Summer 2005

SCS

Integrating Advanced Computing with Science, Engineering and Liberal Arts

School of
Computational Science
at Florida State University

Laser Beams and Water Efficiently Remove Nano Dirt

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Computers, cell phones, and digital cameras keep getting faster, more powerful and smaller at a mind-boggling rate. A typical computer chip, the size of a fingernail, can contain millions of components. Today's scientists even talk about assembling electronic elements from individual molecules.

Nanoscale structures (from nanometer, one billionth of a meter) are manufactured in super clean environments, but it is not yet possible to totally avoid all contamination. Micro- or nanoscale particles may sneak into electronic or optic systems and disrupt their function or durability. To avoid this problem, we need micro- or nanoscale cleaning systems.

STRONG FORCES OPERATE

It might seem easier to remove small particles rather than large, but as size decreases, gravity loses its impact and very strong molecular forces start to dominate. A particle less than one thousandth of a millimeter in size can adhere to a surface with a force that is over a million times its weight.

Current micro-cleaning systems often use liquid chemicals, which are sources of contamination in themselves, and they may harm the surface of the material to be cleaned. Additional motivation for society and industry to find better alternatives is the worldwide phasing out of freon and its chemical relatives. Once popular cleansers, these are now known to deplete the ozone layer and contribute to the greenhouse effect.

A thin film of water is deposited over the dirt particle (orange) adhering to the surface. Laser heating of the water and the surface vaporizes the base layer of the water, lifting both water and particle from the surface that needs cleaning. Numerical simulation by K. Smith, S. Sablin, and L. Gelb. Visualization by B. Futch, K. Beason, and D. Banks.

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A friend once remarked that university campuses ought to be designated as permanent construction zones because every campus always has new buildings under construction and old buildings under renovation, year in and year out. This is true at all levels; at SCS, we are renovating our main computer room, not too long after adding power and power storage to the facility and following an extensive renovation that created our computational science classroom. We seem always to be having construction meetings for something.

The visible construction reflects what occurs on the inside; that is, university programs and departments are constantly changing and redefining themselves in response to new discoveries, new ideas, and new ways to bring the excitement of discovery to students. We are no different at SCS. As you can read in one of the articles in this issue, in the last year, some of our faculty members taught new courses, revised existing courses, and proposed additional novel courses for subsequent years. We have talked about ideas for new training programs and some of us are moving forward to turn those ideas into plans and, ultimately, students.

In my ideal world, we would have a column every year about new courses and new ideas for programs. This is not to write that we shouldn't have continuity; to the contrary, good programs succeed and endure through continuity and stability. But continuity and stability are aspects of a program and are not to be confused with its content. In that sense, I expect that the SCS will have continuity and stability as a program but that the teaching and research within the program will be dynamic – we should always reflect the leading ideas in computational science, even as they themselves grow and change.

Joe Travis
Director, SCS

Luckily, less damaging methods are on the way. One of the new cleaning techniques uses high energy density laser beams and water as the main components. In short, a thin water film (its thickness measured in nanometers to micrometers) is deposited on the surface that needs to be cleaned. The water film is brought to an explosive boil by the energy from a laser beam, and the dirt particle lifts from the surface. The water with the contaminants can then be removed by suction.

The method has proven to be very efficient, removing nearly 100% of the unwanted particles after a few repetitive treatments.

THREE APPROACHES

A group of present and former FSU scientists and students have investigated this cleaning system both in a chemistry/physics lab (Drs. Susan Allen and Sergey Kudryashov), and in simulation experiments performed on the FSU Eclipse supercomputer (Dr. Yousuff Hussaini).

To add even more to the understanding of the cleaning process, visualization researchers led by Dr. David Banks have used simulation data to make image sequences showing how the dirt particle is removed from the surface.

The explosive boiling of the near surface water film, and the subsequent particle removal, happen within a fraction of a second. Nonetheless, each computer simulation was run in 30,000 time steps, allowing an extremely detailed study of the molecular movements.

Several simulations were made, in order to study the effects of different temperatures and various water layer thicknesses.

HIGH RESOLUTION

In high-performance computer modeling, you can follow the movements of individual molecules, and you have perfect control of the system that you study. This resolution makes it possible to see things that cannot be seen in a wet lab experiment.

The models will not only make it possible to improve industrial techniques, but will also give us insights into fundamental physics. Because, as Professor Hussaini points out, even seemingly familiar processes like vaporization are not yet fully explained on the molecular level.

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New Graduate Courses in Computational Science

In all fields of science, the use of mathematics and computers is increasing quickly. Sooner or later, students in physics, biology, geology, meteorology, chemistry, engineering, or other disciplines, face problems that can only be solved with computational tools.

There is a strong demand for researchers with a working knowledge of computational tools and algorithms. Even more important is the ability to combine these computational tools with knowledge of the applied sciences.

NEW GRADUATE COURSES

The FSU School of Computational Science is developing innovative new graduate courses, which will serve computational disciplines campus wide. The courses will also be core or elective courses for the new graduate degree programs that SCS is developing.

The courses listed below are new, and will be offered by SCS in the academic year 2005–2006, along with courses like *Introduction to Computational Biophysics*, and *Introduction to BioInformatics*, which have been taught before. At least two additional courses will be introduced in 2006–2007, *Applied Computational Science I* and *II.* In both courses, lectures will be combined with computer labs.

FALL COURSES 2005

Introduction to Scientific Programming, which will be taught by Dr. Gordon Erlebacher, is viewed by SCS faculty as being a core course, which will serve as a foundation for the majority of computational courses offered by SCS and other disciplines. Students will be introduced to the basic elements of the computing languages Fortran 90, Java, and C++. A student completing this course will be comfortable thinking in objected oriented terms, will know how to manipulate objects with dynamically changing information, access elements of one language from another, learn to construct software libraries and more.

Dr. Bernd Berg will teach the course *Markov Chain - Monte Carlo Simulations* out of his own text book from 2004. MCMC simulations have become a major enabling technique in the applied sciences. The course will include not only Monte Carlo methods themselves, but also the statistical foundations and background necessary to analyze data from these methods. Applications will be drawn from statistical physics as well as other areas.

A wide range of biological applications – including identifying pathogens and tracing viral transmission pathways – rely on inferring the evolutionary history of the organisms involved. A course on *Computational Evolutionary Biology*, taught by Drs. Beerli and Ronquist, will cover the methods used for evolutionary inference, the principles they are based on, and how they are implemented. In a lab session, the students will get hands-on experience in developing computational software implementing these methods.

SPRING COURSES 2006

During spring, two courses on the numerical solution of partial differential equations (PDE's) will be offered. In Dr. Michael Navon's course *Computational Finite Element Methods*, theory will be combined with numerical illustrations of test cases of available finite element software. The applications will be geared towards engineering applications.

The other course on PDE's, *Survey of Numerical Methods for Partial Differential Equations* will be given by Dr. Janet Peterson. This course is intended for students who want an overview of available techniques for approximating the solution of PDE's.

Dr. Hugh Nymeyer is planning to teach a course called *Computational Methods in Biochemistry* in the spring. The course will be focused on molecular dynamics methods for studying the dynamics and equilibrium properties of large molecules.

MORE INFORMATION

Detailed information as well as updates concerning courses in Computational Science can be found on the SCS homepage. www.csit.fsu (click Education).

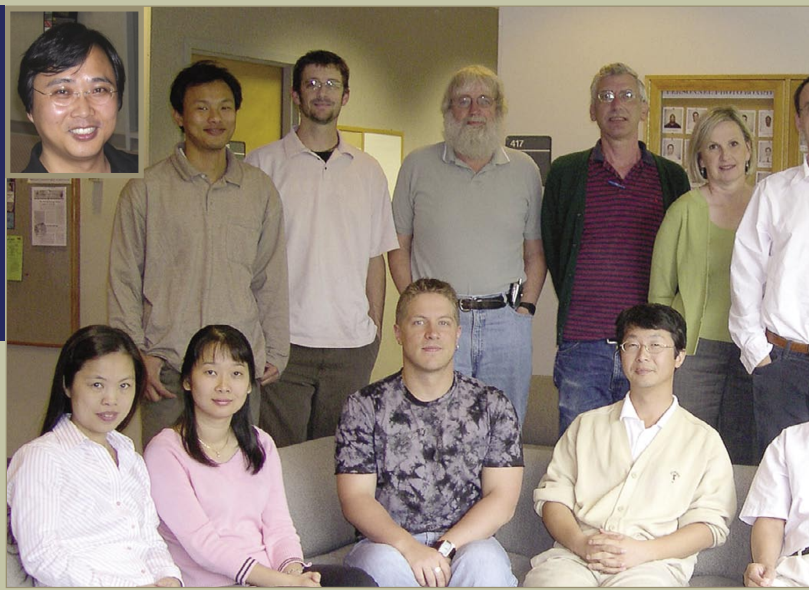
Computational Math: Connecting and Enabling the Computational Sciences

If mathematics is indeed the language of science, then partial differential equations (PDE's) make up a large part of its vocabulary and grammar. They are the mathematical structures most often used for the study of the behavior of physical systems and to effect technological advances. PDE's are used to describe phenomena ranging from the electronic structure of atoms to the formation of stars, and everything in between.

Unfortunately, except in some grossly simplified settings, PDE's are not amenable to exact solution; one must instead rely on finding approximate solutions using computers. In fact, the modern digital computer was invented in order to solve PDE's and even today, this task remains as the main motivation for the development of supercomputers!

Solving PDE's on computers is the primary research interest of the numerical PDE group at SCS. Specifically, the group does research in mathematical modeling (writing down mathematical relations that describe a phenomena), the analysis of the mathematical models (to answer questions about their validity), and the development, analysis, and implementation of algorithms (methods that can be programmed into a computer). Our central goal is to develop methods for determining approximate solutions of PDE's using computers and to use those methods to solve scientific problems.

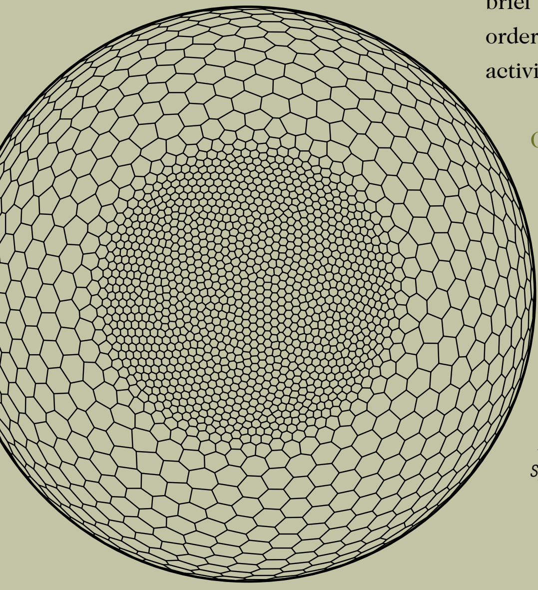
The numerical PDE-group at the School of Computational Science.
Standing, from left: Haomin Lin, Hugh MacMillan, Max Gunzburger, John Burkardt, Janet Peterson, Catalin Trenchea, Marcus Garvie, Yuki Saka, Zheng Chen, and Wan Kan Chan.
Sitting, from left: Wendy Cheng, Hoa Nguyen, Clayton Webster, Sung-dae Yang, and visitor Hong Chul Kim.
Inserted: Xiaoming Wang
Missing from picture: Yanzhao Cao.



We now describe, in very brief terms and in no particular order, some of the research activities of the group.

COUPLED MULTIMODEL PROBLEMS

In many situations, e.g., the flow around an airplane, one has to simultaneously solve for more than one physical phenomenon. We study novel, optimization based methods for the efficient solution of such problems that allow the user to use codes developed for each constituent model without change.



A locally refined grid on the sphere.

GRID GENERATION

Many methods for solving PDE's on computers rely on first subdividing the domain of interest into small regions which collectively are called a grid or a mesh. We are developing statistical sampling-based approaches for generating high-quality meshes.

FINITE ELEMENT METHODS

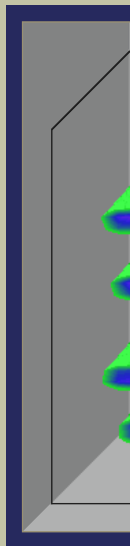
This is a very popular class of grid-based methods that are used to solve PDE's on computers. We are involved in the development of improved FEM's based on modifications of the PDE and replacing the PDE with an equivalent minimization problem.

MESHLESS COMPUTING

Generating grids is a complicated task, but is a necessary step in standard methods for solving PDE's. We are developing a new class of methods that do not require a grid by combining statistical sampling techniques with optimization-based characterizations of PDE systems.

CONTROL AND OPTIMAL DESIGN

In addition to using computers to predict what a physical system will do, one also wants to use computers to tell us how to control or design a system. Although we cannot control the weather,



there are lots of things we can control, e.g., chemical plants, robots used in factories, and the response of an airplane to wind-shear events, to name three of the countless instances. We can also try to design cars and airplanes that have less drag, or bridges that use less steel, or securities portfolios that yield the best return, etc. A major thrust of our research is the development of algorithms for the control and design of systems that are described by PDE's which could potentially include the applications just mentioned and others.

REDUCED-ORDER MODELING

Standard methods for solving PDE's on computers require massive amounts of computing power. We are developing clustering-based, reduced-order methods that are much less expensive to use compared to standard methods.

UNCERTAINTY

All real-world systems involve uncertainties in data and prediction. We are developing methods for solving PDE's that incorporate the effects of uncertainty, using reduced-order methods to greatly cut down on the cost of sampling-and-averaging techniques.

SUPERCONDUCTIVITY

Superconductors, which can transmit current without resistance, can sometimes be modeled using PDE's. We are currently involved in a material optimization study that is aimed at determining the optimal placement of nano-impurities in superconductors that are crucial to their performance.

FLUID FLOWS

Fluid flows play a central role in, e.g., the aerospace, automotive, petroleum, and chemical industries as well as in medical and environmental applications. One project involves using a novel scale-dependent technique for treating notoriously difficult turbulent flows.

IMAGE PROCESSING

A non-PDE related project is the development of inexpensive, effective methods for image compression (approximating an image using much less data), segmentation (dividing an image into segments that contain related elements), and reconstruction (filling in incomplete parts of an image). For these tasks, we have developed efficient and effective statistical clustering techniques – yes, the same ones we use for grid generation, meshless computing, and reduced-order modeling. This is one of the great beauties of mathematics: seeing connections between seemingly disparate notions.

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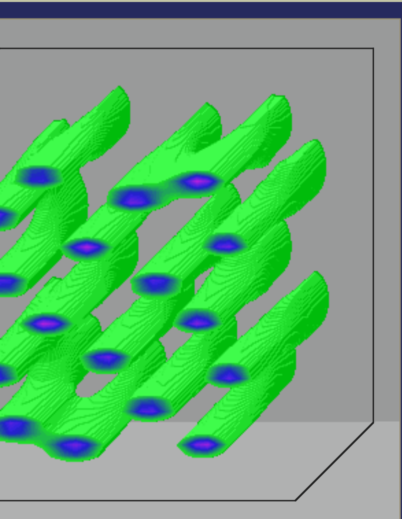
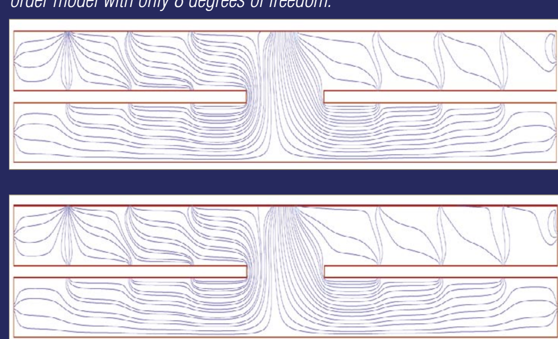


Vortex tubes in a 3D anisotropic superconductor



The flow in a prototype public building determined by an expensive finite element method with thousands of degrees of freedom and with a reduced-order model with only 8 degrees of freedom.

"Europe-by-Night" image and its segmentation into three segments.

Computer Room Upgrade

If you've been on southeast side of Dirac's fourth floor during the months of April and May, then you have probably heard the banging of hammers and the buzzing of saws. On April 4th a major renovation and expansion to the SCS computer room was started. This upgrade was made necessary by a growing demand for computer clusters to support diverse research requirements. The new commodity clusters soon exceeded the available space and the electrical and cooling capacity of the room.

The room was originally designed to accommodate a single computer, the Thinking Machine; however, by the beginning of 2005 this same space held over 500 servers and computational nodes. More space was made available by expanding the west end of the computer room into Dana Lutton's and Elaine Dennison's old offices.

A 40-ton HVAC and a raised floor will triple our current cooling capacity and will help to effectively distribute the cool air throughout the western half of the room. Electrical upgrades to the room were made in 2001 and 2003 and will accommodate present and future demands.

The upgrade is scheduled to be completed in late May or early June. As soon as the room is ready, the cluster nodes and computational servers will be moved from the eastern half of the room into the new space. This will clear the way for the second phase of the computer room upgrade – replace the old AC units and continue the raised floor over the eastern half of the room.

The eastern half of the room is designed to house core services machines, which are currently being temporarily housed in the computer shop.

www.csit.fsu.edu/twiki/bin/view/TechHelp/ScsClusters

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Personnel News

Two of our long-term colleagues have left SCS. **Fred Koerner** of the technical support group has reached retirement age, and is about to start a new life in Arizona with his wife and his Harley Davidson. Good luck Fred, and thanks for all your patience over the years..

Fiber structure in the brain, reconstructed from diffusion MRI data. Image by Y. Yagi, K. Beason, and D. Banks, SCS Visualization Laboratory.

Susan Greenwalt, who has been with SCS for several years in different administrative positions, has moved to the FSU College of Law. All the best to you, Susan, and thank you.

SABBATICALS

Professor **David Banks** will be on sabbatical during the upcoming academic year. Dr. Banks, Director of the SCS Visualization Laboratory, plans to spend this time visiting Harvard Medical School, Johns Hopkins University, and Emory University to collaborate with colleagues in the area of brain imaging.

Professor **Michael Mascagni** will take his whole family to Zürich, Switzerland, where he will be on sabbatical as Gastprofessor in the Seminar for Applied Mathematics (SAM) at the Eidgenössische Technische Hochschule (ETH). He will be teaching a two-term graduate course in advanced Monte Carlo methods. Notes for this course will be made into a book to be published by the European Mathematical Society. In addition, he will be continuing his research in Monte Carlo methods and random number generation with his ETH-SAM colleague Wesley Petersen. Dr. Mascagni will be on historic grounds. ETH, celebrating its 150th anniversary, is the institution where Albert Einstein did his thesis work, although he received his Ph.D. from the University of Zürich.

NEW POSTDOCS

Guoquan Chen has started in Dr. Hussaini's group. **Alexei Vezolainen** joined Dr. Erlebacher's group, and **Li Yin** joined us as a new postdoc of Dr. Cao's. Two biology postdocs started in Dr. Ronquist's lab, **Andy Deans** and **Matt Buffington**.

Five Questions for Joe Travis, Interim Dean of Arts and Sciences

Q *Congratulations, Joe! Tell us, please: How come you accepted this position? We thought you wanted less work, not more.*

A Several considerations in combination led me to accept the position. First, the university and the College have been very good to me and I believe strongly that one ought to return the favor when called. It's a bit of an "old school" mentality that I carry around with me. Second, there is a real opportunity in this position to help multi-disciplinary programs like SCS move forward.

Q *What goals do you have as Interim Dean?*

A Many areas of scientific training and inquiry are changing and we're moving into an era in which our administrative structures don't always reflect the structures within which students need to be trained. We're going to see more "interdisciplinary" and "multidisciplinary" programs being developed. One of my goals will be to help set up policies and structures that can help all of these programs grow and thrive.

In addition, I considered the opportunities to continue to support the remarkable strengthening of many of the programs in the humanities that has marked Dean Foss' stewardship; these seemed awfully enticing to me.

Q *In what way will you deal with SCS issues as Dean?*

A Until we have a plan from the Provost to replace me, I'll continue to function as SCS Director. My guiding principle for SCS will be to act in the best interest of its long-term success as a genuinely interdisciplinary academic program.

Q *What will happen to your research?*

A I hope it will keep moving forward because I agreed only to serve as Interim Dean. Fortunately, I have excellent students who are able to help me through. We have already started experiments and other plans for the coming summer and autumn and that work is under way on its own momentum now. My biggest concern is being able to give my graduate students the attention they deserve, so I am trying to figure out ways to ensure that I carve out the time for their benefit.

Q *Will you come back to SCS after this year?*

A Right now I'm more concerned with how we'll sustain SCS's growth while I am serving as Interim Dean.

One Score or 20 Years Ago....

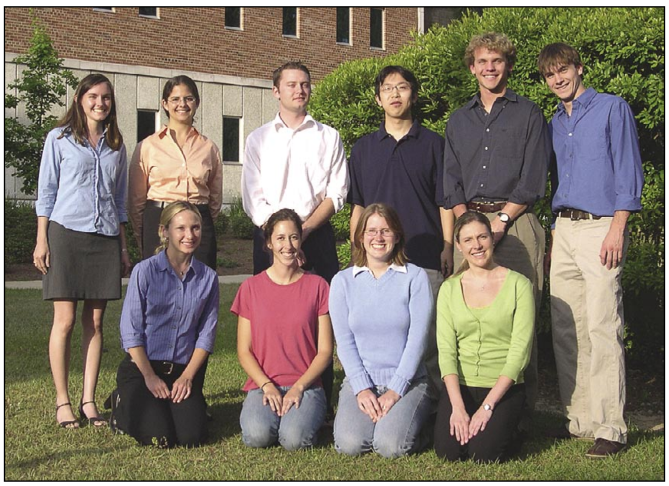
In May of 1985, the era of supercomputing on the Florida State campus was inaugurated, with the arrival of the Control Data Cyber 205. Researchers were eager to pounce on this top of the line machine. One of the special features was a pair of vector pipelines, which allowed it to perform some repetitive tasks even faster than the clock speed would seem to allow. The Cyber was a "massive" machine, with 32 megabytes of memory and a peak speed of 400 MegaFLOPS. It is instructive to realize that today, an ordinary desktop computer exceeds the power of the Cyber.

The Cyber served until October 1989; its most recent replacement is Eclipse, with 512 processors. Every one of Eclipse's processors has 2 gigabytes of memory, and the entire machine can run at a peak speed of 2.2 TeraFLOPS – 5,500 times faster than the Cyber. In other words, calculations that took four days to perform on the Cyber can be completed in one minute on the Eclipse.

"Gaining Computer Knowledge is Like Growing an Extra Arm"

A group of talented FSU students have spent their senior year gaining knowledge about the use of math and computers in modern biology. A year ago, these students were selected from many applicants to be the Hughes Fellows of 2005–2006.

In addition to taking classes in mathematical or computational biology, each student was paired with an FSU Science Faculty member to carry out a biological research project with mathematical and computational components. Since the Fellows studied full time in the fall and spring, most of the research was planned and conducted during the summer between their junior and senior years. Each of them was awarded a $ 5000 stipend to cover their educational costs.



The 2004-2005 Howard Hughes Fellows. Standing, from left: Fiona Smyth, Kimberly Nevader, Michael Miller, Yang Liu, Aaron Kline and Christopher French. Sitting, from left: Carolyn Hemmer, Theresa Landon, Jennifer Walker and Kimberley Thornton. Missing is John Jacobs.

Yang Liu is one of the graduating Fellows, and the one to compare his new knowledge to growing an extra arm. With his mentor, Dr. Thomas Houpt, he studied disturbed locomotion pattern in rats, by recording and analyzing the movement of each of the four paws. The research could be used to add to the understanding of Parkinson's disease, which is characterized by movement difficulties.

While Yang Liu has always been interested in programming, that is not the case with all the students. Most of them are biology majors and their math and computer skills vary. One of the students, Jennifer Walker, describes herself as a former computer illiterate, but after a year of computational science training she surprises not only herself but also people around her with what she can accomplish with the help of a computer.

The computer proficiency and the knowledge of computational resources in general – online databases, for instance – are what the graduating students tend to mention first when they describe their year as a Hughes Fellow. In addition, they appreciate the opportunity to get involved in a research lab and to work closely with senior scientists. The experience of being a Hughes Fellow also included fun times, and, for some, new friends.

www.csit.fsu.edu/HHP

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.

Please visit our website at www.csit.fsu.edu.

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