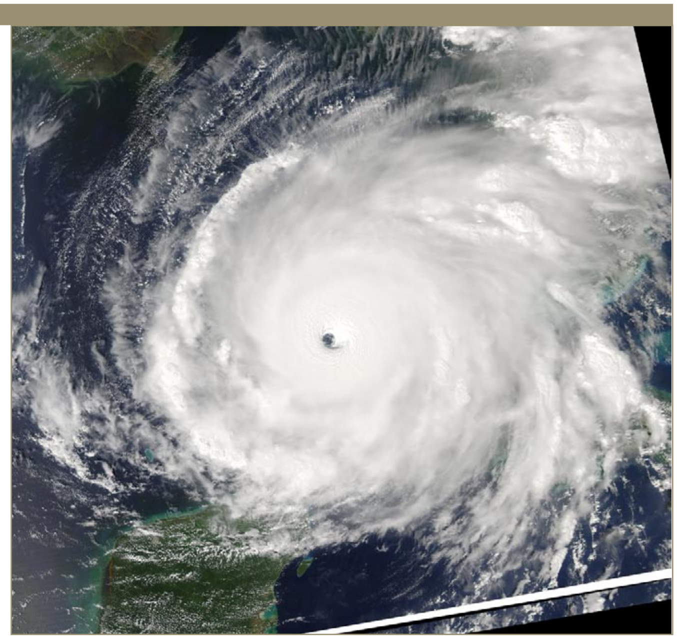
SCS

Integrating Advanced Computing with Science, Engineering and Liberal Arts

School of
Computational Science
at Florida State University

How Mathematics Saves Lives

INSIDE THIS ISSUE



Hurricane Rita, here on its way across the Gulf of Mexico, made landfall in Texas on September 24, 2005. Image courtesy Liam Gumley/UW-CIMSS.

This past hurricane season has once again proven that mathematics can literally save lives. The amazingly accurate hurricane forecasts, which are all based on equations and observations, give authorities and residents time to evacuate threatened areas, and take other precautions to protect people and property. Unlike the people in Galveston in 1900, we are no longer taken by surprise by the storms.

Hurricane models are continuously upgraded and refined by our most skillful mathematicians. Dr. Michael Navon at SCS is one of them. He and his group, and collaborators across the US, are working on improving the mathematical foundation of the models. One of the questions currently occupying his time is the question of data assimilation.

Simply speaking, data assimilation is about how to update your model with new data from observations, and about how much you should trust new measurements compared to the well-founded data from the model, which is based on thousands of measurements.

DOES REALITY COUNT?

We all know that if the map differs from reality, reality counts. But if a measurement of say wind, humidity, or temperature – all of which are important factors in hurricane prediction – differs from what your model predicted, then what do you do? The new data could very well contain important information about an unexpected turn in the hurricane trajectory, or an increase in strength. However, it could also be the result of an inaccurate measurement, or be within the range of normal variation at that spot in the atmosphere. Scientists thus need to be able to balance the predicted value, which is based on thorough research, with the actual observations at each moment.

Mathematicians talk about the variance of an observation, which measures its uncertainty. Dr. Navon is working with a calculus method called Kalman filters, which is a set of mathematical equations that provides an efficient computational (recursive) means to estimate the state of a process, in a way that minimizes the mean of the squared error. The filter is very

continued on page 2

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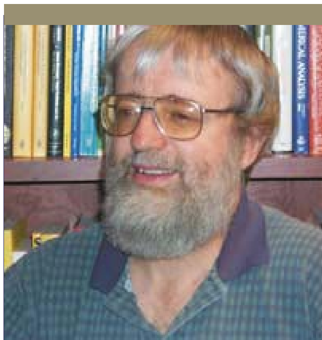

Joe Travis has been appointed Dean of the College of Arts and Sciences, and I have been appointed to replace him as the Director of the School of Computational Sciences. We all want to thank Joe for his years of service as director and wish him luck and success in his new position.

I am excited about taking over the leadership of the SCS. We have in place an outstanding interdisciplinary faculty, superb facilities, and an excellent support staff. The goals of the SCS remain as they have been: (1) to develop innovative interdisciplinary graduate training programs in scientific computing and its applications, (2) to foster research in scientific computing and its applications in a variety of disciplines, and (3) to provide a supportive environment for computing on the campus.

We have accomplished much towards meeting the last two goals, and this year, we will be developing and implementing degree programs. We have submitted preliminary proposals for two new degree programs, described on Page 3, which we plan to have in place by the Fall 2006 semester. It is important to note that these new programs do not duplicate existing programs at FSU; instead, they will complement them to provide FSU students with new choices for learning about scientific computing.

This year we will also be hiring additional faculty to further enhance our research and teaching. We also hope to host several interdisciplinary workshops and visitors. All in all, building on the progress made in the last few years, this should be the year the SCS fully matures into a top-notch unit providing excellent research and education to FSU and the scientific community worldwide.

Max Gunzburger,
Director, SCS

powerful in several aspects: it allows estimations of past, present, and even future states, and it can do so even when the precise nature of the modeled system is unknown. It does so in a way that minimizes variance and gives the best possible state for the computer model for the next prediction of updated forecasts.

PROFESSOR KALMAN

Rudolf E. Kalman, who is Hungarian by birth, is a professor emeritus from University of Florida. He started to develop the Kalman filters in 1959. Since that time, due in large part to advances in digital computing, the Kalman filters have been the subject of extensive research and application, particularly in the area of navigation. They have been used on spacecrafts like the Apollo, but they have been difficult to use in weather models because they demand an unreasonable amount of computer resources.

Dr. Navon and his colleagues at CIRA, Colorado State, are working on a modification, called Ensemble Kalman Filters (EnKF). This was first proposed in 1994 by Dr. Geir Evensen, Nansen Environmental and Remote Sensing Center, Bergen, Norway. The modification will bring down the computational complexity, and eventually enable the useful Kalman filters to find wider use in numerical weather prediction.

www.cira.colostate.edu/nsf/default.asp
www.nersc.no/~geir/EnKF/
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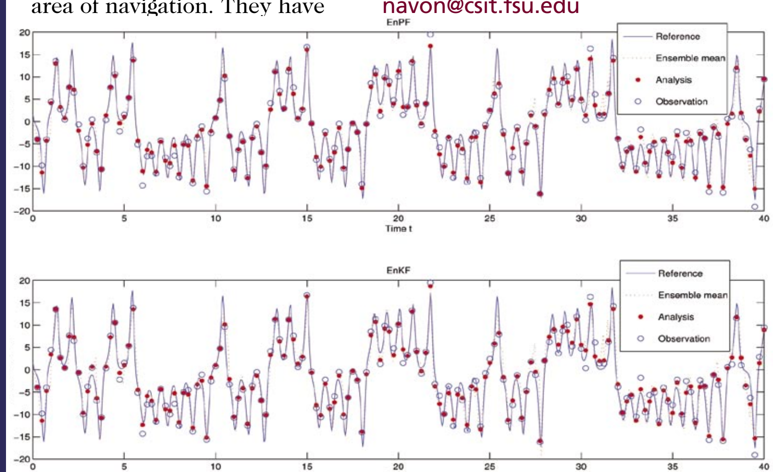

The EnKF is a sophisticated sequential data assimilation method. It applies an ensemble of model states to represent the error statistics of the model estimate, it applies ensemble integrations to predict the error statistics forward in time, and it uses an analysis scheme that operates directly on the ensemble of model states when observations are assimilated.

New Graduate Degree Programs at SCS

The SCS has formally submitted paperwork to begin the process of getting two new graduate degree programs established. The degree programs consist of a doctoral program and a professional master's degree which is known nationwide as a Professional Science Master's (PSM) degree. The initial phase of the process to establish a new degree program is to complete a "Proposal to Explore" for each program; this proposal must be approved at various levels of the University. At the September 11 meeting of the Science Area Chairs, the two proposals were unanimously approved.

The proposed Ph.D. degree is in computational science. This degree program is in answer to the national need for individuals trained in an interdisciplinary environment with a strong computational grounding.

The program will strive to integrate computational science and an applied science and prepare students for positions in academic environments as well as the industrial and laboratory settings.

The proposed PSM is a two year, professional degree program which prepares students to work outside of an academic setting in industry, government or a national laboratory. The goal of the program is to train students to be technically adept in computational science, to acquire knowledge of an applied science as well as to be able to manage a project, work in teams and to effectively communicate ideas and results.

Since the SCS lies at the intersection of applied mathematics, applied science, computer science and engineering, it has the unique opportunity to train students in areas which cut across disciplines. These areas include topics such as visualization, multi-scale analysis, data analysis, algorithm development, etc.

The SCS consists of faculty trained in application areas such as biology, chemistry, engineering, geology, and physics as well as faculty concerned with data analysis and algorithm development, analysis, and implementation. Consequently, SCS is uniquely situated to provide an interdisciplinary environment to foster graduate training of the nature described.

If the new degree programs are approved in a timely fashion, the School anticipates accepting applications for the 2006–07 academic year for the Ph.D. program and in the following year for the PSM program.

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Scientific programming

Becoming a multidisciplinary scientist requires versatility and the ability to adapt to a changing environment. This is particularly true with programming languages, which form the backbone of virtually all areas of scientific research that involve computers. While many students at FSU have elementary knowledge of a single compiled language such as C and Fortran, or of an interpreted language such as Matlab, this knowledge is insufficient for the development of large-scale scientific codes, which require abilities such as multi-file programming, multi-language programs, benchmarking, and more.

To remedy the situation, we have developed a course on scientific computing to provide students with a working knowledge of Fortran 90, C++ and Java, three languages of wide-spread use in scientific computing. Working knowledge of one of these three languages is a prerequisite for the course, which ensures that the other languages can be learned relatively easily by concentrating on their similarities. The students are taught to solve problems at the conceptual level using mainstream object-oriented programming ideas. They are also taught to benchmark and document their codes.

Fourteen students are participating in this first offering of the Scientific Computing course. They are a mix from the departments of Mechanical Engineering, Physics, Mathematics and Meteorology. This course will be required of all students enrolled in master's and Ph.D. programs at SCS.

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Shark Scientist Swims Against the Tide

Gavin Naylor is one of four professors in the group of evolutionary biologists at SCS, but while the other three are busy developing state-of-the-art computer models for the study of evolution, Gavin Naylor is more interested in testing the models with empirical data.

He focuses his research on the evolution of sharks. However, if you expect him have gruesome stories to tell about encounters with these mighty animals, you will be disappointed. It is true that he gets to travel widely around the world, collecting specimens for his research, but he rarely goes fishing for live ones. Instead, he goes to smelly, local fish markets to buy the animals that he needs.

“Reality is usually quite boring”, he says with a laugh.

SHARK TEETH

As a biologist, interested in evolution over long periods of time, he has found sharks to be the perfect model animals.

“Sharks have a much better fossil record than most animals”, explains Dr. Naylor. “They can afford to shed their teeth regularly, since they are cartilaginous fish and don’t need as much calcium for their skeleton as bony fishes. Thus, shark teeth from the latest 200 million years can be found in fossil deposits and compared with teeth from living sharks, to provide a sense of their evolutionary history.”

Like all evolutionary biologists, Gavin Naylor works with evolutionary trees, showing how today’s organisms are related, and which their ancestors were. While evolution as such is undisputed among modern biologists, the exact look of the gigantic tree of life is largely unknown.

Evidence is gathered branch by branch, twig by twig, through meticulous comparisons of different species. Data is stuffed into computer software, which, in turn, calculates the most likely family tree for the studied group of organisms.

EVOLUTIONARY LEAPS

The dominating view among biologists is that evolution takes place in small steps, or incrementally. Gavin Naylor, however, is of the opinion that sometimes evolution may take leaps rather than tiny steps, and he gives the example of the hammerhead shark.

When analyzing DNA from different shark species, he discovered that the family tree challenges the former theories on shark evolution. The dominating view has been that the extreme head shape of the hammerheads has developed gradually, via species with intermediately wide heads. Dr. Naylor suggests the opposite, saying that the most basal hammerhead shark likely had the most extreme head shape and that sharks with intermediate heads represent evolutionary steps away from, not towards, extreme heads. He also suggests that the hammer-like head may be the result of one single mutation with drastic effects. Now, how would that be possible?

ALTERED FUNCTION

A mutation causes a change in the blueprints used to make proteins in the cell. A single mutation might cause one single amino acid in the protein to be exchanged for another one, which, chemically, is a small change. However, if the new amino acid has a different charge than the one it replaced, it might twist the whole amino acid chain and cause it to fold in a totally new fashion, which will inevitably give a new function to the protein.

Most mutations this drastic would die out quickly, but in a few cases they would survive because they provide some kind of advantage to its bearer. Dr. Naylor argues that something like this may have occurred initiating the origin of hammerheads. A single mutation in a regulatory gene might have caused a differential growth pattern in the head, giving a poor shark a head that the oceans

School of hammerhead sharks. The eyes are placed at the end of each side of the broad and flattened head. front of the head these sharks have sense organs, detecting changes in pressure and electrical fields. The h acts like a wing, probably improving maneuverability. Photo courtesy Seawatch.org.

had never seen before. The reason that a fish with this odd look could survive is possibly an advantage that the hammerhead has when it comes to navigation and the search for food.

Evolutionary leaps might also give an answer to the question about “missing links”, the intermediate species that one would expect to find as evidence of the gradual evolution from one group of species to the next, but that researchers have failed to find in the fossils. Gavin Naylor’s idea is that, in some cases, these forms may have never existed.

On the ... ead also

SMART SIMPLIFICATION

Gavin Naylor represents the users rather than the developers of computational methods. He humbly claims to be a poor mathematician, but also recognizes this as a possible advantage:

“Since I don’t understand the most complicated calculations, I have to look for the simplest solutions to scientific problems,” he says.

What he calls simple, others would call brilliant. Together with his former graduate student Olivier Fedrigo, he has designed a novel DNA sequencing chip, which is subject to a pending patent application, and which could be potentially useful for computational biology.

DNA sequencing is widely used to compare an unknown species to its known relatives, to figure out its place on the family tree. The method is theoretically simple: you paste small sequences of DNA onto a chip, flood the chip with a preparation of the unknown DNA, and check for matches. Even with short strands of DNA this creates a big task, requiring a big chip, since there are so many possible combinations of the four existing nucleic acids. (Imagine how many different necklaces could be made from beads of four colors.)

Gavin Naylor’s idea is that in reality, the number of combinations is much more limited, since most of the theoretically possible DNA sequences would result in non-functioning proteins. Evolution may have already produced most of the viable variations. If you limit the DNA on your chip to permutations based on DNA from all known species, the resulting chip will be a whole lot smaller and easier to produce and use, and the results easier to analyze.

So while others at SCS strive to find faster algorithms for the software that analyzes DNA sequences, the Naylor lab tries to cut computation times from the other end, by reducing the search space of necessary computations.

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The Naylor lab: Standing, from left: Clemens Lakner, Neil Aschliman, and Vicente Faria. Sitting: Jun Inoue and Gavin Naylor.

Professor **Gavin Naylor’s** research addresses issues like why there are so many different organisms on earth, and how the genetic variation maps to the visible, or functional, variation in plants and animals. His favorite model organisms are sharks, because they shed their teeth regularly, leaving behind an abundant fossil record. Comparisons of fossil teeth and more recent ones allow evolutionary studies over a period of 200 million years, back to the dinosaur age.

Dr. **Jun Inoue** is a post doc from Japan. He is interested in the molecular phylogenetics of fishes, especially ancient fish. Among other things, he has worked on how to estimate the divergence times using sequence data. At FSU, he started the development of novel molecular evolutionary models for vertebrate mitochondrial genomes.

Neil Aschliman is a Ph.D. student, interested in vertebrate evolution and diversity. He studies the systematics of batoid fishes (skates, rays, and sawfishes) from molecular and morphological perspectives. He also enjoys scientific illustration.

Vicente Faria is a PhD candidate, trying to find out how many species of sawfish there are. The taxonomy of this group is among the most confused of all sharks and rays. His dissertation research centers around characterizing genetic variation within and among species for all taxa in the family, from all parts of the globe.

PhD student **Clemens Lakner** is interested in methods for reconstructing the evolutionary history of organisms, especially statistical methods. Bayesian inference methods allow dealing with parameter rich, complex models that take protein structural information into account. His main interest is to identify structural constraints and to use this information for phylogenetic inference.

Personnel Update

Our new director, **Max Gunzburger** is a Francis Eppes Professor of Mathematics. He came to FSU in 2002, after stepping down as chair of Iowa State University's math department. Together with his colleague Janet Peterson, Max Gunzburger has assembled a large group of students and post docs in computational mathematics at SCS. Dr. Gunzburger presents some of his plans in the director's column on page 2.

SCS also proudly recognizes that our former director, **Joe Travis**, has been appointed permanent dean of the College of Arts and Sciences, after only a few months as interim dean. Congratulations from all of us!

Four postdocs have been hired. **Sangbum Kim** adds to the group of Janet Peterson and Max Gunzburger. **Naveed Aslam** is working with Yousuff Hussaini, **Jun Inoue** with Gavin Naylor, and **Donghong Min** (below) with Wei Yang.

The MorphBank project keeps growing, and **David Gaitros** has been hired as a project manager to maintain order, while working on "community annotation", a system for communication within a database.

The Technical Support Group has lost two members, and gained one. **Mimi Burbank,** our (La)TeX expert, has left FSU, which she has served since 1984. Retirement for some people means relaxing, but Mimi plans to buy a one-way airplane ticket for Uganda, where she will work with the people of the Diocese of Kasese. Good luck, you brave woman!

Danny Loughlin left our TSG in early summer to take a position at the FSU/FAMU School of Engineering. Danny contributed significantly to the growth and maintenance of SCS research clusters, network monitoring, and systems support. Thanks, Danny!

Tim Nguyen-Pham (right) has been hired as a senior member of the technical support staff. He will be working with faculty and students to help fine-tune our clusters and servers so that these systems better satisfy our research requirements.

Professor Wei Yang

Dr. Donghong Min

Wei Yang, assistant professor of chemistry and biochemistry, has joined SCS to further strengthen computational biophysics. He is the third SCS professor in this area, along with Huan-Xiang Zhou and Hugh Nymeyer. Wei Yang obtained his B.S. degree from Tsinghua University in China, and got his PhD from SUNY at Stony Brook, New York. He was a post doc at Harvard before moving to Tallahassee with his wife and their little son. To relax, Wei Yang loves to skate and play soccer.

Wei Yang has hired a post doc, **Donghong Min**, who comes from Louisiana State University with a Ph.D. in computational materials science. She will be working with the development of efficient stochastic sampling methods to simulate biomolecular motions.

Raul Tempone is a new assistant Professor with SCS and the Department of Mathematics. He was born in Montevideo, Uruguay, where he also obtained his degree in Mechanical Engineering. After defending his PhD thesis at the Royal Institute of Technology in Stockholm, Sweden, he spent two and a half years as a postdoc at the Institute of Computational and Engineering Sciences, University of Texas, Austin. His area of interest is applied mathematics, in particular the approximation of deterministic and stochastic differential equations. Dr. Tempone is excited to join SCS and looks forward to interacting and collaborating with fellow faculty at SCS.

Tim Nguyen-Pham

New Research Grants

Three research grants have been awarded to SCS recently, all collaborative grants with other universities or FSU units.

SCS Professors **Michael Navon** and **Gordon Erlebacher**, with collaborators at Portland State University, were awarded a NASA/Modeling, Analysis and Prediction grant for their project on "Adaptive observations". This project is about the most efficient way to gather data like like moisture, wind velocity, and temperature for weather models. Some observations contribute more than others to the quality of the forecasts of extreme events, such as hurricanes. "Adaptive observations" is about making it easier to choose the best locations and times to make critical observations using adjoint model sensitivity.

The total support for the first year will be about $125,000. Parts of the grant will be used to support a full time graduate student at SCS.

Dr. **Max Gunzburger** and his collaborators from Sandia National Laboratories, Colorado State University, and Rensselaer Polytechnic Institute have been awarded a grant on "Atomistic-to-Continuum (AtC) Coupling" by the Department of Energy.

AtC coupling has emerged as a critical component in computational materials science and other applications. Past research in AtC model and algorithm development has paid off in the formulation of effective procedures for specific applications. However, much less effort has been directed at the mathematical theory of AtC methods. Dr. Gunzburger and his colleagues will develop an operator based mathematical formalism that addresses and quantifies critical formulation issues such as well-posedness, stability, error estimation and the inherent uncertainty of the AtC coupling process.

The total grant is $2.3 million, and the SCS portion will be used for at least one graduate student and one post doc position.

Dr. **Fredrik Ronquist** and the interdisciplinary MorphBank team has been awarded an NSF grant, which will allow development of the image database both technically and geographically. As the database expands, several research challenges regarding database technique, information technology, networking, and user communication need to be addressed. The mere size of the database is also a challenge, as well as communication between the planned nodes of the global network.

The total FSU grant is $2.25 million. The SCS share will be used for programming staff, graduate students, summer salaries and more.

Courtesy of Carsten Heckmann, Leipzig University

Berg 21st Leibniz Professor

Leipzig is a town of half a million people in the former East Germany. The town hosts Germany's second oldest university, which will celebrate its 600th birthday in 2009. Gottfried Wilhelm Leibniz, who is best remembered for inventing calculus independently of Newton, was born in Leipzig in 1646. Indeed, in 1675 Leibniz was the first to write down the modern $\int f(x)\,dx$ integral notation, which since then has caused nightmares in billions of school kids. A bitter priority fight with Newton followed in the early 18th century, perhaps the first of its kind in science. Leibniz also tried to construct a mechanical calculating machine, which failed, and developed the binary system of arithmetics, which is used in modern computers.

Every year Leipzig University honors its famous son, whom they once refused their Ph.D. degree, by naming two Leibniz Professors. This year one of the Leibniz Professorships was awarded to Dr. Bernd A. Berg for his achievements in computational physics. Dr. Berg is a FSU professor since 1985, who is tenured in the Physics Department and holds an appointment with the School of Computational Science.

The Leibniz lectureship is endorsed with a competitive stipend and comes with the obligation to teach one course and a seminar series. At the award ceremony, Dr. Berg gave a public lecture with the title "The Computer Revolution and Computer Simulations".

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Some of the MCM conference participants outside the Turnbull Center at FSU, where the conference was held.

The Science of Rolling Dice

The Fifth IMACS Seminar on Monte Carlo Methods was held at FSU in May, 2005. This was the first of these seminars to be held in North America, the four previous installments all having taken place in Europe.

The attendance at the Tallahassee edition, chaired by FSU professor Michael Mascagni, included over one hundred researchers from 15 countries from North America, Asia, and Europe. Many of the large Eastern (ex-Soviet bloc) and Western research groups were represented. Thus, the Seminar provided a rare opportunity for Monte Carlo researchers trained in differing scientific cultures to begin discussions and plan future collaborations.

Topics ranged from Monte Carlo theory, random number generation, solution of partial differential equations, financial modeling, to statistical mechanics. Leading Monte Carlo researchers and practitioners from Berkeley, Harvard, Michigan, and Montreal, as well as from the national laboratories and Wall Street, gave plenary talks. The program committee made the conscious decision to select all of these speakers from North America to highlight the high level Monte Carlo work found on the continent.

The meeting was a very congenial affair, which included alligator watching at Wakulla Springs. All participants received a pair of "fuzzy dice" as one of the welcoming gifts. Since Monte Carlo methods are computations that use random numbers, and originated from the study of games of chance, dice are often used symbols in the field. Fuzzy dice are a peculiar Americanized version.

For a pdf-version of the abstract book, and for more information, please visit the conference web site at mcm2005.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.

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

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