SCS
Integrating Advanced Computing with Science, Engineering and Liberal Arts

School of
Computational Science
at Florida State University

The Co-Evolution of Landforms and Ecosystems in Salt Marshes

INSIDE THIS ISSUE

Salt marshes are complex environments located between the sea and land. While they are now widely recognized as invaluable ecosystems, their importance to society was long unknown or ignored. As a result, over half of the original salt marshes in the U.S. have been destroyed to create more land for agriculture, housing, or industries. However, substantial efforts are being made to restore salt marshes now that their economical and ecological values are appreciated.

RICH MARSH LIFE

Despite the fact that very few plants can tolerate regular flooding with salt water, tidal marshes are surprisingly productive ecosystems. Vegetation, especially grasses, provides both protection and an abundance of food to a variety of animals.

Many species of fish, crab, and shrimp use the salt marshes as their nurseries. The marshes also provide excellent habitats for birds, including egrets, herons, and game birds.

The typical marsh grasses have very tough root systems, which reinforce the soil. This is important, because the marshes take the first hit of storms and floods. Their ability to absorb energy from the storms moderates the effects on upland areas. The marshes also act as filters, preventing pollutants and some sediments from reaching the oceans. Sediments, along with organic residues from marsh plants, add to the buildup of soil and eventually to new marshland.

Since tidal marshes are constantly changing, they involve specific challenges for the scientists who study them. Geology professor Sergio Fagherazzi at FSU is one of them, and he is particularly interested in the formation of channels in these wetlands.

IMPORTANT EXCHANGE

Channel networks are important for the exchange of water, sediments, and nutrients between the marsh and the

Tidal marshes in Chassahowitzka National Wildlife Refuge, Florida. Photo courtesy U.S. Geological Survey

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At this time of the year faculty members tend to be quite distracted because we are planning next year's teaching. At the same time we are concentrating on getting the spring semester's courses off to a good start. At SCS this year the distraction coefficient is even higher because, for the first time, we're planning next year's teaching schedules as part of a long-term curriculum.

When I look at the courses that SCS faculty members have offered in the last two years, and that they will offer next year, I am struck by how this initiative has broadened the opportunities for students.

Some of these offerings are novel varieties of existing courses, like the Computational Genomics module of the long-running Experimental Biology course in Biological Science. Others, like Scientific Visualization, Numerical Linear Algebra, and Computational Methods in Bioinformatics, have been completely novel. Some courses, like Markov Chain Monte Carlo Methods, are definitely esoteric, while others, like Introduction to Scientific Computing and Survey of Numerical PDEs, serve broader audiences.

And SCS faculty have also taken turns in long-standing courses like Calculus, General Physics, and even Conservation Biology.

When I looked at this list for the first time, I found it overwhelming. But when I looked again, I saw the teaching and training phase of this initiative emerging. Not that it wasn't there without the list, but when I think in terms of advising faculty members and working with each one individually, thinking about one course at a time, it's easy to miss the larger shape of the program. That shape is looking very gratifying to all of us who thought we could make a difference.

Joe Travis
Director, SCS

ocean. They are formed when tides move large volumes of water back and forth over the marsh platform. While there is an element of randomness in their formation, they share basic geometrical properties with other natural networks.

COMPUTER MODELING

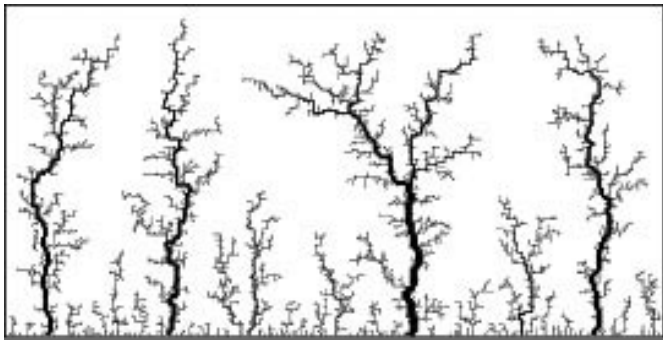
Sergio Fagherazzi is currently developing a computer model to help him explain how the channels are established. He is also one of the co-editors of a recent book, called "The Ecogeomorphology of Tidal Marshes". As the title suggests, he recognizes the fact that biologists and geologists have to work together to understand the formation of these landscapes.

Many factors affect the establishment of wetland channels, such as the slope of the land, the rate of the tidal flow, and vegetation. Along with components like biomass production, they all have to be taken into consideration in the modeling framework.

The final goal of Dr. Fagherazzi's research project is the development of a numerical model that links phenomena occurring at different spatial scales. The model will be able to follow the physical evolution of salt marshes and to predict the impact of human intervention, restoration projects, and sea level rise on these delicate environments.

Since the biological component is of paramount importance in tidal marshes, the model will include vegetation encroachment on the marsh surface, belowground root production, and sediment trapping by marsh canopy.

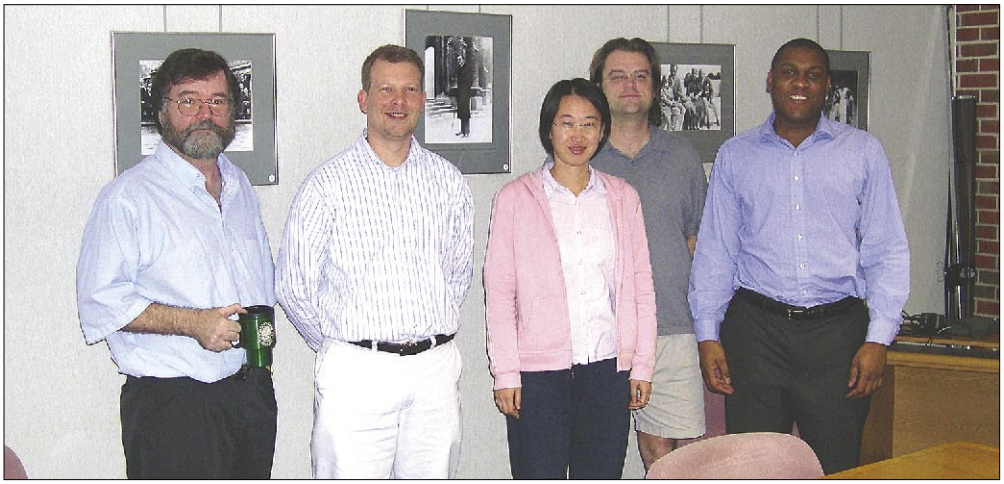
sergio@csit.fsu.edu



Simulation results of channel development in a tidal marsh.

New Math Speeds up Scientific Calculations

An NSF-funded research project, led by FSU professors Robert van Engelen and Kyle Gallivan, has generated results that will prove important in many areas of computational science. The project dealt with a basic, but crucial, task for computers: determining in which order to perform the millions of calculations that make up computer programs. For each piece of software, the right answer to that question might multiply the computing speed. Since some scientific tasks take months to perform even on modern supercomputers, the possibility of shortening the running time is critical to many scientists.



From left: Kyle Gallivan, Robert van Engelen, Yixin Shou, Burt Walsh, and Johnnie Birch.

A typical computer program used for numerical scientific calculations contains instructions to access data in tabular form, such as matrices and grids. Sometimes, the computer is instructed to take the result from one operation and use it for the next one, which makes it necessary to perform all the calculations in a specific order.

Usually, however, this is not the case. Large parts of a computer program consist of series of operations that can be calculated independently or can be changed to operate independently. Here is where you find chances to speed up the processing. If you can tell the computer which parts of the computer program that can be performed simultaneously – parallelized – you can multiply the computing time with the number of processors available.

The trick is to identify which parts are independent of each other, without actually running the program. For relatively simple, linear indices into the tables and matrices, the prediction can be made automatically, using compilers. Compilers are specific computer programs necessary for translating high level software, that people normally write in, into machine code specific to a particular computer and operating system. Compilers, for instance, make sure that our common word processors may run on different computer brands and operating systems.

For nonlinear numerical expressions and table indices, compiler tools cannot distinguish between dependent and independent operations, but this is where the FSU team has made its important contribution. Drs. Gallivan and van Engelen, with the help of doctoral students Johnnie Birch, Yixin Shou and Burt Walsh, have developed a new compiler, based on a new type of "recurrence algebra" that is more efficient in analyzing these nonlinear functions.

engelen@csit.fsu.edu
gallivan@csit.fsu.edu

Unfolding the Nature of Proteins

Virtually everything that happens in our bodies, as well as in other living organisms, is regulated by proteins. Proteins rule our wellbeing and our diseases. They function as hormones, antibodies and enzymes, or as catalysts that modify the speed of the chemical reactions in the cell. They are also building blocks in muscles and other body tissues.

Every protein molecule has a three-dimensional (3D) structure that is specific for that protein and of crucial importance for its function in the cell. The 3D fold decides which parts of the molecule are exposed on its surface and thus determines which molecules the protein can react with. For instance, some protein parts bind easily to fatty substances, while others have positive or negative charges that are attracted to water and other polar molecules.

FATAL MISFOLDING

When the fine-tuned processes of protein folding are disturbed, the consequences can be dramatic. The dreaded Alzheimer's disease illustrates this. While the primary cause of this condition is not yet fully understood, it is clear that the protein α-synuclein in the brain starts to fold in an erroneous way. This starts a chain reaction of misfolding, and the resulting abnormal proteins clump together to form what is known as amyloid plaques in the brain.

Professor Huan-Xiang Zhou at FSU uses the example of Alzheimer's disease to explain the importance of protein folding and binding, the focus of his research, which is supported by the National Institutes of Health. Professor Zhou is with the Department of Physics, which at first glance might seem surprising. However, physics has lent much of its advanced theories and technologies to biology, allowing a detailed study of molecules in the scientific branch called biophysics.

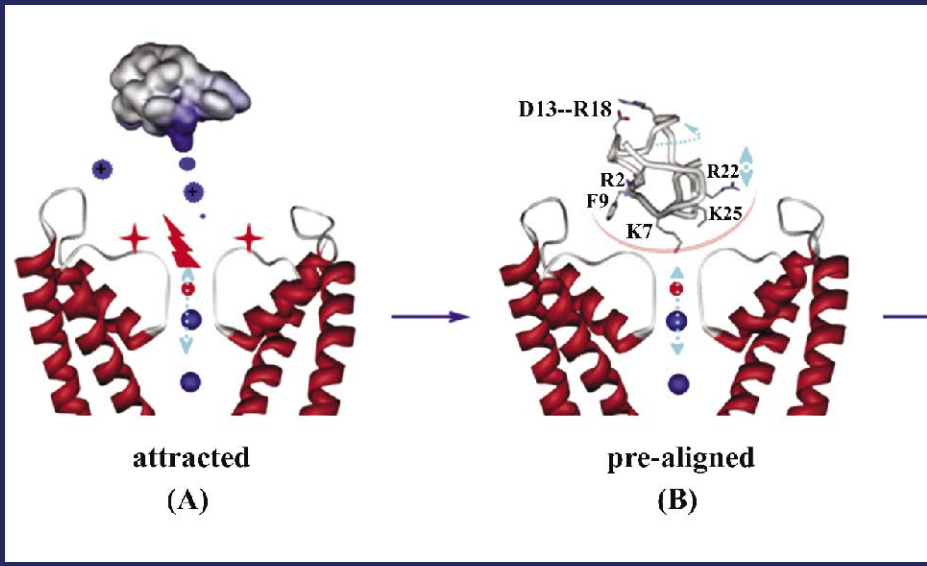
Professor Zhou came to FSU in 2002 at the start of the Computational Structural Biology initiative of the School of Computational Science. In 2004, Professor Hugh Nymeyer joined this effort, and the recruiting process for a third professor is on its way.

DRUG DESIGN

Protein structure can be studied in lab experiments or through computer modeling. Determining protein structure in the laboratory is expensive and time-consuming, and it is hoped that computer modeling will offer a complementary approach for purposes like drug design. Creating computer models of potentially useful drug molecules, and even making the initial screening in the computer, could be a way to multiply the rate at which potential drugs can be made.

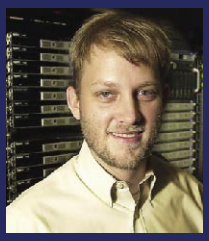
Just as there are research databases for protein sequences, there are others for protein structures. Professor Zhou and his group are making use of these databases to predict the formation of protein-protein complexes based on the structures of the individual proteins.

In a fascinating worldwide effort called CAPrI (Critical Assessment of Predicted Interactions – http://capri.ebi.ac.uk), computer predictions of protein complexes are compared to the structures revealed by X-ray studies. Scientists that are about to publish structures determined by X-ray agree to announce the imminent publications, while computational scientists race to come up with the most accurate computer model of the same protein complex.



The figure illustrates the binding of a toxin from the fish-hunting purple cone snail to a potassium ion channel in the cells of its prey. The snail paralyzes its prey in a second. The toxin, illustrated as the large grey molecule, rapidly finds the ion channel of the prey. The ion channel has a concentration of negative charges (red zig-zag) around its entrance in order to induce the passage of the positive (blue) ions. The snail toxin has evolved to have many positive charges around the surface, and the attraction of opposite charges works across a long distance. The attraction orients the toxin as it approaches the ion channel (panel a to panel b). Once in proximity, the toxin and the channel undergo fine adjustments and finally form a very specific complex (panel b to panel c). The toxin plugs the hole and stops the normal ion exchange. These steps were modeled on the computer by Xiaoqin Huang (former postdoc at CSIT). In the simulations, the motions of the molecular system, consisting of 72,700 atoms, were followed 2 femtosecond ($2 \cdot 10^{-12}$ s) at a time up to 13.2 nanoseconds ($13.2 \cdot 10^{-9}$ s). The simulations took about eight months on the SP4 supercomputer.

Professor Huan-Xiang Zhou and his group: Standing, from left: Jyotica Batra, Ke Xu, Debangshu Samanta, Daniel Spencer, Ramzi AlSallaq, Harianto Tjong, Johan Bredenberg. Sitting, from left: Tjipto Juwono, Huan-Xiang Zhou and Myunggi Yi.



Professor Hugh Nymeyer

The models from dozens of groups of computational scientists (including Dr. Zhou and his collaborator Dr. Bovin, the Netherlands) are then compared with the experimentally determined structure. In the scientific discussion that follows, the limitations of the different models are scrutinized and improved.

MEDICAL APPLICATIONS

Chronic myeloid leukemia (CML) is caused by impaired protein interactions in the cell. It is known that CML patients have an enzyme that is too active due to a specific mutation. Professor Zhou is investigating how the protein action is regulated under normal conditions. CML can be treated if diagnosed early.

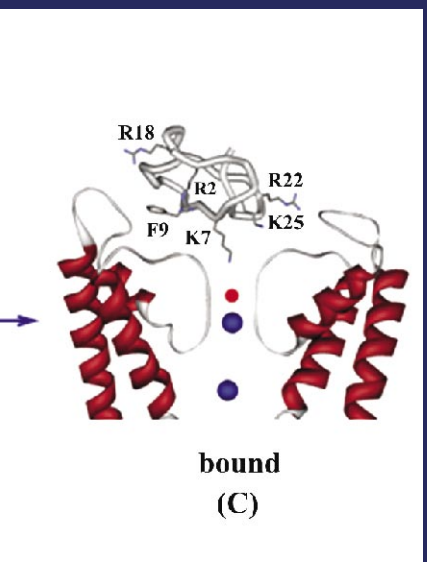
The group is also analysing a toxin from purple cone, *Conus purpurascens*, a venomous snail which can be found in tropical waters. The toxin is positively charged, and functions by blocking the negatively charged channels through the cell membrane usually used for the vital transport of potassium ions. Many different snails produce powerful toxins, some of which are being tried as drugs, for instance as painkillers or cancer treatments.

MEMBRANE PROTEINS

The potassium channel affected by the snail toxin is a special type of protein called a membrane protein. About 30% of our proteins are membrane proteins. These proteins reside in the cell walls and organelles. Some selectively allow ions or small molecules to cross the cell wall, while others just work to carry messages from one side of the cell wall to the other side. The most important proteins involved in photosynthesis and metabolism reside in the membrane.

Because of the difficulty in handling and crystallizing membrane proteins, much less is known about them than other types of protein, making computational studies especially important. Professor Nymeyer and his group are using special computer algorithms to study the interactions that stabilize and position proteins in the membrane. The forces that stabilize membrane proteins depend on the composition and structure of the cell wall. Also, small molecules like cholesterol and many common anesthetics dissolve into the cell wall and can affect the structure and function of the membrane proteins inside.

hnymeyer@fsu.edu
zhou@sb.fsu.edu



Genes & Proteins

The human genome consists of 30 000 genes, containing information about the traits that children inherit from their parents. A gene can be described as the blueprint for a specific protein. All vital processes in all organisms are regulated by proteins, and to understand the nature of heredity and genes, you have to study the structure and action of the proteins that the genes code for.

A protein is a chain of amino acid molecules. There are twenty different amino acids, and they have a similar basic composition, mainly consisting of carbon, oxygen, hydrogen, and nitrogen. A small protein might be a relatively short string of 50 amino acids, while the large ones may contain thousands. Short chains are usually called peptides.

The exact order of the amino acids in a protein is crucial, since it determines the protein's properties. Small mistakes in the synthesis of a protein, caused for instance by a mutation in the corresponding gene, can severely affect the protein's function.

As soon as the long protein molecule is formed in the cell, it bends and curls to form a 3D structure that is as unique and important to its function as the amino acid sequence.

New and Familiar Faces at SCS

Both our technical and adminstrative staff have undergone personnel changes during the past months. Office assistant Pam MacManus got a new position at the FSU School of Criminology. Our Systems Manager, Gary Eggebraaten, left SCS in January for the College of Engineering, where he will be the Director of Communications and Multimedia Services. Gary leaves behind a long list of accomplishments at SCS. Thank you, Pam and Gary, and the best of luck to both of you.

TSG CHANGES

Jim Wilgenbusch has taken over the supervision of the Technical Support Group (TSG) while continuing his work in phylogenetic research and application development in the Computational Evolutionary Biology group. Jim will be assisted in his administrative duties and in project planning by the Local Systems Committee (Gordon Erlebacher and Kyle Gallivan). The LSC is currently leading a search for a Senior Systems Administrator as a replacement for the position held by Gary. However, the new position will not have administrative duties. Therefore, this person will have more time to work on systems projects.

Jim Wilgenbusch

Daniel Whelan, a familiar face to many in SCS, has traded in his part-time position for a full-time one in the TSG. In his full time capacity, Daniel will continue to apply his strong technical skills in the area of server administration, as well as, taking on a more prominent role in the management and documentation of some our ongoing systems projects.

NEW POSTDOCS

The four postdoc positions in Computational Biology that were advertised jointly last summer have all been filled, and three of these postdoctoral fellows came in January. The first of the three to show up was **Koffi Sampson**, who has a PhD in mathematics and is Peter Beerli's postdoc. He will be working on problems in population genetics using coalescence theory. **Paul Van Der Mark** has joined Fredrik Ronquist's group and is working on the development of MrBayes, a program for the Bayesian estimation of phylogeny. Paul has a background in computer science and is interested in parallel and distributed computing. **Johan Nylander** will work with David Swofford on convergence diagnostics for MCMC methods applied in phylogenetics. It is Johan's second appointment at SCS, since he did some of his PhD work here at the end of 2003.

A British addition downstairs is **Simon Rycroft**, whose duties include creating web services and a new layout for the MorphBank site. Simon, who's originally from England, has studied in Glasgow, Scotland, where he worked on SID, another image database.

SCS welcomes a new office assistant, Lynn LaCombe, who has taken over travel, purchasing and personnel issues from Pam MacManus. Lynn is well acquainted with those duties after almost 18 years at FSU. Before coming to SCS, she also worked in Strozier Library, Purchasing, Physics, and Family & Child Sciences. A Tallahassean since childhood, she still lives in our city with her husband and two daughters.

Risette Posey has joined SCS to work for David Swofford on the Howard Hughes program. Risette works half-time, and devotes the other half to her doctoral dissertation on strategic technology management. She has also worked at the FSU Office of Technology Integration, Florida Department of Insurance, and the Supreme Court of Florida. In her spare time, Risette grows an organic vegetable garden and walks her dog.

Howard Hughes – More Than Aviator

In an FSU press release, dated July 2002, you can read the following: "FSU has received $1.6 million from the Howard Hughes Medical Institute to enhance its undergraduate computational biology curriculum over the next four years. FSU is one of 44 research universities across the nation that received $80 million from HHMI for their biology program".

Since then, the field of mathematical biology has certainly increased at FSU, and the Howard Hughes funds for developing undergraduate courses have played an important part in this expansion. The money has been used towards two main objectives: First, to increase the amount of mathematical and computational biology taught to all biology majors, and second, to make it possible for students to specialize in computational biology. The latter has been made possible by the creation of a "Mathematical and Computational Biology" track with specialized classes within the biology major. Also, up to 12 FSU students a year, called Hughes Fellows, receive financial support to pursue a research project in computational biology during their senior year.

The Department of Biological Science, together with SCS, has developed new courses in bioinformatics and programming for biologists. A new computer lab has been set up at SCS, and professors and teaching assistants have been hired with support from the Howard Hughes program.

However, not only the biology department is involved in this endeavor. The Department of Mathematics is likewise deeply engaged, and has developed a course called "Mathematical modeling in biology" for biology OR mathematics majors. Also, the Department of Statistics teaches a course for biologists on applications of statistical methods in biology.

Biology professor John Elam originally administered the grant, but last fall professor David Swofford at SCS took over the coordinating function. Dr. Swofford explains the importance of the program:

"All fields of science have become more mathematical as they have matured, and biology is no exception. Students interested in pursuing biological and medical research, who are also comfortable with math and computation, will be at a clear advantage."

Dr. Swofford and his assistant Risette Posey (p. 6) are now encouraging juniors to apply for the third term of Hughes Fellowships. They are also planning an event in May, where the 11 current Hughes Fellows will get a chance to present their research on topics ranging from anticancer drugs to zebrafish genes.

The eccentric Howard Hughes has been portrayed lately in both the blockbuster movie "The Aviator" and the documentary "Howard Hughes: The Real Aviator". With a fortune generated from his father's patented oil drilling equipment, the young Hughes Jr. pursued his two great interests: film-making and aviation. In 1953, he also founded the Howard Hughes Medical Institute to support medical research and education.

www.csit.fsu.edu/HHP
swofford@csit.fsu.edu

Japanese Pioneer to Visit SCS

In February, Professor Mutsuto Kawahara from Chuo University in Tokyo, Japan, will visit FSU with a group of 38 students and scientists. Professor Kawahara has been collaborating for many years with Professor Michael Navon at SCS, the host of the group. A workshop called "Applications of optimal control and EnKF to Flow Simulation and Modeling" will be held on February 23 to 24. The program (link below) also includes prominent speakers from FSU and other U.S. universities.

Professor Kawahara is a pioneer in many areas of computational science, civil engineering being one of them. Already a couple of decades ago he had the vision of engineering experiments being performed in the computer, as a complement to hands-on experiments with physical models. Professor Kawahara and his group contributed greatly to the early work in mathematics needed to create the computer methods for engineering that are now widely used around the world.

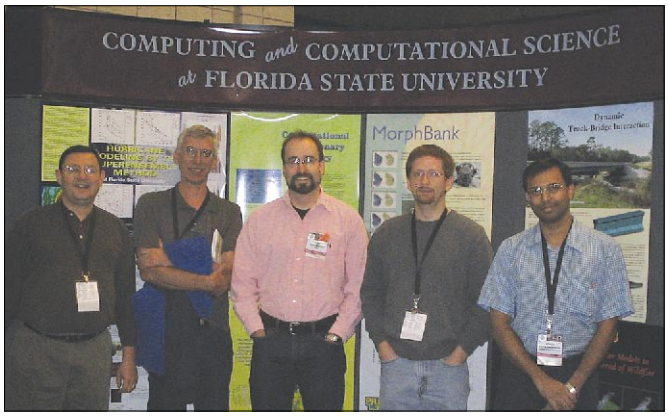
Professor Kawahara's work has plenty of connections to everyday life. His publication list in the field of fluid dynamics contains articles on blood-flow in the arteries, water pollution, and operation of dam water gates, as well as tsunami wave propagation.

www.csit.fsu.edu/~navon
navon@csit.fsu.edu

FSU Research Shown at Supercomputing Conference

The annual IEEE Supercomputing conference, SC2004, was held in Pittsburgh in November, 2004. The FSU booth included general information on computing capabilities at FSU. It also highlighted certain computational science projects ongoing at FSU. This activity was organized by Michael Mascagni (Computer Science and SCS) and Ashok Srinivasan (Computer Science).

The "Supercomputing" conferences are important venues for universities and other research organizations working in high-performance computing and scientific computing. Over the years, the conference attendees have become a cohesive community, and thus this conference series has become the premier venue to interact both formally and informally with this community. Not only is a large fraction of the institutions involved in this work represented with research exhibits, but the conference brings a consistently large and diverse group of program managers from most of the federal funding agencies.



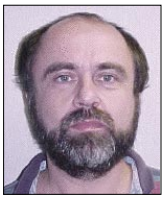
The FSU booth was set up and presented by Michael Mascagni (CS, SCS), John Burkardt (SCS), Clint Whaley (CS), Chuck Fleming (CS, SCS), and Ashok Srinivasan (CS).

Thus, participation, at the level of a research booth, is a signal that an institution considers its activities in these areas of significance. The FSU research booth, though modest, was well received, and certainly served this purpose.

www.sc-conference.org/sc2004
sc05.supercomputing.org
www.csit.fsu/pittsburgh
www.cs.fsu.edu/~mascagni

Bernd Berg Fellow of APS

Prof. Bernd A. Berg, SCS and FSU Department of Physics, has been elected Fellow of the American Physical Society. This great honor is bestowed upon prominent physicists by their peers. The society elects only a half percent of its members to Fellowship each year. The citation reads: "For pioneering lattice gauge theory simulations, innovative contributions to Markov chain Monte Carlo algorithms and their applications to Statistical Physics."



berg@csit.fsu.edu

SCS — School of Computational Science

The mission of SCS is to be the focal point of computational science at the Florida State University. The school supports and develops a variety of high performance computing facilities, accessible to the university community. SCS is designed to overlap with existing departments and schools to provide a venue for interaction among faculty and students across many disciplines.

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SCS
Dirac Science Library
Florida State University
Tallahassee, FL 32306-4120
Telephone: 850 644-1010
Fax: 850 644-1593

Director: Dr. Joseph Travis
850 644-7024

Editor: Eva Ronquist
850 644-0196
evaron@csit.fsu.edu

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