Department of Alabama A&M University.
George Seweryniak, DoE Computational Science Division
Dr. George Seweryniak is a program manager in the Office of Advanced Scientific Computing Research of DOE.
Debbie McCoy, Oak Ridge National Lab

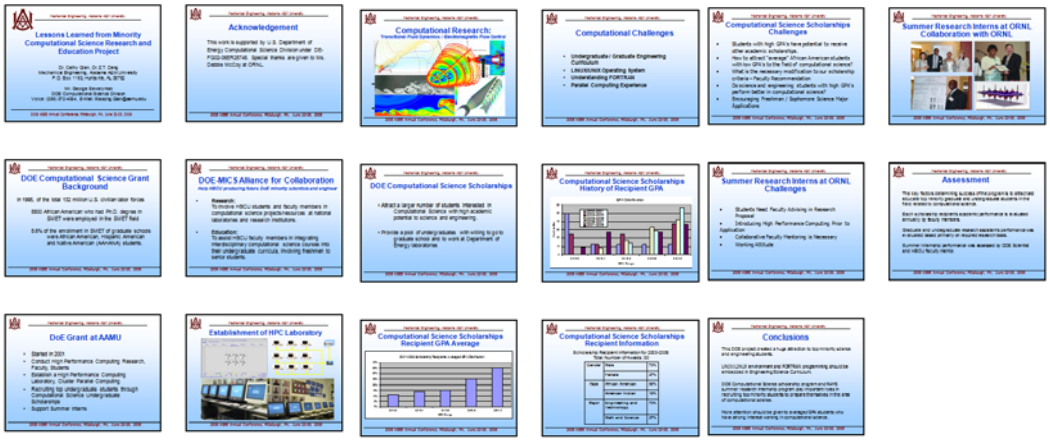
Abstract

The Research Alliance in Math and Science (RAMS) program is a twelve-week summer research internship program for under-represented students majoring in computer science, mathematics, engineering and technology. It is carried out through the Computing and Computational Sciences Directorate at Oak Ridge National Laboratory (ORNL). The objective of the RAMS program is to identify students and faculty members in computer sciences, mathematics, engineering, and technology disciplines for summer internships in support of the long-term goal of increasing the number of under-represented minorities with advanced degrees in the workforce. In the past eight years, more than 100 student interns have been appointed and mentored in the ORNL computing directorate. The RAMS program continues to create high impact on Historically Black Colleges and Universities (HBCU) and other minority educational institutions. Alabama A&M University (AAMU) has been collaborating with ORNL since 2001. This paper describes the RAMS program impact on undergraduate computational science activity in AAMU. The RAMS student research activities indicated that the RAMS summer intern research program provided excellent training for minority undergraduate science and engineering students at AAMU in the area of computational science. The RAMS program opened students' eyes to the fascinating world of scientific computing.

ASEE AC-2007-1103 Presentation:



ASEE AC-2008-763 Presentation:



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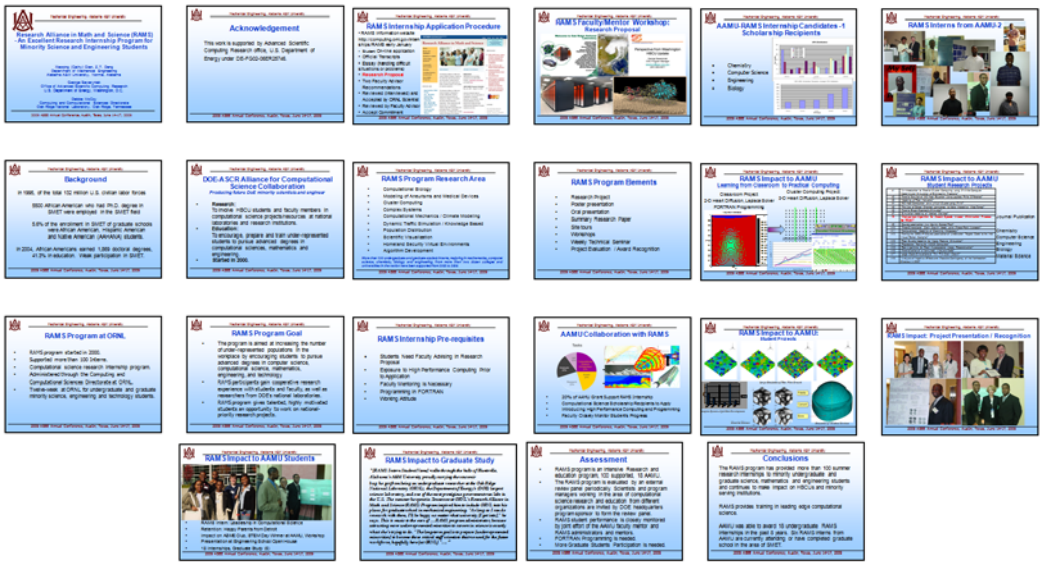
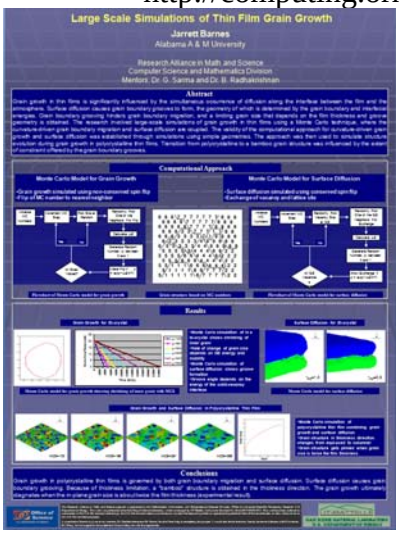
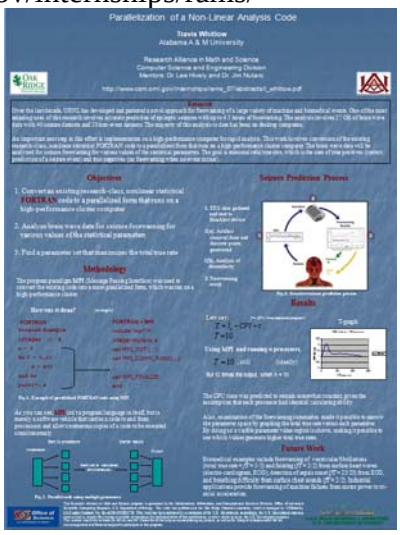


APPENDIX B
Sample AAMU-RAMS Internship Reports
http://computing.ornl.gov/internships/rams/



RAMS 2007-1



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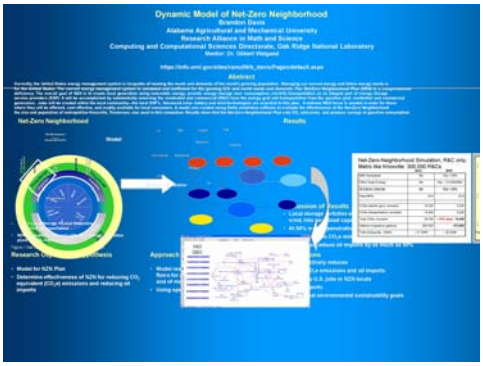
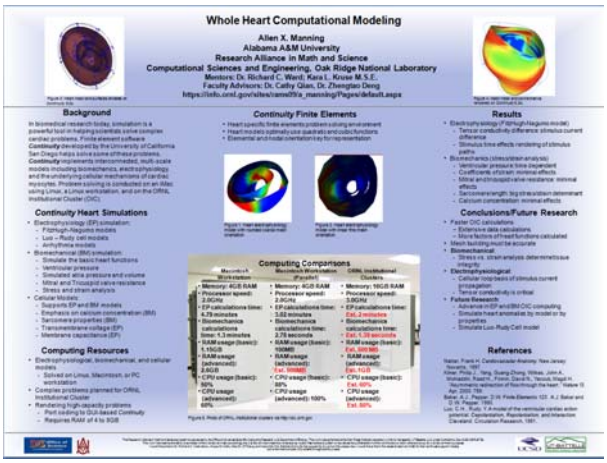
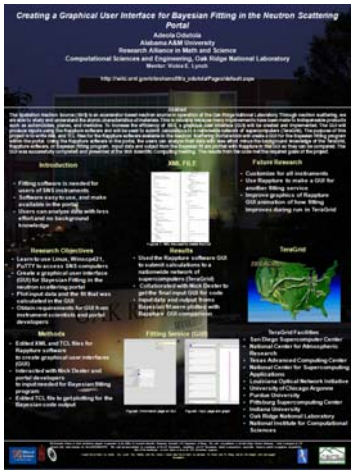


RAMS 2009-1

RAMS 2008



RAMS 2009-2



RAMS 2009-3