SCS
Integrating Advanced Computing with Science, Engineering and Liberal Arts

School of
Computational Science
at Florida State University

Image Database Spawns Technological Advances

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Whitetop pitcherplant, Sarracenia leucophylla, *is a rare, insect-eating plant, native to the Southeastern U.S. The photograph of this R. K. Godfrey herbarium specimen was submitted by herbarium director and MorphBank team member, Dr. Austin Mast.*

In recent years, large scientific collections of plant and animal images have started appearing on the Web. Detailed digital photos require so much disk space that in the past large image databases have been difficult to assemble.

MorphBank is one of several open Web databases for biological images. The name refers to the term morphology, which is the study of the shape and structure of plants and animals. The database was started in 1998 by a Swedish-Spanish-American team of insect specialists who wanted to share their microscope photos with colleagues around the world. Dr. Fredrik Ronquist brought the database to FSU in 2003. Since then, the project has expanded rapidly thanks to an interdisciplinary team of FSU scientists from biology, computer science, information studies, mathematics, and statistics (see MorphBank.net).

NOT JUST STORAGE

Much of the development of MorphBank is driven by the database users, whose wish list inspires researchers in different fields to find new technological solutions.

One important addition is the capability of the database to function not just as storage space, but also as a venue for communication between scientists. David A Gaitros (Dept. Computer Science) will present his doctoral thesis in spring on community annotation, which allows scientists to enter notes of their own observations to the database. Every note, and the specific location on the image that the note refers to, will be stored in the database. This makes it easy for biologists to rapidly share information and discuss their findings.

The image annotations need to accommodate conflicting views. What is a fossil zebra bone to one scientist may look like a horse

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So much is happening at SCS that it might be easy to overlook some of the quieter events. This would be unfortunate; some quiet events are very significant.

One of them occurred this summer when Vanessa Jackson defended her M.S. thesis in Biological Science. Vanessa was among the first students to come to FSU specifically to study one of the computational sciences with a faculty member at SCS.

Her thesis, directed by Dave Swofford, was an insightful examination of a popular computational method in comparative biology. As in the best theses, Vanessa's work produced some surprising results and opened up unexpected new questions. Vanessa's success is gratifying at many levels. But for SCS and FSU, her success reinforces our commitment to training students in computational science. Vanessa, it turns out, majored in computer science as an undergraduate and had little formal training in biology. But her talent and energy allowed her to learn new areas and develop a contribution that will change the way some biologists do their research.

This is precisely what is supposed to happen in an interdisciplinary training program. Best of all, this happened even without formal course requirements or protracted negotiations about counting student credit hours — Vanessa studied what her mentors suggested, the Biological Science Department approved her program, and the results speak loudly and clearly.

We have learned that computational science can happen at FSU; now our goal is to pave the way for more students to succeed as well as Vanessa.

Joe Travis
Director, SCS

bone to another. Drs. Peter and Corinne Jörgensen (School of Information Studies) help tailor the annotation technology to biologists and their needs. For instance, different contributors can be ranked by their peers to help users evaluate the quality of the notes in the database.

In the future, it may be possible to take a photo of a plant or an animal, send the image to the database, and get back a reliable species identification. Dr. Anuj Srivastava (Dept. of Statistics) and his group of students are doing research on shape recognition and how it can be used in image matching.

GRID TECHNOLOGY

An important goal for the computer scientists (Drs. Robert van Engelen and Greg Riccardi) is to enhance the database using Web and grid technology. Distributing the images on several computers insures that there are back-up copies, and can also reduce the amount of disk space required on each machine. The latter is important since MorphBank is growing explosively. The number of images is expected to reach 1,000,000 before the end of next year. Grid technology can make all image servers act together as one huge machine.

A SILENT REVOLUTION

The MorphBank group is collaborating with other similar groups in creating international standards that will make it possible for biological image databases around the world to talk to each other. That will give biologists access to a wealth of photos with a wide range of uses. One example is that comparing newfound organisms with images of the ones already known, will speed up the efforts to identify, describe, and protect the endangered species of our planet.

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MorphBank images of similar butterfly species: Agrodiaetus transcaspicus (left) and A. theresiae (right). Photo courtesy Dr. Martin Wiemers, University of Bonn.

Classroom Computers Double as Cluster

Creating the computer classroom has been a big task for the Technical Support Group over the last year. Now the classroom is in full use for the second semester, and its computers are on a busy schedule.

The room contains eighteen computer stations for students, and a mobile one for the instructor. The computers are connected to form a mini cluster, which can be used for research tasks when the classroom is not in use. The cluster is managed by the Condor software.

The computers are modern Linux machines with Intel processors. While the Linux system is what most faculty want to use, the computers also have "virtual Windows", so that Windows based software can be run.

With the recent addition of "Centers of Support" within SCS, the classroom is now a Center of Support with Matt Clausen as the contact person. mclausen@csit.fsu.edu

5 Questions for Hugh Nymeyer

Dr. Hugh Nymeyer has joined the SCS faculty as a Professor of Molecular Biophysics.

Q Welcome to SCS, Dr. Nymeyer. Please tell us a little bit about yourself.

A I grew up in Chicago and went to college in Michigan. After that, I went to graduate school at the University of California, San Diego. I did my postdoc at Los Alamos in New Mexico, which is also where I met my wife Tracy, who is a financial advisor.

Q What brought you to FSU?

A I have been impressed by FSU. It might not be one of the most well-known universities, but there are some very good people here.

Q Which scientific field are you interested in?

A I work with proteins and their three-dimensional structure. I study how they fold and how folding changes their properties. I make computer models of proteins and their environments and study the interactions.

Q What is the advantage of the computer over experiments?

A One of the problems with traditional experiments on protein folding is that things happen so quickly that it's hardly possible to detect the middle steps of a reaction. You know what you have initially and what you end up with. In the computer I can see what happens in between, and I get some really interesting results.

Q You are teaching a lot during this first semester at FSU. Why is that?

A I actually asked for it. I enjoy teaching.

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Welcome — and Good-bye!

Dr. **Hugh Nymeyer** (see article to the left) has joined the SCS faculty as an assistant Professor of Molecular Biophysics. Two visiting professors will spend their sabbaticals with SCS. They are **Hong-Chul Kim**, who is in Dr. Gunzburger's group, and **Jae Woo Lee** in Dr. Rikvold's group.

Several postdocs have started over the last months, including **Hongmei Chi** (group of Dr. Beerli), **Daniel Robb** (Dr. Rikvold), **Debra Murray** (Dr. Ronquist), **Hatem Touil** and **Betul Unlusu** (Dr. Hussaini), and **Sung-Dae Yang** (Dr. Gunzburger).

Wilfredo Blanco, who was in Dr. Bank's visualization group for two years, started working as a research assistant on the MorphBank project in October.

While we welcome our visitors and new colleagues, we say thank-you and good luck to **Hugh Brown**, formerly of our Technical Support Group, who is now working for ACNS at FSU.

Physicist Outside the Box

Per Arne Rikvold, professor of physics at SCS, enjoys crossing borders. Not only did he leave his native Norway for the U.S., stopping in Japan for a couple of years; he has also refused to stay put within the traditional boundaries of physics. He is a convinced interdisciplinary scientist who doesn't let traditional specializations define the limits of his research, and his group investigates things as diverse as magnetism, electrochemistry, evolution, even fluctuations of the stock market.

CROSSOVER SCIENCE

How can that be? What would a physicist have to add to the area of biology, or economics? "Physicists have a reputation of arrogance, of trying to work on subjects that they know nothing about," says Rikvold, jokingly — himself anything but arrogant. He continues, more seriously: "Theoretical research is often interdisciplinary by nature, since the methods we develop can be applied to many different problems."

The new School of Computational Science was created for scientists interested in scientific borderlands, and Rikvold was delighted when given the possibility to join SCS. He has high expectations for cooperation and knowledge transfer among the different groups that make up the new school, and he takes an active part in its shaping. But then again — we should not expect him to settle down behind his SCS desk. With his laptop in the backpack, he'll keep rushing between SCS and three other FSU organizations where he has collaborators: the Physics Department, MARTECH, and the NHMFL (Center for Materials Research and Technology, and National High Magnetic Field Laboratory).

Dr. Rikvold's group is often called the SCS Materials Science Group, though that must be taken in a very wide sense, he says. The common denominator of the diverse work of the group is statistical physics — or rather methods developed in statistical physics — that can be used for exploring all kinds of phenomena.

INTERACTING PARTICLES

The systems that the group studies involve large numbers of interacting particles. When applied to biological macroevolution, the "particles" are individuals of different species, interacting with each other, such as a predator interacting with its prey. When applied to surface electrochemistry — think for instance of plating car bumpers with chromium — it is about how molecules and ions in a

Per Arne Rikvold and his group

Professor Rikvold was born and raised in Northern Norway, and earned his Master's degree at the University of Oslo in 1976. He moved to Kyushu University, Japan for a graduate fellowship, and took the opportunity to study Japanese along with the research work. After two years in Japan, and two more in Oslo, he headed for Temple University in Philadelphia, Pennsylvania, where he earned his Ph.D. in 1983. A post-doc position at State University of New York at Stony Brook was followed by two years as Senior Research Chemist at ARCO Chemical Company in Pennsylvania. In 1987 Rikvold became an associate Professor of Physics at FSU, where he also got involved in the Supercomputer Computations Research Institute (SCRI), predecessor of SCS and CSIT.

Over the years, Rikvold has been granted several honors and awards in Japan, Norway, and the U.S. In the summer of 2004, he was named the James G. Skofronick Professor of Physics at FSU.

Rikvold's group includes three Physics graduate students: **Ibrahim Abou Hamad** from Lebanon, who specializes in simulation studies of electrochemistry, **Sam Hill Thompson** from the U.S., who studies dynamics of magnetic nanoparticles and ultrathin films, and **Volkan Sevim** from Turkey, who works on macroevolution. Postdocs are **Stefan Frank** from Germany (electrochemistry) and **Daniel Robb** from the U.S. (dynamics of nanoscopic magnetic systems). **Greg Brown** from the U.S., a research scientist with Parallax, Inc. of Tallahassee and a former postdoc in the group, shares his time between SCS, Parallax, and Oak Ridge National Laboratory in Tennessee. At SCS he works on problems both in magnetization dynamics and electrochemistry.

Standing, from left: Ibrahim Abou Hamad, Stefan Frank, Per Arne Rikvold, and Daniel Robb. Sitting: Sam Hill Thompson, Greg Brown, and Jae Woo Lee. Missing are Volkan Sevim and Gloria M. Buendía.

Physics professor **Jae Woo Lee** of Inha University, Korea, recently joined the group for his sabbatical year. He is interested in the statistical description of time series and surfaces, and currently he is working on an application to stock market fluctuations. A regular visitor and collaborator with the group is physics professor **Gloria M. Buendía** of Universidad Simón Bolívar, Venezuela. She works on problems in nonequilibrium statistical mechanics related to both magnetism and surface chemistry.

solution interact with each other and with metal surfaces.

Electrochemistry is the research for which Rikvold gets the most attention right now, and also the most invitations to give talks. However, much of his work is in another area, magnetic nanoparticles, which are being used in computers to store data.

When computers get smaller, so do the particles used to store the zeros and ones that make up all software and data in the computer memory. However, information stored on very small particles becomes sensitive to both thermal fluctuations and to weak magnetic fields, such as the earth's magnetic field, or metal detectors at airports. Since "you don't want to have to carry your laptop around in a bottle of liquid helium in the future," as Rikvold puts it, it is crucial to understand how to keep those minute magnetic moments stable in our everyday environment.

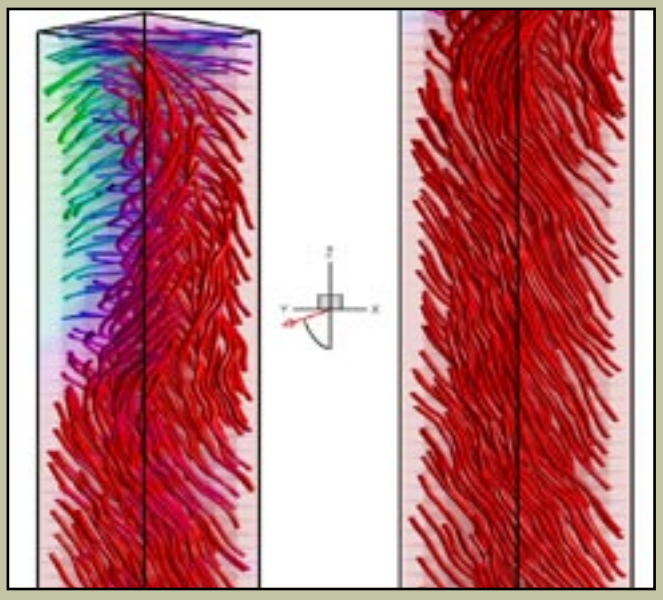
TECHNOLOGY BOOST

The theoretical understanding of nanoscale magnetism demands huge computations, and so do the other problems mentioned above. The more refined and fast the computer models and computers get, and the larger mathematical models they can handle, the more details start to show in the results of the computations. Meanwhile, the experimental research also develops quickly. Using surface chemistry and magnetism as examples, Rikvold continues: "The development of better microscopes has been explosive since the 1980s, and scientists can study smaller and smaller systems. Today, it is actually possible to look at individual atoms with equipment like STM or AFM (Scanning Tunneling Microscopes or Atomic Force Microscopes)."

"While the experimental scientists look at the atoms in a microscope, those of us who choose the theoretical approach can study and predict the movement of atoms in a mathematical model, run by fast computers. We have reached a point where the systems that experimentalists and theorists can study begin to overlap, which is truly exciting."

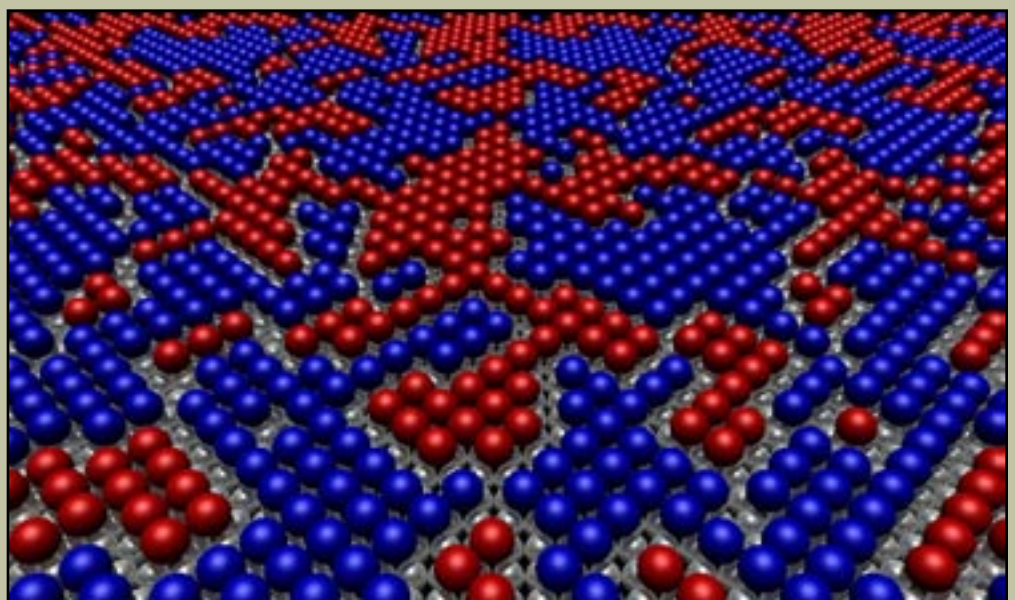
ACKNOWLEDGEMENT

Rikvold's research is funded in part by The National Science Foundation.



Magnetic flux lines inside a simulated iron pillar (9 x 9 x 150 Ångström), modeled after nanoparticles that are synthesized by MARTECH at FSU. The pillar is caught in the act of reversing its magnetization from antiparallel (red) to parallel (green) to the applied magnetic field (the red arrow in the coordinate system in the middle). Left: top of pillar. Right: middle of pillar. Visualization by grad student S. H. Thompson.

A simulated layer of bromine (Br) on a silver (Ag) surface. The Br atoms are too large to sit in nearest-neighbor positions on the surface, so they fill one of two sublattices (red or blue), like the black and white squares on a chess board. The "red" and "blue" domains are separated by domain walls, where the Ag atoms (silver) can be seen between the Br. Visualization by former grad student Steven J. Mitchell (now at The University of Georgia).



Consolidating the School of Computational Science

Last April, Provost Larry Abele issued revised guidelines for the School of Computational Science. Besides changing the name from Computational Science and Information Technology (see What's in a Name?), these guidelines ushered some significant changes for us.

The changes were prompted by our desire to develop training programs in computational science and our difficulty in doing so in the past. In fact, the revised guidelines actually begin with a clear description of SCS's responsibility for developing and delivering new graduate programs in computational science and outline how those programs will be structured administratively. The plans being developed include so-called stand-alone programs as well as joint degree programs with individual departments.

INCREASED AUTONOMY

With increased autonomy over faculty assignments comes increased accountability. The guidelines include benchmarks against which the school's progress will be assessed after five years. These benchmarks include the number of students in the programs, the number of other departments served by computational courses, and the research productivity of the faculty, among other measures.

The guidelines describe an interim assessment after two years that will be used to gauge how well our present level of autonomy is helping us achieve our goals.

The Committee for Curriculum and Recruitment at work. From left: Wendy Cheng, Janet Peterson, Huan-Xiang Zhou, Bernd Berg, Michael Navon, and Max Gunzburger. Gordon Erlebacher and Gavin Naylor are missing in the picture, but part of the committee.

And with these changes in organization and responsibility, there is much to be done. We have assembled several faculty committees who are working on tasks from writing by-laws for a governance structure to developing short-term and long-term faculty recruitment plans. Of course, the largest committee is working to develop the degree programs and curricula that will, more than anything else, define the school.

CHANGES FOR FACULTY

The consolidation of the School has brought some changes but not a wholesale revolution. The major changes are administrative. In the past, each faculty member received his or her assignment of responsibility from the chair of the home department, with the Director contributing the "CSIT portion" of the assignment. Now, the process is reversed. The SCS Director makes the assignments with a contribution from the department chair. This change should bring more stability to faculty assignments and permit the offering of new courses and programs. Faculty members remain in individual departments and will still devote teaching effort to courses offered in their departmental programs.

FOCAL POINT

The more important change is the higher visibility that this consolidation will give to computational science

"The more important change is the higher visibility that this consolidation will give to computational science on the campus."

on the campus. To be sure, computational methods are used by many research programs all across the campus and instruction in those methods takes place every day somewhere on campus. We will be a focal point for research and training in the development of these methods and in the study of their effectiveness.

Indeed, as increasingly sophisticated computations are used more widely, the study and development of those methods become increasingly important. So the real news is the affirmation that computational science, as a discipline, belongs on the FSU campus.

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SCS Faculty, September 2004

David Banks
Peter Beerli
Bernd Berg
Dennis Duke
Gordon Erlebacher
Sergio Fagherazzi
Kyle Gallivan
Max Gunzburger
Yousuff Hussaini
Michael Navon
Gavin Naylor
Hugh Nymeyer
Janet Peterson
Per Arne Rikvold
Fredrik Ronquist
David Swofford
Huan-Xiang Zhou

What's in a Name?

While the discussions about consolidating the School's faculty were occurring, the School of Information Studies was developing new degree programs in information technology. When those programs were approved, Dean Jane Robbins asked if we would consider changing our name to minimize confusion and help make clear that Information Studies was the campus home for degrees in information technology. As it was, we did not anticipate that information technology would become a major part of our curriculum, although some information technology must be a part of any computational science curriculum. But in the larger framework of the campus, it seemed wise to follow Dean Robbins' suggestion. These changes will be submitted to the Faculty Senate and its committees for approval this year.

Prominent Math Visitor

Professor Peter Lax. Photo courtesy of New York University, Courant Institute of Mathematical Sciences.

In the week of November 15, Professor Peter Lax from the Courant Institute of Mathematical Science, New York University, will visit FSU. Professor Lax is a Member of the National Academy of Sciences of the U.S. He has also been awarded the National Medal of Science and the Wolf Price.

Professor Lax is the first one in a series of eminent mathematicians to receive the new Sir James Lighthill Distinguished Lectureship Award. This award was established to honor leaders in mathematical sciences, and to attract them to visit the Florida State University to give lectures, inspire and interact with the faculty and students. The Provost confers the award, which was established following an initiative by SCS Professor M. Yousuff Hussaini.

Sir James Lighthill was a great mathematical scientist of the twentieth century, whose contributions in the diverse field of fluid dynamics were insightful, fundamental and enduring. He had an uncanny ability to find mathematical descriptions of physical processes that were deceptively simple and yet captured the essence of complex fluid dynamical phenomena in such fields as aero-acoustics, water waves and bio-fluid dynamics.

For more than half a century the famous Lighthill acoustic analogy has formed the basis of procedures for computing the noise produced by aircraft engines. His formulation of the general principles of fluid waves has led to greater understanding and prediction capabilities for ocean currents and flood movement. His pioneering, interdisciplinary contributions to bio-fluid dynamics ranged from blood motion to animal flight.

Faculty who wish to meet with Dr. Lax while he is here may call Susan Greenwalt at 644-0601.

Research Tryout for Students in Mentorship Program

Undergraduate students from universities all over the nation visited FSU during the past summer. They all took part in a mentorship program called "Research Experience for Undergraduates", or REU. This was made possible due to a collaboration between Dr. M. Yousuff Hussaini from SCS, and Dr. Steve Blumsack from the FSU Mathematics Department.

Based on their research interests, the students were assigned to work on small projects for various faculty members and postdocs at FSU. These mentors were Steve Blumsack, Jerry Magnan, and Mark Sussman (Mathematics); James O'Brien, (COAPS); and Shannon Grady, Mohamed Jardak, Jinquan Xu, Marwan Al-Haik and Svetlana Poroseva, (SCS). Susan Greenwalt carried the administrative load, while Mimi Burbank and Adrian Petrisor provided the technical support that made the venture possible.

Adrian Petrisor

The mentorship program gave the students a chance to try research before choosing their careers. Hopefully some will come back for graduate studies at FSU.

SUPERCOMPUTER ACCESS

Mentor Shannon Grady says: "My student was great. He worked on wind turbines, and produced some useful results. He also enjoyed working on a supercomputer, which was an opportunity he would not have had at his small home college." During their eight weeks at FSU, the students attended short courses and seminars in mathematics and science, given by FSU faculty including Dr. David Swofford (SCS); Dr. David Loper, (GFDI); Dr. T.N. Krishnamurti (Meteorology), Dr. DeWitt Sumners and Dr. Steve Bellenot (Mathematics); and Dr. Jim O'Brien (COAPS).

The program concluded with a poster session followed by a dinner and an appreciated talk by Provost Larry Abele.

NEW STUDENTS NEXT YEAR

NSF funded the program together with the Department of Defense (DoD). Stipends, travel, and living expenses were paid for all 16 students, who were selected from 70 applicants. The program will continue in summer '05 with another group of students.

For an in depth look at the mentorship program, please see http://www.cespr.fsu.edu/people/myh/reu.html

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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