5th Computational Science Workshop for Underrepresented Groups

Collaboratory for Advanced Computing Simulations
College of Letters, Arts, and Sciences
Viterbi School of Engineering
5th Computational Science Workshop
for Underrepresented Groups

January 4-10, 2006

Organizing Committee

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Preface

The fifth Computational Science Workshop for Underrepresented Groups (CSWUG) was held January 4-10, 2006 on the campus of the University of Southern California in Los Angeles. Twenty-four undergraduate students and twelve faculty mentors, primarily from Historically Black Colleges and Universities (HBCUs) and Minority Serving Institutions (MSIs), participated in the workshop. Ten graduate research assistants from USC and the three of us conducted the workshop activities.

The workshop gave the participants hands on experience in computer hardware, parallel computing, and scientific visualization. At the workshop, student and faculty participants built a parallel computer cluster from components and then used it to perform selected parallel computing exercises. To prepare for the exercises, the students learned parallel programming techniques and interfaces. Eight experts gave presentations on emerging opportunities for research and education in computational science. At the end of the workshop, each student participant received the computer they had built to bring back to their institution.

Patricia Wong, Richard Clark, Yi-chun Chen and Richard Seymour played a key role in organizing and running the workshop. We would like to thank them and our graduate students, Hsiu-Pin Chen, Zhen Lu, Ken-ichi Nomura, Takehiro Oyakawa, Weiqiang Wang, Cheng Zhang, and Sijie Zhang. The workshop was partially supported by the National Science Foundation and the Programming Environment & Training (PET) element of the DoD High Performance Computing Modernization Program (HPCMP).

Rajiv Kalia, Aiichiro Nakano, and Priya Vashishta
Introduction

This is a report of a workshop held at the University of Southern California to support undergraduate education in the field of computational science. The workshop was supported by the National Science Foundation and the Department of Defense HPCMP.

The Computational Science Workshop for Underrepresented Groups has a mission to provide hands-on experience in a) building a PC cluster, (b) designing parallel algorithms for scientific applications, and (c) utilizing the power of parallel computing. In addition, there were several lectures on emerging trends in computational science and engineering, as well as computer science.

The sponsors of the workshop further facilitated continued learning in those topics introduced at the workshop, by the generous donation of computers to the students. The Computational Science Workshop for Underrepresented Groups has made a real difference in the participants scholarly lives by building on investments by the NSF and the Department of Defense, the Collaboratory for Advanced Computing and Simulations at USC has created an opportunity for training promising young researchers. In this workshop, our country’s future scientists, mathematicians, and engineers can begin to collaborate and build on each other’s unique talents. This program significantly enhances the quality of the participant’s education and provides the highest quality of computational science training to all the students.

Richard Seymour
Student Profiles

Samantha A dato
Mary Baldwin College, Virginia

I am a sophomore and a part of the Program for the Exceptionally Gifted (PEG) at my college. I am a Computer Science/Math major. I am very involved in College Against Cancer, Relay for Life, SIFE, and I am a member of Miscellany, the literary magazine at Mary Baldwin College. I am also a teacher’s assistant for College Algebra, secretary for the Class of 2008, and part of my campus’ Judicial Board. I plan on going into the design of pediatric orthopedics or biomedical engineering, or working with the American Cancer Society to develop new drugs for cancer treatment.

When I came to this workshop, I intended to learn more about computer programming, programming languages, and their uses. I was also interested in learning about what the different options were for students with strong backgrounds in computer science. The workshop has been very informative and stimulating, and I have learned many new things including how to build a PC, new programming languages, and how many other fields rely on the computational sciences for their work.

My favorite activity was assembling the PC on the first day and then learning how to use Unix, which I had used before. I enjoyed meeting the many diverse people at the workshop and learning about everyone’s backgrounds and what they plan on doing with their degrees. I also found it amazing that such a diverse group could come together and all learn to do the same things on a computer, applying those skills to what they are doing on an everyday basis at their own schools.

Olaniyi Bajulaiye
Benedict College, South Carolina

My name is Olaniyi Bajulaiye. I am an undergraduate majoring in Computer Science at Benedict College, Columbia, South Carolina. I have a strong passion for computer-related concepts, especially computer programming. Last summer, I had a summer research with the Center for the Study of the Origin and Structure of Matter (COSM) at Hampton University in Virginia. During the program, I worked on Grid computing. I developed some UNIX scripts to identify information about sites on a grid, in other to enable communication between sites on the grid. I also wrote a C++ program to test a large number for primality on the grid. The program scaled the range of divisors for the number and used each range as a set of inputs for each “condor submit file” generated by the C++ program.

My decision to attend the CSWUG 2006 was borne out of my desire to learn about the different areas of computational science. Attending this workshop has been very beneficial to me. The PC building, Fortran programming and parallel computing sessions were very enlightening. In addition, The MPI programming and Molecular Dynamics sessions have stimulated me to learn more about those areas of computing.

The workshop environment has also been very conducive. The instructors, mentors and students have been very friendly. After my first degree, I intend to conduct research in the areas of Mobile Computing and Artificial Intelligence, and attending this workshop has fueled my desire to achieve my career goals.

I thank the sponsors and organizers of the CSWUG 2006 for this golden opportunity and above all I am grateful to almighty God for the grace to partake of the workshop.

Shanequah Brison
Langston University, Oklahoma

I am working on a minor in Mathematics. Some organizations that I am a part of are Beta Kappa Chi Scientific Honor Society, Alpha Chi Scholarship Honor Society, Scholar’s Club, and L.I.O.N.S. Community Mentoring Program.

This conference has exposed me to things that I wouldn’t have learned at Langston such as Parallel Computing, Message Passing Interface (MPI), and parallel molecular dynamics simulations. The thing that I enjoy the most was building my very first PC cluster and using it to do parallel programming. The lectures that were presented were very interesting in how Computational Science is being used from Chemistry to prediction of earthquakes.

My future goals are to pursue a Masters in Computer Science or Information Sciences, and I would like to work in the area of databases. I would like to thank the National Science Foundation (NSF), Department of Defense (DoD) and the University of Southern California (USC) for this great opportunity to participate in such an informative workshop.
Charles Brown  
University of Arkansas at Pine Bluff, Arkansas

I am currently a sophomore majoring in Computer Science. After obtaining my degree, I plan on attending graduate school to pursue a Masters degree in Computer Science. There is a wide range of careers that I am looking to pursue from programming to software engineering. Since I am not deep into my major, I have not quite narrowed it down on which career to pursue.

Attending the Computational Science Workshop for Underrepresented Groups 2006 has been very helpful and has given me further insight on computer science. At first, I was sort of lost, because I had not taken any computer science courses that dealt with what we went over. With the help of the instructors and the graduate students, it became easier to understand. The information I have learned here in CSWUG06 will be used towards my future classes. I have greatly enjoyed this program, and I will always remember this experience.

Naomi S. Brown  
University of Hawaii, Hawaii

Currently a junior at the University of Hawaii, I’m majoring in physics with an emphasis on astronomy. I’ve seen how large the role of computers is in both of these fields, so I’m always interested in learning more about how technology and science come together. I have some programming experience with astronomical data analysis, but the Computational Science Workshop has helped me gain a better understanding of what’s involved. The basics of computing are clearer, and I’ve been able to see what types of modern-day problems can be addressed with the help of computers.

Career-wise my interests lie mainly in the physical sciences, using physics with astronomy and geology, but I’m also interested in the fields of linguistics, diplomacy, and foreign policy. The workshop lectures included practical applications of technology within many of these fields, which helped broaden my views even more. My goal of this workshop is to leave with a stronger foundation in computing for future physics courses as well as programs, internships, and careers that I might wish to pursue. I want to be competitive in my field, so in my undergraduate career I’m focusing on research, internships, and programs that will provide more knowledge and skills. When I’m not in school or at work, I spend my time hiking in the mountains, reading, surfing the net, playing an instrument, travelling, or practicing martial arts.

Joy-Ann T. Colbourne  
University of the Virgin Islands, St. Thomas

I was born on the exotic island of Antigua, but I currently reside within the United States Virgin Islands, where I received my secondary education. I am currently a sophomore on the island of St. Thomas, and I am enrolled in the co-op program between my university and Columbia University in which I will receive a dual degree: a Bachelor’s of Science in both applied mathematics and engineering. After graduating, it is my dream to become a member of the Hovensa Oil Refinery in St. Croix (in the U.S. Virgin Islands), where I will specialize in chemical engineering.

This workshop allowed me to build a PC, giving me the opportunity to focus on a different aspect of science. It also reinforced my basic programming skills and enabled me to work in different computer languages such as Fortran 77. Even though this conference is coming to an end, I want to establish a hold on the information I have learned here, especially on parallel programming.

During this workshop, my perspective has changed about computer science. The lectures and hands-on learning sessions have established a yearning desire to learn more about programming. As I return to school for the spring semester, it is now my goal to minor in computer science.
I hail from Lagos, Nigeria. I am a junior majoring in Electrical Engineering. Last summer, I conducted my research at Hampton University in Virginia with the Center for the Study of the Origin and Structure of Matter (COSM). I conducted research in physics using ROOT, a software designed for physicists. It was really a wonderful learning experience, but this summer I seek research in nanotechnology. I have also considered internships in the networking and wireless communication industry. I especially believe that an internship opportunity is necessary, as it prepares me for graduate school. After I get my Bachelor’s degree, I intend to pursue a Master’s degree in Electrical Engineering with a concentration in Communications Engineering at Caltech. I hope to obtain a high GRE score to secure a scholarship.

From this program, I intend to gain a lot of practical knowledge about computers, simulations, programming and more. I already enjoyed the fact that we got to assemble our own computer. This is something I have always wanted to learn how to do. I have learned to perform simulations on parallel computers, and I dare say that the presentations have broadened my horizon on a lot of things.

I enjoyed the presentations from Professors Rajiv Kalia, Aiichirio Nakano, William Goddard, and the ever-knowledgeable graduate students. I particularly enjoyed Thomas Jordans presentation entitled Computational Challenges in Earthquake System Science.

Overall the program has being interesting and educational, and I totally welcome the idea of coming back here next year to gain some more knowledge of computers, if given the opportunity.

I am originally from Milwaukee, WI, but I currently live in Atlanta, GA where I am a senior at Spelman College in Atlanta, GA. I will be receiving a B.S. in Mathematics with a minor in computer science. Upon graduating from Spelman College I plan to attend graduate school in mathematics, particularly in the field of applied mathematics or interdisciplinary sciences. My ultimate career goals (subject to change) are to continue in industrial research and eventually become a teacher.

In coming to this computational science workshop I hoped to learn more about exactly what computational science entails. I expect my graduate studies to be computationally intense and this conference is the perfect opportunity to get a first-hand look at research possibilities in the field and what I can expect as a graduate student. I especially enjoyed being able to build my own PC and I found the presentations very informative. I would recommend this conference to any student with an interest in applied sciences. It was extremely beneficial.

Mary Baldwin College is a women’s college in Staunton, Virginia. I am working towards degrees in both Mathematics and Studio Arts with an emphasis in painting. I will be graduating in May 2007. My plans for after I graduate from Mary Baldwin College are to go to graduate school and work towards a PhD in Mathematics. With a PhD in mathematics I want to pursue mathematical research.

I have always had an interest in Computer Science and programming, so when I heard about the Computational Science Workshop for Underrepresented Groups it sparked my interest. Since being here, I have learned a great deal, including how to put together a PC and also a new programming language. Through a variety of different presentations and lessons, I have learned how computational sciences are affecting the modern world and the future. By going through this workshop, I hope to gain a better understanding of the computational sciences and, also, to see how mathematics affects the computational world. I am very thankful for the computer I was given at this workshop. I intend to use this gift to further the knowledge I received from this program.
Duvano Garnes
Livingstone College, North Carolina

Hi! I am a native of the Republic of Trinidad and Tobago and a graduating senior of the class of 2006. As a chemistry major, my interest in science and technology has developed to the point where I believe that I can pursue a career as a research scientist in the near future. For this reason, the workshop here at the University of Southern California was beneficial value to me.

Throughout the workshop, the environment was both intellectually and socially stimulat- ing, I learned about PC building, OS installation, Fortran, MPI, and many other higher-level operations which, overall, increased my knowledge base of computer science and technology. The staff, professors, faculty mentors and participants of this program have all added to the fantastic experience not only at the USC campus but in Los Angeles in general. I will definitely carry this experience of my first trip to California with me and have good stories to tell. Thank you!

My hobbies include playing soccer and the steelpan, hanging out with good friends, and going to a good party once in a while. I have a great appreciation for all genres of music: classical, 70's and 80's music, R & B, soca, calypso, reggae, Latin, you name it! More importantly, my ultimate goal is to use the benefits of my academic experience to make a significant contribution in the field of science and technology, and to share my expertise to create opportunities for present and future generations.

Saenya M. Grant
Oakwood College, Florida

My name is Saenya M Grant. I was born on the beautiful island of Jamaica, and I now reside in Ft. Lauderdale, Florida. I presently attend Oakwood College in Huntsville, Alabama, where I'm a junior majoring in Chemistry and minor in mathematics.

I aspire to be an undergraduate Chemistry and Mathematics professor when I finish school. To assist me reaching my aspirations I work as a tutor in calculus and organic chemistry. Being a tutor has really helped me reach out to students who were in need, which is something I like to do. I also had the opportunity to work as a physics lab instructor, which gave me the ability to gain more skills working with others.

At Oakwood College, I'm a member of Mkon-Nia drama ministries, alpha Chi honor society, student government, where I'm the senator of my dorm, and Sigma delta Alpha math and Computer Science club. I'm also a member of the national Dean's list and American collegiate scholars.

Being a part of the math and computer science club has opened my mind up to more than just things in chemistry. Through the club I found out about this conference. At first, I didn't see how computer science could help me in chemistry, but once I received more information about the conferences I realized that, if I attended I could learn more about computers and how they operate. I realized that I would have the chance to be exposed to an area that I never understood.

Attending the conference at USC has helped me to learn things that I never found interesting before now. I learned how to build a computer, which was a tremendously exciting experience. I’m also gaining knowledge about computer programs, like FORTRAN and MPI. I knew very little about how programming languages operated, but daily I'm learning more, which is helping me understand this area of computers better.

Being involved in this conference has given me the opportunity to meet students and faculty from other colleges all over the United States and other parts of the World. When I leave this conference I hope to gain an understanding of computer programming languages and how to create different programs. I hope to gain information about the parts used to build the pc and how the parts make the computer what it is. I also hope to gain information that I can share with students in the mathematics and computer science club. Finally, I hope to learn things that can help me with career in chemistry in the future.

Vincent Hall III
Edward Waters College, Florida

I am from Fayetteville, North Carolina and attend school at Edward Waters College in Jacksonville, Florida. I am currently a sophomore, seeking a Bachelor of Science in Computer Information Systems.

I became interested in this workshop because I wanted to learn more about computer programming, parallel computing, and building a PC. The program is a great networking tool to other professors, colleges, programs, and internships at the University of Southern California, and other colleges. The most enjoyable part of the program was building a PC.

I plan on using my degree and skills learned at this workshop to attend graduate school, possibly at USC for a Masters Degree in Video Game Programming, or working for the Department of Defense.
Student Profiles

Mikia A. La Rue  Delaware State University, Delaware

As a junior at Delaware State University aspiring toward a dual degree in computer science and mathematics, I have worked to build a rapport among students and faculty as a leader, a role model, and a scholar. I am not only active in the enhancement and empowerment of the campus community but also in the community surrounding the university. As the president and member of several organizations such as AMP, MAA, NSBE, and NAACP, I have lead my fellow members in several charitable events to lend assistance to those in need across the country. I have maintained a GPA that keeps opportunities knocking and scholarships available to her dispose.

As my future progresses towards graduate studies, I will be able to use the information and connections I have obtained to encourage my classmates to continue their educations and to empower themselves through programs such as CSWUG. I am extremely grateful to the DoD, NSF, and USC for providing such a beneficial and memorable opportunity.

Cindy J. Mondragon  University of Arkansas at Pine Bluff, Arkansas

As a native of Lake Village, Arkansas I attend the University of Arkansas at Pine Bluff. On May 13, 2006 I will obtain my bachelors degree in biology, chemistry. After graduating I plan to enroll in a masters program in public health administration and later attend medical school.

Furthermore, as a UABP student I am actively involved in numerous organizations: honors college, Alpha Chi National Honors Society, Ronald McNair Scholars Program, LULAC, NAACP, Tau Iota Mu, INSPIRE, RISE, STEM, SNMA, and Union Programming Board. My intense participation in extracurricular activities and academics motivated me in attending CSWUG 2006. The reason for applying to the program was because I wanted to learn how to use computer programs and how they influence every field of study in life. Indeed the workshop has broadened my understanding in computational science although it did get confusing. Personally, I have learned so much in such a few days about simulations in Parallel MD, MD, and atomistic simulations. Physically interacting with the construction of the CPU was the most interesting activity. After all putting all the pieces together is not as difficult as it sounds. I thank the CSWUG committee for giving me the opportunity to learn computational science and the programming techniques.

Steve Mondragon  University of Arkansas at Pine Bluff, Arkansas

My name is Steve Mondragon. I am from a small town in southern Arkansas. I am currently a junior at the University of Arkansas at Pine Bluff and I am working on my B.S. degree in Fisheries Biology. Furthermore, I hope to pursue graduate studies in wildlife law enforcement. At UABP I am not only I academically oriented but also involved in several school organizations: Honors College, American Fisheries Society, Arkansas Fisheries Club, LULAC, Navigators, and TAU IOTA MU. My interest in learning more about computers inspired me to attend the 2006 CSWUG workshop. I can satisfactorily say that I have learned more than I ever thought I could. The exercise which I enjoyed the most was the one on constructing the computer itself. I can successfully say that this workshop has really broadened my understanding in computational science. Lastly, I plan to use all the skills that I have acquired during this workshop in future computer assignments.
I. Sandrine Nana

I am originally from Burkina-Faso, a small French-speaking country in West Africa. When I was in high school back in Burkina Faso, the trend was to pass the national high school exam and to secure an admission at the University of Ouagadougou, the only public university in my country. Although I knew that my parents could not send me to a private university or to a university abroad, I still wanted to get a better education that the education provided at hometown University (where classes are often canceled due to protests and riots).

After I graduated from high school, I applied to study at the United World College (UWC), which is an international baccalaureate program. I was offered full scholarship to study at the UWC of New Mexico. After two years at the UWC, I went to Hood College, Frederick, MD, where I am currently pursuing a double degree in computer science and business Management.

My short term goals are to graduate with a double degree in computer science and business management (with a concentration in international finance and economics) and to get one or two years work experience in one or more of the following fields: software engineering, web services/web design and modeling and simulation. Then, I intend to pursue a master degree in software engineering and information technology (and maybe also a master in international economics).

This workshop was a great opportunity for me to learn more about computers in general and to be introduced to the use of computations in various areas including physics, chemistry, defense, biology, etc. I intend to use the knowledge I gain from this workshop by investigating more about modeling and simulation and by taking the opportunities available for undergrad students (such as internships and research opportunities). Another thing that I found beneficial during this program is the fact that I was thought how to assemble a computer from components.

I never hesitate when it comes to learning new things and I am glad that the 2006 computational workshop gave me the opportunity to increase my knowledge in computer applications, parallel programming and to be exposed to new ideas and knowledgeable professors and students at USC.

Gavin-Ajani N'avarro

My name is Gavin-Ajani Navarro, and I am a 18 years old junior at the University of the Virgin Islands, St. Thomas campus. I was born on the beautiful Island of St. Croix to Maria Navarro. I graduated salutatorian of my high school class and is currently major in chemical engineering. I am enrolled in a co-op program between University of the Virgin Islands and Columbia University. When I finish with college, I would like to have several degrees including a Bachelor of Science in Applied Mathematics and Bachelor of Science in Chemical Engineering.

After college, I plan to become employed by the Hovensa Oil Refinery on St. Croix for several years. After establishing myself in good standing amongst chemical engineers, I would like to explore other corporations for employment. I plan to becoming a senior chemical engineer of a major corporation before I retire.

I am attending the Computational Science Workshop for Underrepresented Groups (CSWUG) to gain more understanding about computer and computer science. I am still deciding whether if I should obtain a associates degree in computer science or not, so I hope that this program would help bring me closer to my decision.

Christopher A. Norris

As a Officer Candidate Surface Warfare (SW) I am dual enrolled at the University of Texas and Huston-Tillotson University in Austin, Texas. I currently studying for a Bachelor of Science in Computer Science. Once earned, I will be commissioned as an Ensign in the United States Navy. My aspirations for the future lie in gaining a position as a pilot with the National Aeronautics and Space Administration (NASA), opening a baseball pitching and hitting clinic in order to do research in human molecular movement via computer simulation to decrease injuries in baseball pitchers, to further grow his business that he currently owns and operates in New Braunfels, Texas, and engaging in any other opportunities that may come my way that I may not even know about at this time.

The Computational Workshop at USC, up to this point, has been phenomenal. As stated above, there are so many opportunities that I do not have the knowledge of. Being accepted to this workshop it has been a pleasure and an honor. I will continue to Network with the individuals that are participating in hopes of learning about more opportunities where my services can be rendered helpful. I am always open to opportunities that I can help others as well as gain the knowledge they have to offer in the process. Thanks for selecting me for this workshop, and I hope to visit this campus in the future to learn more in the computational sciences.
Danielle Roberson

I am a young man with aspirations in the interactive entertainment, or videogame, industry as well as teaching computer science. Because I have played videogames since childhood, I find videogames and their production very interesting. I have attended the last three Innovation, Creativity, and Capital (IC3) Institute programs (which is a University of Texas company) on videogames, conferences on artificial intelligence, game simulation and networking. I believe I can help mold new minds in the computer sciences and attending two education seminars has helped to reinforce this belief.

To help myself along, I have completed Associates of Art in Local Area Network Administration, and I am currently working on my Bachelor of Science in Computer Science. I am apart of Huston-Tillotson University’s (HTU) Student Government Association Rules and Regulations Committee as well as HTU’s Linux Group. I have built a Linux lab under the regulation of the Information Technology (IT) department at HTU, as well as design labs for the Linux lab to be used on the network I have built.

Gary Roberts

I currently attend Florida Memorial University in Hialeah Florida. I am in my Junior year. I plan to earn a Bachelor of Science degree in the field of Electrical of Engineering. Furthermore, I am considering doing a double major in Computer Engineering as well to further help me in my interest to work for a power company, however my mind is open to other options as well. My aspirations also include obtaining a Master’s Degree in Business and Electrical Engineering. Also, I want to get my PhD, however at this time I am not sure exactly in which field to focus, however I will choose a field close to Electrical Engineering. There is no area of scientific study that doesn’t stimulate me, but my favorite area of study has to do with physics and closely related research.

The Computational Science Workshop for Underrepresented Groups has given me a chance to work programming scientific applications. I have gotten a feel for programming in Fortran and computing across multiple CPUs.

Aduramigba Sopeju

My name is Aduramigba Sopeju, and I am a junior majoring in Electrical Engineering and Physics. I have a very strong affection for computer hardware and programming.

In the past, I have had multiple programming assignments, which included writing a data acquisition program for a new Keithley multimeter, designing and implementing a student database system and also writing a client email program. Last summer, I was a research intern at the European Organization for Nuclear Research [CERN] in Geneva, Switzerland. I worked on the assembling, testing and calibration of the “Forward Calorimeter” for the Compact Moun Solenoid [CMS]. This will be an integral part of the Large Hadron Collider [LHC] being constructed to investigate the Higgs boson. During my work at CERN, I was able to pinpoint the possible sources and avenues for light leaks, which had been a persistent problem for the group. I also tried to eliminate these light leaks as much as possible.

Upon graduation, I will pursue a Ph.D. in the area of nanotechnology. I decided to attend this workshop to broaden my understanding of parallel computing and also learn some principles behind the implementation of the Grid. At the conference, I was able to learn how to use FORTRAN and MPI programming, which I believe would be useful for my career in experimental research. I am very thankful for the PC that was given me, because it will help me continue to practice and advance my skills acquired at this conference.
Gabriel J. Williams, Jr.  
Morehouse College, Georgia

Currently, I am a Senior Mathematics and Physics major at Morehouse College. My interest in mathematics dates back to high school where I excelled in AP Calculus. I learned throughout my matriculation process that mathematics is a very exquisite art form with intrinsic beauty. However, my interest in physics occurred in college when I began to take several physics courses. After taking these courses I realized the interconnectedness of mathematics and physics. From my physics courses, I saw that beauty of mathematics intertwined with the applicability of physics. I learned that mathematics wasn’t just a form of art, but it is the language of nature. Because of my love for both subjects, I plan to further my study in physics and mathematics.

After graduating from Morehouse, I plan to obtain a Ph.D. in Applied Mathematics because of my interests in mathematics and its various physical applications. After obtaining my Ph.D., I would like to become a research professor at a research-oriented institution. I believe that one of the keys in growing the economy of a nation is in developing the infrastructure of the science and technology sector, which includes both the education and research of science and technology. Therefore, during my career as a successful researcher, I would like to help develop the science and technology sector in other underdeveloped countries around the world.

The CSWUG 2006 conference has been very helpful in developing my skills as an applied mathematician. In today’s society, an applied mathematician must also be proficient in computational science as well as theoretical mathematics. This conference has helped hone my programming skills in FORTRAN as well as teaching me the fundamentals of parallel computing. Also, the presentations have given me many ideas concerning the use of computer simulation and modeling in many different areas of science. The networking opportunities with students and faculty at this conference are extremely valuable as well.

Shelby Wilson  
Spelman College, Georgia

I am a native of Milledgeville, Georgia and currently a graduating senior at Spelman College. In May of 2006, I will be receiving a Bachelor’s of Science in Mathematics and Computer Science. After graduation, I plan on attending graduate school in applied mathematics, where I intend to concentrate in computational mathematics. Following graduate school, I plan on going into the industry to conduct research in mathematics.

I came to this program to learn more about interdisciplinary research and how my background in mathematics and computer science can be applied to other areas of science. I am very interested in computer simulations and modeling and the talks on application areas of computer simulations and modeling have sparked my interest.

I particularly liked creating a simulation of atom interactions using FORTRAN. My experience in the Computational Science Workshop for Underrepresented Groups has further confirmed my goals for doing graduate study in the area of computational mathematics.

Briana Young  
University of Arkansas at Pine Bluff, Arkansas

I am a senior majoring in Computer Science and Information Systems. At this time, I am exploring several options of what I would like to do after graduating from college. I am currently seeking internship opportunities to gain experience in my field of study. My ultimate goal is to work for a large communications company, such as SBC.

The reason I wanted to attend this workshop was to gain more knowledge about computer science and to get the hands-on experience with computers that I have not been about to receive while attending UAPB. The second reason for attending this workshop was to have the opportunity to meet students from other universities who are majoring in computer science and to learn about the direction in which they have chosen to take in this field. It has been beneficial to talk to the graduate students and learn about their experiences in undergrad and what they did after graduating.

While attending this workshop, I have learned so much. Some of the things I learned include proper way to build a PC, load the operating system, and learning about programs funded by the Department of Defense.
Cynthia Brooks  Bennett University of Arkansas at Pine Bluff, Arkansas

I currently serve as a Computer Science Instructor at the University of Arkansas at Pine Bluff. I teach programming languages, networking technology and information science. My current interests include database design and web technology. The University is collaborating with the National Science foundation (NSF) with our STEM project. The STEM project has attracted a very intellectual group of students, who have been exposed to a vast array of computer concepts. The computer science unit will place a great emphasis in providing a new and challenging curriculum for those students who enter our program having already been exposed to similar subjects. The attendance of our faculty and students to programs such as the CSWUG is only the beginning which will also enhance faculty teaching and research capabilities.

Angela Daniels  Philander Smith College, Arkansas

My name is Angela Daniels, and I am an Adjunct Professor of Mathematics and Computer Science in the Natural and Physical Sciences Division at Philander Smith College. With an approximate enrollment of 1000 students, Philander Smith College is a private HBCU located in Little Rock, Arkansas.

I received a B.S. in Mathematics and Computer Science. During my undergraduate career, I worked on numerous research projects through the National Science Foundation in conjunction with Xavier’s AMP (Alliance for Minority Participation) and Dwight D. Eisenhower Fellowship through the Department of Transportation. After graduation, I received a position at the Arkansas State Police as a Senior Programmer/Analyst. This position allowed me to merge my interests in Intelligent Transportation Systems with my skills in Software Engineering. During this period, I completed a M.S. in Operations Management from the University of Arkansas, Fayetteville.

Currently, I am working on a Ph.D. in Industrial Engineering with an emphasis on Optimization. My research interests include Intelligent Transportation Systems, Combinatorial Optimization, Graph Theory, and Software Engineering. I am hoping to do my dissertation in the area of Vehicle Routing Problems with an emphasis on Real-Time and Time Windows.

My hope from attending this workshop is to come away with enough experience to spark interest among my college in the area of Computational Science. Furthermore, I hope that this workshop exposes me to areas of Computational Science that will aid me in the preparation of my dissertation.

Khalil M. Habash  Wilberforce University, Ohio

I am an Assistant Professor of Electrical Engineering at Wilberforce University in Wilberforce, Ohio. My areas of interest include digital design, integrated circuits and electronics. I am involved in advising and monitoring my students for the Ohio Space Grant Consortium Scholarship (OSGC) and the Students Achievement in Research and Scholarship (STARS) programs.

The courses that I teach include Circuit Theory, Analog Electronics, IC design and Computer Literacy. What I hope to achieve from attending this workshop is the involvement with underrepresented groups and the knowledge that I will gain in building a PC cluster, designing parallel algorithms and the use of grid computing.

I hope that I can apply these skills and knowledge in my classes and pass the experience to my students to raise the awareness and the importance of Computational Science.
Ayivi Huisso, Ph.D.  
Florida Memorial University, Florida


For devices operation and performance, the study of the fluctuations of transport coefficients is important. We use stochastic Boltzmann equations to evaluate correlations in single particle state occupancies leading to the noise calculations in the mesoscopic devices but for submicron devices we use the quantum statistical many-body master equation for reduced density operator and the correlations and quantum noise are computed. Our present challenges are to apply the quantum statistical model for coefficient fluctuations in nanodevices through analytical and simulation methods.

This computational science workshop is an important avenue for me to learn new topics such as parallel programming, atomistic simulations and MD simulations applicable to my research fields. The presentations give a great opportunity to exchange directly ideas with the authors. Thank you very much for inviting me to attend this computational science workshop and for all your financial support.

Dr. Sharon Lewis  
Langston University, Oklahoma

In December 2002, I received my Ph.D. from the University of Oklahoma, Department of Chemistry/Biochemistry. In August 2003, I became an Assistant Professor of Chemistry at Langston University, in Langston, Oklahoma. Since I have experience in human, bacterial, and plant functional genomics, I established a bioinformatics lab at LU in August 2004 where I have mentored 25 scholars in molecular biology and bioinformatics.

I am the campus coordinator for the NSF funded Oklahoma Louis Stokes Alliance Minority Program (OKAMP) which is in its third phase of transitioning ten undergraduate scholars to doctorate programs.

I am also the campus coordinator for the Academy for Applied Science funded, Research and Engineering Apprenticeship Program (REAP). Six unique high school students work in my lab during the month of June gaining valuable hands on experience with the Human Genome Project, Functional Genomics, Molecular Biology, and Bioinformatics.

I have a collaboration with Dr. Hugh Nicholas, Jr., of the Pittsburgh Supercomputing Center (PSC) to establish a bioinformatics course, curriculum, or Masters Program in Bioinformatics.

Participation in the 5th Computational Science Workshop for Underrepresented Groups will has allowed me to expand the scope of my bioinformatics lab to include allowing the interns to build a PC, teaching UNIX and using it for DNA sequence analysis, adding Fortran or Java programming to some aspect of the sequence analysis for generating primers, computational chemistry from PSC, using chemical simulations during teaching and for poster presentations during symposiums, using molecular dynamics and quantum mechanics while investigating the properties of asphalt.
Dr. Xinlian Liu

I am an assistant professor in the department of computer science at Hood College in Frederick, Maryland.

I received a PhD in computer science from LSU with the group. Attending CSWUG is like a homecoming experience, especially during a college football season. Geaux Tigers! I would like to explore opportunities to reach out to people with similar interests in high performance computing (HPC), and build collaborative research ties.

My primary research interests lie on the computer science side of HPC, include algorithmic development and performance analysis in the theoretic aspect as well as scientific visualization and data mining in the applied sector.

I also hope to use this workshop to stimulate interests in computational sciences among our students. Midway through the workshop, I learned from colleagues back in Maryland that the student I brought here already wrote home about what she had learned here enthusiastically. A loud applause for the organizers!

For students interested in working with computer simulation at Hood College: Frederick, Baltimore and Washington D.C. formed the Mid- Atlantic Triangle, with 40 miles apart each other. You will find good food, good weather with all four seasons, and close approximate to federal agencies and the I-270 Technology Corridor. Graduating seniors are welcome to apply to our MS programs in computer science and information technology at Hood.

Julia Oroian

I am professor of Computer Science and Computer Engineering at Benedict College, in Columbia SC. Having earned a Master’s Degree in CS and CE from USC (University of South Carolina), I am continuing with a doctoral degree at the same university.

My interests lie in the field of Bioinformatics and Genomics. The most important and captivating work in this field that I have done so far is participating in a two-year research project funded by USDA and HS aiming the design of a computational tool able to assist humans in determining if an unknown pathogen is a naturally emerging one or an engineered one. The latter situation is thought of as being mainly with bioterrorist intentions. A recent example of the occurrence of a new pathogen is SARS, the avian virus that naturally (without human intervention, happily) mutated to attack new hosts: humans.

In the light of my interests CSWUG is most valuable. Supercomputing, parallel computing, the main topics at CSWUG06, are a must in applications having to deal with genetic information. I am very grateful for the opportunity of participating to such an enriching workshop, in which the intense hands-on applications, alternating with interesting presentations and talks are extremely inspiring. But probably the most important aspect to mention is the binder of this scientific manifestation - the warm, encouraging, and dedicated atmosphere created by the wonderful CACS team at USC.

Besides the immediate scientific enhancement that all of us here have been so generously exposed to, the long term profit I hope to achieve as an outcome of my participating to CSWUG 2006 is continuing and initiating scientific and research activity in my school, back in SC.
Dr. Tony Lee Perry  University of the Virgin Islands, Virgin Islands

My goals include providing educational opportunities to my students. I’m interested in developing computer perspectives to my drug discovery program of Natural Products, Synthesis and Molecular Modeling. I’d like to develop combinational therapy using nano-second high frequency pulse to enhance the potential of small molecules. This combinational therapy will be used in conjunction with differential gene expression (DGE) data in toxicology profiling. This will provide new information on anatomic, physiologic, biochemical, immune, and other underlying factors that drive mechanisms of tissue responses to noxious agents.

My research involves the use of computers to model drug/receptor interactions. Pharmacogenomic and toxicogenomic applications to drug development has led to a significant increase in the use of computers to minimize late-stage development failures. This workshop provides training, as well as a prospective view to key application issues and questions that are confronting medicinal chemistry investigators. I’m extremely interested in building PC Clusters and to apply this knowledge to drug discovery.

The experience gained through CSWUG has encouraged my efforts to develop a computational chemistry curriculum at the University of the Virgin Islands.

Periasamy Ramalingam  Albany State University, Georgia

The main objective of my coming to this Workshop is to gain an insight into effectively using computing in my teaching. I currently teach Physics and Pre-Engineering courses at Albany State University (ASU), Albany, GA. The Pre-Engineering courses are highly computing intensive. These courses are Engineering computing, signal processing using Matlab and computer architecture. All these are transfer credit courses for students under the RETP program (Regents Engineering Transfer Program) and bound to Georgia Tech at the end of the second year at ASU.

Attending this workshop will also provide me some intuition to apply mathematical modelling for some physical problem such as pollutants discharge from industrial sites. My current research are Optical interferometry and the use of Laser Raman spectroscopy to determine the stress induced phase transformation of partially stabilized zirconia ceramics.

Currently involved in HBCU-UP and MBRS-RISE programs in my campus which focuses on gate keeping courses and also on transfer to graduate schools. My school encourages faculty to gain professional development and provides opportunity to implement such new ideas by obtaining grants from various government organizations.
Dr. Marwan Rasamny  
Delaware State University, Delaware

I am an Associate Professor and Chairperson of the Department of Computer and Information Sciences at Delaware State University in Dover. In addition to teaching the standard data structures and algorithms courses, I have been involved in designing and teaching parallel processing and compilers courses. I have also taught computer networks and operations research.

My main research areas of interest include first principles and other (both formal and computational) approaches to electronic, magnetic and structural properties of condensed matter systems. I have worked on understanding binary alloy phase diagrams using a combination of first-principles calculations and statistical mechanics. I have engaged in the development of parallel computational first-principles techniques to study defects and other properties of Ni-Al and Pd based systems; the later with particular emphasis on improving catalytic properties. I have an interest in developing quality interatomic potentials from first-principles calculations for use in molecular dynamics calculations to study large complex systems.

As an educator and chairperson, I have been very interested in ways of improving student advising. I am currently engaged in developing a data-base supported system for undergraduate student advising and tracking as well as a collaborative university course scheduling system. Since finding optimal or good solutions for scheduling problems, I believe that this is an excellent opportunity to get students involved in developing and implementing parallel algorithms that provide good solutions.

The mentor-student approach of this workshop will allow me to get students involved in computational science and parallel code development and should prove valuable to faculty members in the Department. This workshop has also given me insight and ideas into having a workshop for our department that will help get faculty in my department started in applying the parallel processing paradigm to their research in video surveillance and tracking.

Nakamuthu Sundaralingam, Ph. D.  
Edward Waters College, Florida

I am an Associate Professor of Physics and Chairman of the Division of Mathematics and Sciences at Edward Waters College, Jacksonville, Florida. I graduated from Tufts University, Medford, Massachusetts and I did research on Cosmic Ray Physics. My current interest is in computer simulations using parallel computing. In fact, I have built my first 24 nodes Beowulf parallel computing cluster at Edward Waters College. I am planning to utilize this cluster to extend my research activities in cosmic ray simulation.

I am also a Principal Investigator/Director for the two programs at Edward Waters College supported by Department of Army, Army Research Laboratory. I am expecting to work at Army Research Laboratory along with three of my students during this summer 2006.

My interest in this workshop is to learn about programming for parallel computers and to learn how parallel computer cluster works. This is great opportunity for me and one my student who came to participate. This workshop also gives me an opportunity to meet several other people particularly doing research using parallel computing techniques.
Ahlam Tannouri  
Morgan State University, Maryland

I am a Senior lecturer in the Department of Mathematics at Morgan State University. I hold a PhD in Mathematics from Paris VI, Pierre and Marie Curie, France. My research interest is shifting from mathematical modeling of dynamical systems to computational biology.

I am currently developing new applied Mathematics courses for our newly established M.S. in Bioinformatics, and computational Mathematics courses for our engineering students. I have a strong background in theoretical applied Mathematics; I came to the CSWUG 2006 workshop hoping to deepen my understanding and broaden my experience in hands-on simulation. Learning MPI, parallel MD and grid computing has added a new dimension to my research goal, which in fact will help me to expand the opportunities for my students in the Sciences and Engineering.

The CSWUG 2006 was intensive, extremely beneficial, very well organized and run by an excellent and dedicated team from USC. My Future Plans include writing proposal to implement similar computational science workshops in other countries.
Patricia Wong
I am the budget coordinator for CACS. I worked on organizing CSWUG 2006. I was very happy to see so many polite students eager to learn and network. Their level of maturity and teamwork impressed me. It has been a great experience and I look forward to organizing CSWUG 2007.

Yi-Chun Chen
I am focusing on nanoindentation and friction in energetic materials. Using the reactive force fields method (ReaxFF) we can introduce chemical reaction into the simulations, allowing us to discover new properties. While working on my PhD in Physics, I am also pursuing a Master’s Degree Computer Science. The CSWUG program gives us graduate students a great chance to meet people who share the same interests and enthusiasm.

Zhen Lu
I am currently a Ph.D student in Material Science and also pursuing a Master’s degree in Computer Science. My major research focus are cracks under compression, focusing on MD simulation of crack initiation and propagation. Other topics include stress corrosion and indentation simulations. I have been to CSWUG before and I enjoy participating. It is a wonderful experience to help such enthusiastic students.

Weiqiang Wang
I am a student in the CACS group working on my PhD in Materials Science. I have taken part in the CSWUG three times. Each time, I enjoyed having the opportunity to meet with new students and help them gain more knowledge in computational science. It is always my great pleasure to help participants get started in the field.

Ken-ichi Nomura
I am currently pursuing a Master’s Degree Computer Science and a PhD in Physics. I am also working for CiSoft program between USC and Chevron. My current interest is an atomistic approach to material modeling utilizing hierarchical nature of a given system. Implementing such models on high performance parallel/distributed computing architecture is my specialty. Participating in CSWUG gives me a great opportunity to share my work with smart students interested in the things I like to do.

Hsiu-Pin Chen
I am a PhD student in Materials Science and I will also pursue a Masters degree in Computer Science. My research is currently focusing on nanoindentation simulation on different crystallographic directions of 3C-SiC. Nanoindentation on nanophase materials is my next topic of interest. This is the second CSWUG that I have participated in with CACS and I look forward to spending time with students next year!

Richard Clark
I am pursuing a Master’s Degree in Computer Science and a PhD in Physics. My interests include large scale simulations with semi-classical potentials to model the behavior of nano-explosives and nano-composites. I am studying the uses of Lattice Boltzmann techniques and time-accelerated methods to allow for the bridging of many different scales - both temporal and spatial. It was a pleasure to organize the CSWUG this year with the help of Yi-Chun and other members of CACS. A conference like this is always a lot of work, but with their help it was possible. The opportunity to meet such a great group of participants certainly made it all worth the effort.

Sijie Zhang
I am a PhD student in physics and pursuing a Master’s degree in Computer Science. The focus of my thesis is on the charge transport in a polymer or protein system. I combine the quantum mechanics calculations and classical Molecular Dynamics to approach this problem. I have taken part in three CSWUG events, and worked as one of the two organizers in 2005. Each has been an exciting and valuable experience for me.

Takehiro Oyakawa
I am a Master’s student in Materials Science and Engineering. I enjoyed working with the students participating in CSWUG 2006.
Building your own computer
presented by Rich Seymour - CACS USC

Summary by Naomi Brown - University of Hawaii, Hawaii and Danielle Roberson - University of Texas & Huston-Tillotson University, Texas

With mentors and grad students dispersed throughout the room, we were given the task of putting together a computer from parts. Table space was limited, and once all the students began the process, there was just enough room to do what was necessary. Cramming 40 computers into a room and teaching all 40 students to build their computer is no easy task for those teaching, however, and it was actually very convenient having assistance within reach.

What are the necessary steps for one to build a complete computer system? First, prior to purchase, one must analyze each individual component in order to be confident that each component is compatible with one another. Although research of the components will not be the focus just keep in mind its necessity.

Beginning with the processor, one notices the different dimensions that stand out. First thing that I notice is the notched angle on the upper right corner of the chip with an arrow. This designation shows where the number one pin is located and how it must be placed in the socket. After removing the motherboard from the box, one and looks for the socket in the processor will be seated. From the socket you notice a lever in the socket locks and the name of the socket (remember the need to research components). The lever is a locking mechanism for the processor to be secured in place.

Next component to be installed is memory. Memory has identifying marks that help prevent one from installing in the wrong way. On the motherboard the memory slots will have matching notches to match memory stick and locking clamps that secure them. After the memory, one prepares the case for the motherboard. Add extra risers to secure total perimeter of the motherboard. If necessary replace io plate to match io connector configuration. Now mount the motherboard on the risers while matching the io connector to the faceplate. Now for the hard-drive, where the operating system will be installed, needs to be connected, using red SATA cable to black SATA connector number one. Mounting to case is very simple. In this order you will find a few five and a quarter, two three and a half inch bays and several three and a half inch bays with out open faces. Place hard-drive in any of the bays in the third area and secure with screws. The next step is installing the compact disk read only module in the five and a quarter inch bay. One should use the round flat screws during installation.

Now for the video card, installing installation will take the correct connector whether it be AGP, PCI, or PCI-E. This in our installation will be using we used the AGP connector. A distinguished connector will be used that is the same size as the PCI with a locking lever. After one has installed the video card in the correct manner, one can go in and zip tie individual and groups of cabling in order to give a more professional appearance as well as maintaining space for cooling, components, and a more dust free environment. Double check your work and make sure that every connector is properly secured. Once these particular steps are completed, one can power on in order to make sure that the proper error message is displayed. And once the proper error is displayed, the individual can close the tower and begin installing the OS of choice.
OS Installation
CentOS [the Community ENTerprise Operating System]
presented by Rich Seymour - CACS USC
Summary by Sandrine Nana - Hood College, Maryland

Each student went through the process of installing the Linux distribution CentOS on their computers. This was an interesting process as we learnt the tricks of successfully installing the OS. I personally learned the importance and the purpose of the system gateway and the primary DNS.

During the process we were also introduced to other OS distributors such as Debian, SUSE, Redhat, Gentoo, etc. After installing the OS, we also installed MPI which is the program that would allow us to do parallel programming.

The presentation on Unix/Linux allowed the students to discover that the Unix system is described by Kernel and shell systems and that it is a multiuser and multiprocess system. The tutorial introduced the basic steps and commands needed to write programs using editors such as nano, vi, etc.

Supervisor: Dr. Liu, Xinlian

Unix Tutorial
presented by Richard Clark, Weiqiang Wong - CACS USC
Summary by Tamara Flourny - Spelman College, Georgia

The Unix operating system is categorized as a kernel and shell operating system because the kernel and the shell are the two essentials for the system. The kernel is the main component of the system and contains the CPU, hardware, memory, etc. The shell is the way in which the user interacts with the kernel. Almost everything in Unix—data, directories, processes—is expressed as a file. These files are stored in a tree structure called a directory. There are several important directories.

The top directory is known as the root directory and is denoted by “/”. Branching off from the root directory are several more directories. Among those is the home directory, which is where the user stores most files. The user is able to make additional directories using the mkdir command, but there is a major precaution in naming directories and files. The user should be aware that Unix is case sensitive. Therefore, the following are distinct: computational science, COMPUTATIONAL SCIENCE, CoMputation Science.

In order to create files, directories or do just about anything on the Unix system the user must use the shell and the correct command. There is an almost endless number of commands, but there are a few very useful commands. One is ls which lists the visible files in the current directory. A related command is Is –al. This command is an example of another way to use commands. After the command the “-l” denotes the usage of an option. In this example the ‘a’ tells the system to display all files, including the hidden files. The ‘l’ tells the system to display the information using a long format. The permissions and file size are among the information displayed in this long format.

Another useful command allows the user to move between directories, cd (change directory). There are several ways to move within the directories. In order to move from one directory to another the command cd can be used, but this option is limited to the directories within the current directory. The other way is to specify the path to the file. There are two types of paths, absolute and relative.

An absolute path is the complete trail to the file from the root directory. The relative path is relative to the current directory. Each file and directory has a set of ten letters associated with it. The first space is used to indicate whether the file is a directory. The next three are the permissions for the user. Permissions specify what the user is allowed to do to the file. There are three different actions that can be performed on file. The first is the ability to read the file. This is indicated by an “r” in the first space (of the set of three). The next space is used to indicate whether the user can write to the file and “w” is used here. The last possible action is to be able to execute the file and “x” is used here. The remaining six spaces denote the permissions for the group and for the world. In many cases a user is working with other users on a large project. This collection of users can form a group and share files through the network.
Introduction to MPI
presented by Hsiu-Pin Chen, Zhen Lu, & Sijie Zhang

Summary by Briana Young - University of Arkansas at Pine Bluff, Arkansas and
Saenya M. Grant - Oakwood College, Florida

What exactly is MPI, you may ask? MPI is a Message Passing Interface which is used for interprocessor communication through nodes. In this presentation given by Hsiu-Pin Chen, students had the chance to learn about eight major MPI subroutines calls in Fortran and how to use them.

Initializing was the first subroutine that the student learned about. It is used to activate the MPI environment by using the command MPI_INIT(ierr). Within this subroutine, the integer ierr, which is an error code, was introduced. The error code is a value that would be zero if there is no problem. On the other hand, if there is a problem in the program, the value of the error code would not be zero.

After initializing, students learned that it was necessary to know the rank for each processor. There are a total of six processors in the domain, ranging from zero to five. The students then learned that they also needed to know the number of processors in the MPI environment, which is represented by MPI_COMM_WORLD. The MPI environment is the world, which is made up of the number of nodes or hosts. In order to find the amount of processors in the environment, students had to use the command MPI_COMM_SIZE (comm, size, ierr).

Once the ranks were known in a particular domain, students learned how to send and receive messages from one node to another. To send a message from one node to another, the following command is needed: MPI_SEND(buf, count, datatype, dest, tag, comm, ierr). Once the message is sent, it can be received by using the command MPI_RECV(buf, count, datatype, source, tag, comm, status, ierr).

Commands for sending messages from one node to another were discussed. Another avenue of sending a message is by broadcasting. This involves sending messages from one node to all the nodes in the MPI environment. To execute this subroutine, the command MPI_BCAST(buf, count, datatype, root, comm., ierr) is used. However, to collect messages from everyone in the MPI environment, the following command is used: MPI_REDUCE(input, output, count, datatype, op, root, comm, ierr). Once the messages are collected, the results are stored in the output.

Finalizing was the last subroutine the students learned about. In this subroutine, one node is released for other nodes to access. The command used to finalize and put the finishing touches on the program is MPI_FINALIZE(ierr).

All in all, by learning about the eight major MPI subroutines in Fortran and how they operate, students gained the ability to communicate through nodes by sending, receiving, broadcasting, and reducing messages.

Sijie Zhang and Zhen Lu both graduate students at the University of Southern California were the speakers for MPI Test programs. Sijie Zhang discussed the first portion of the topic. She mainly explained how to run an MPI program. On behalf of her request, four groups were formed and asked to create host files. Moreover, she presented the variables: rank, size, mpierr, tag, and status. According to Ms. Zhang these variables are used for messaging, sending, and receiving. The message command identifies what is being sent. She ended her presentation by making sure that everyone had created and sent the host files to three other computers. Zhen Lu covered the second part of the MPI test program. Mr. Lu stated that the calculation of the value of pi is complicated. Both Sijie Zhang and Zhen Lu covered their portion of the MPI test program successfully.
Parallel MD Simulation
-Performance Measurement-
presented by Zhen Lu, Cheng Zhang, Ken-ichi Nomura, Weiqiang Wong

Summary by Julia Oroian - Benedict College, South Carolina and Naomi Brown - University of Hawaii, Hawaii

After getting a flavor of the problem at hand: atomistic simulations, by writing the Fortran code for the linear and 2-D dimension problem, and after having had exposure to basic MPI instructions to understand the mechanism of the communication process between processors, Professor Vashishta took the stage to make all of us understand what results we should expect for different options of decomposing the problem.

The following concepts were very clearly explained:

1. Range of addresses for 32b, 64b processors – this can be a limitation of how much data can be handled by one processor. For example for our problem a 32b processor can deal with approximately 1 million atoms (taking into consideration all data that pertain to one atom: 3-D position, velocities)
2. Periodic boundary condition – In order to be able to have complete information at the atoms close to the boundary of each subsystem it is important to create copies of neighboring subsystems, or wrap around the boundaries of the subsystem.
3. Partition size – With respect to this concept there are two aspects to focus on:
   3.1 The limit of how small a partition can be (this is imposed by the specific of the real problem to be resolved; the model is the one to set this limit, that is equal, for our problem, to r – the radius of interaction of atoms, more precisely: 30Å.)
   3.2 The determination of the optimum size of a grain – because, as we see through the following three sets of experiments, up to some point, communication gets more efficient, but beyond that point it turns to be less efficient.

As a verification of the concepts presented the following considerations should be made:

Looking for example at lines 2 and 3 in experiment #1, lines in which we recorded the times for the MD simulation for 1000 atoms/processor, on 4 processors in line 2, and on 8 processors in line 3, the communication time does not double from 4 to 8 processors. The explanation is that latency is still dominating in these configurations.

Comparing all the results in experiment #1 we have too many processors with small grain size is not a very good idea, because the communication time grows to largely exceed the computation time. Thus, for experiment #1 it is obvious that beyond 4 processors the communication process becomes ineffective.

Experiment #2 is similar to #1, but with a larger number of atoms/processor: 4000 instead of 1000.

A new perspective is brought in by experiment #3. This time the total number of atoms for all processors stays the same: 12000. The last 4 lines, pertaining to experiment #4, in the table below show the time when the process is run on one processor, versus the time when the process is parallelized on 4, 8, 12, respectively 24 machines. We found that parallelizing up to 8 processors resulted in both computational and communicational times that were efficient for the system, but beyond that, the communication overhead spiked. The explanation for this was that the switch was overloaded, leading to a bottle-neck effect for the computations. Therefore, the computational efficiency decreased greatly.

So, as a conclusion, it is very important to assess what the machine performance is, what the switch performance is and establish the best trade off.
Parallel MD Simulation Results

**Experiment #1**
Constant grain

<table>
<thead>
<tr>
<th># Processors</th>
<th>Total N of Particles</th>
<th>Total Time</th>
<th>Computational Time</th>
<th>Communication Time</th>
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<tbody>
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<td>0.976</td>
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<td>4</td>
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<td>12</td>
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<td>0.997</td>
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<tr>
<td>24</td>
<td>1000 x 24</td>
<td>18.33</td>
<td>0.985</td>
<td>17.34</td>
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</table>

**Experiment #3**
Constant total size

Total number of particles = 12,000

<table>
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<th># Processors</th>
<th>N of Particles per processor</th>
<th>Total Time</th>
<th>Computational Time</th>
<th>Communication Time</th>
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User Productivity Enhancement and Technology Transfer (PET)

presented by Dr. Susan Brown University of Hawaii, Hawaii

Summary by Cindy M ondragon - University of Arkansas at Pine Bluff, Arkansas

Dr. Susan Brown’s presentation on the responsibilities of the User Productivity Enhancement and Technology Transfer (PET) and its collaboration with the Department of Defense (DOD) indeed was very informative and educational to all of the students attendance at CSWUG 2006. PET assists and trains DOD HPCMP users in an attempt to improve user productivity. In other words, as long as PET and DoD work together, the pace in sharing such valuable information will remain accelerated.

PET is comprised of four components: Dayton, OH; Aberdeen, MD; Vicksburg, MS and Stennis Space Center, MS. Hence, it transfers the most updated technology that is held by the governments, industrial and academic HPC communities into DoD. PET is also involved in assisting ten of the DoD computational technology areas such as: Computational Electromagnetics and Acoustics, Computational Electronics and Nano-electronics, Computational Fluid Dynamics, Computational Structural Mechanics, Climate/Weather/Ocean/Modeling and Simulation, Environmental Quality Modeling and Simulation, Focus Modeling and Simulation, Signal/Image Processing, Computational Environment and Enabling Technologies. These areas intensely facilitate the productivity and the security of the DoD HPC community. Personally, I did not know that computational science greatly impacts society and the environment in such extensive manners. Furthermore, participants may have further exposure in all the various technology areas by applying to the PET Summer Internship Program, which is open to only US citizens. The student is introduced to the basics of HPC and scientific applications.

Parallel Programming

presented by Dr. Aiichiro Nakano CACS USC

Summary by Shelby Wilson - Spelman College, Georgia and
Duvane Barnes - Livingstone College, North Carolina

Parallel Computing has advanced greatly in recent history. To put the growth in computing speed into prospective, the computing power generated by 25 processors operating at 1.8 GHz would be able to operate at approximately 67.5 GFlops. This would be classified as the world’s fastest parallel supercomputer in 1993. As of November of 2005, the world’s most powerful parallel supercomputer performed at a speed of 280.6 Tflops. The current trend in parallel computing is heading toward computers that operate on the order of Petaflops.

The interface that enables us to run applications on parallel computers is called the Message Passing Interface (MPI). This interface allows for different processors that are either running the same or different programs to communicate and share data. One major application area that uses parallel computing power is molecular dynamic simulation. In such simulations, atoms are modeled and their movement simulated based on classical mechanics. Some applications of these simulations include drug design, robotics, even in the area of computer simulations for movies.

Another promising supercomputing platform is a Grid of globally distributed supercomputers. Grid computing involves a system in which people have pervasive access to all types of resources (computing, experimental equipment, mass storage, distributed sensors, etc.). The standard software used to implement Grid computing is called Globus. This software enables supercomputers from around the world to interact, work together, and share resources in order to create this world-wide Grid network. One of the applications made possible by Grid computing is hybrid simulation, in which metacomputing allows molecular dynamics simulation to invoke quantum mechanical simulations when and where chemical reactions occur.

There are many applications of parallel computing here at USC. These include simulations of hypervelocity impacts, possible advances in oil field technology, weather forecasting, underwater robots and massive multiplayer online games. All of these applications are made possible through recent advantages in parallel computing.

The lecture has also included a brief summary of parallel computing hardware and digital logic, measurement of network performance, and basics of single program multiple data (SPMD) parallel programming using MPI.
Computational modeling strategies for materials in nanoscience stem from first-principles quantum mechanics, i.e., from the Schrödinger equation. Currently, the technology available forces us that we can model no more than 100 atoms. Macro effects are obtained through multiscale modeling linked with quantum mechanical simulations, which requires simplifying assumptions.

There are several challenges for computational modeling in nanoscience: increased accuracy in quantum mechanical calculations, force fields for chemical reactions and biological systems, and interfacing electronic, atomistic and mesoscale dynamics. The best current approach to those problems is through hierarchal multiparadigm methods, which suggest using several methods based on their efficiency and practicality. Some applications of the hierarchal multiparadigm methods are nanosystems, biotechnology, catalysis, semiconductors, ceramics, polymers, metal alloys, and other environmental applications. Also, nearly all industrial applications require multiscale simulations.

For semiconductors, Moore’s law states that the number of transistors per square inch should double every 18 months. Thus, semiconductors in 2002 have a linewidth of 130 nm; the linewidth has reduced to 90 nm in 2005; and by 2010 it is expected to become 65 nm.

Prof. Goddard also presented simulation results on carbon nanotubes which are excellent candidates for interconnects in devices because of their superior mechanical and electrical properties. The problems for carbon nanotube interconnects construction are minimizing contact resistance, determining the growth of carbon nanotubes, and determining the mechanical stability of contacts. Specifically, the strategy is to deposit metal electrodes in assembled carbon nanotubes, and assemble surface modified carbon nanotubes on top of electrodes. Prof. Goddard described a simulation involving a graphene interface to calculate the contact resistance. The results indicate that titanium minimizes the resistance, which implies that it has the best conduction properties, while gold has the worst conduction properties.

High Performance Computing Modernization Program

Larry Davis, deputy director of the High Performance Computing Modernization Program (HPCMP) at the DoD, gave the final presentation of the workshop. He outlined a broad vision of how advanced computing technology plays an increasingly important role in the development of new fighting techniques and capabilities. We learned how the DoD rolls out and supports their computing infrastructure and the constant process of upgrading the systems for maximum utility. The Major Shared Resource Centers (MSRCs) of the DoD form hubs across the nation for scientific inquiry through massive hierarchical storage systems and advanced HPC compute engines. The Defense Research and Engineering Network (DREN) links 133 sites to the DoD's computing resources.

We also got a look at DoD challenge projects that push the envelope of high performance supercomputing. For example the group at USC has a challenge grant supporting their research into fracture at the nanometer scale in ceramics. Another group simulated the effect of explosives on reinforced concrete walls and another looked at the nonlinear flight dynamics of unmanned aircraft. All of the challenge projects took full advantage of the computing power available through the DoD.

Davis showed us how the User Productivity Enhancement and Technology Transfer (PET) program increases the productivity the DoD user community. This educational program extends hands on training and user feedback driven development into the DoD computing infrastructure. The internship and fellowship opportunities offered by the DoD for students and faculty, such as the summer intern program, sparked the interest of many in the audience.
Chemical and Bio-molecular Defense  
**presented by Margaret M. Hurley- ARL**

Summary by Christopher A. Norris Houston-Tillotson University, Texas

Dr. Margaret M. Hurley is associated with the United States Army Research Laboratory (ARL). In the topic considering the “Defense against Chemical Warfare Agents and Toxic Industrial Chemicals,” Dr. Hurley explains how the research on the mitigation if chemical and biological threats are very important to the national defense and other industrial giants. According to Dr. Hurley, the problem sometimes lies in the complexity of computational mathematics needed in order to build the molecular models that allows one to analyze the reactions between toxins and bio-molecules at the molecular level. Although simulations can be very complex, they are highly informative and provide the ability to safely and effectively satisfy many solutions needed to derive prevention and real-time response strategies. Throughout her presentation, Dr. Hurley illustrated many ways that the ARL is working with quantum chemical methods in order to provide the simulations of utmost interest to the Department of Defense (DoD) and other industrial causes.

In conclusion, the experiments being conducted and the experiments that have been conducted by the ARL, have provided or will provide more innovative ways to design better equipment that is used by the DoD. These particular studies can also lead to ways that mitigate the process a toxin or bio-molecule can destruct the human body.

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Computational Challenges in Earthquake System Science  
**presented by Thomas H. Jordan, Scec Director**

Summary by Allison R. Ford - Mary Baldwin College, Virginia and Adenrele Aphaunda - Benedict College, South Carolina

In this presentation we learned about the history of earthquakes in California, we looked at different ways to model earthquakes and their effects on high risk areas, hazard analysis, and how computational science were used in the study of earthquakes. He mentioned that the study of earthquakes involved three coupled problems namely:

- Fault systems dynamics
- Fault rupture dynamics
- Ground motion of dynamics

California is known as “Earthquake Country” this is because of California’s history of numerous seismic activities. Although earthquakes themselves can not be prevented, the study of earthquake is important because this knowledge could lead to better ways of becoming more equipped in case of this occurrence. Being better prepared for the event of an earthquake is especially important because large urban populations with high density are at high risk of earthquakes. Because the study of earthquakes is of extreme concern among many, many different institutions such as Caltech, Columbia University, and Harvard have become participants in Scec. In addition, Jordan went into the concept of Probabilistic Seismic Hazard Analysis. Probabilistic Seismic Hazard Analysis is basically the specifying the highest intensity of movement expected at a site during a certain time interval. An example of the Probabilistic Seismic Hazard Analysis is the National seismic hazard maps that indicate high risk areas.

He mentioned four SHA computational pathways which use wave equations to predict ground motion. This takes into account the fact that valleys are geographically considered soft settlements. When an earthquake occurs, soft settlement shakes very quickly and immensely. References were made to the destruction that could be caused by earthquakes in the Puente Hills. Simulated damages were estimated at $82 billion to $252 billion dollars, 3,000-8000 fatalities, 142,000 – 755,000 people displaced, 30,000 – 99,000 tons of debris.
USC/DOH CREATE Center
presented by Dr. Randolph Hall
Summary by Xinlian Liu - Hood College, Maryland and Sharon A. Lewis, Ph.D. - Langston University, Oklahoma

CREATE is the first university center of excellence funded by the Department of Homeland Security.

Terrorism causes damage to 1) human lives, 2) infrastructure, such as buildings; 3) economic components, such as the port of L.A. with subsequent impact to national economy. A distinctiveness of terrorism attack from natural disasters is its unpredictability.

The CREATE center was created following the 9/11 commission report’s recommendation ‘to find a way of reutilizing, even bureaucratizing, the exercise of imagination’. Further, Secretary Chertoff indicated that ‘in the long run, a risk-based approach is in everyone’s best interest. Therefore, it makes sense to study the ways to better design of infrastructures to prepare for terrorism attacks, and proper management strategies to deal with the after mass of such attacks, by scientific modeling and simulations.

The center gathers a joint force of multidisciplinary researchers coming from areas such as economics, political science, international laws, policy studies, physicists and computer scientists. The research topics include damages on physical properties, human behavior response and economic consequences associated with human behavior.

The terrorism enterprise is comprised of criminal, coercion and political aims, often with the goal of extirpating the US from middle-east affairs, which is not an acceptable option because of the nation’s dependence upon oil and other resources from that region.

The challenges are to 1) identify threats and vulnerabilities; 2) suggest counter measures; 3) develop tools and analysis to facilitate the decision makings.

In the eight major terrorism attacks targeting the US since year 1983, 4000 American lives have been lost along with small direct money lost in a span of 20 years. The figure itself is relative small comparing to those who died on heart diseases (2000 per day) or traffic accidents (125 per day). However, they changed our style of living permanently because of 1) economic loss by people’s response to the risk of a terrorism attack; 2) the fear factor derived from the inability to predict when and where it will happen.

A four steps modeling system:

A case study example is patient flow, which examines how the current under funded, stretched EM system to cope with the demands after a major terrorism attack. Hall and his team of MDs, Computer Scientists and Engineers modeled the Los Angeles county USC hospitals from top to bottom as an integrated system to identify the bottlenecks and possible improvements of patient flow.

Along with 5 other similar purposes centers funded by the DOH, CREATE offers a summer visitor program, which sponsors teams of faculty and students from MSI to conduct research projects on campus.

Dr. Hall concludes his talk with pictures showing the evolving meaning of protection. He pointed out that the goal was to protect the way of living, including international trades. The US depends on other countries for materials and goods; and other countries depend on the US for innovations.

In the Q&A session, Dr. Hall answered questions on web resources, natural disasters, optimization problems, color coding and signal planning.

Randolph Hall is Vice Provost for Research Advancement at the University of Southern California. A professor in the Department of Industrial and System Engineering, Dr. Hall is a former co-director of the Center for Risk and Economic Analysis of Terrorism Events (CREATE).
ISI was originally funded exclusively by DoD under the Defense Advanced Research Projects Agency (DARPA) programs. It is the birthplace of many technologies which laid out the foundation of the Internet today, such as Domain Name Services (DNS). Nowadays, ISI conducts research in the areas of natural language processing, transition, GRID, and seek funding from NSF, DoD, NASA and ARDA with annual funding of around $70 millions.

Among the 400 some research talents gathered at ISI, there are 28 research faculty, 27 staff scientists and 80 graduate students. ISI sees itself a software development oriented research center conducting applied research. The following diagram shows ISI’s active research areas and components.

One of the interesting projects developed at ISI is the reconfigurable robots. The attendants saw a video of the robots changes its shape from snake-like to butterfly-like to accommodate the terrain changes. The challenge of this project is to make ‘brains’ of each individual block component to coordinate with its neighbor brothers without a global awareness of what kind of creature the entire system represents.

Another project is the tactical language learning, which enables soldiers to practice effective communication skills with help of the computer simulated virtual environment. For example, they need to use proper language and body gestures in talking with local residents to build and maintain trust so that they can extract useful and actionable intelligence. Some soldiers commented that they learned more from this simulated system than their entire Iraq tour.

The favorite project of Dr. Rosenbloom is the contour crafting, which automates the building of a resident house, with the goal of building a 2000 square feet house in a day. The current progress status is building a 5 feet long, 3 feet tall wall.

In the area of computation and high performance computing, ISI conducts research in hardware such as VLSI, chips, bandwidth; software such as compilers; and systems such as reconfigurable devices.

ISI addresses both aspects of GRID, the virtual office and sharing of resources. Illustrated by the collaborated project between ISI and SSEC, people from different agencies at different locations are flexibly assembled to form virtual organizations in performing specific tasks such as conducting a fault system modeling or conducting a rupture dynamic modeling.

In city simulation, ISI technology enabled a scalable system which models millions of entities by partitioning the simulation among distributed computing resources of multi-sites over a wide area network. A significant contribution is a redesign of multicast routing scheme. The current system can scale from 100 thousands people to a million people and from a southwest Asia area to the world.

Some industrial strength efforts of ISE: large scale simulation, tactical language learning, MOSIS, adaptive computing (FPGA), Harrier scheduling and Grid computing.

In the Q&A session, Dr. Rosenbloom answered questions on develop cycles, trends in OSs and roles of mathematicians at ISI. Randolph Hall is a professor in the Department of Computer Science at USC, and associate director of the ISI.