Fall 2006

SCS

Integrating Advanced Computing with Science, Engineering and Liberal Arts

School of Computational Science at Florida State University

High Resolution Hurricane Visualizations with Amira

INSIDE THIS ISSUE

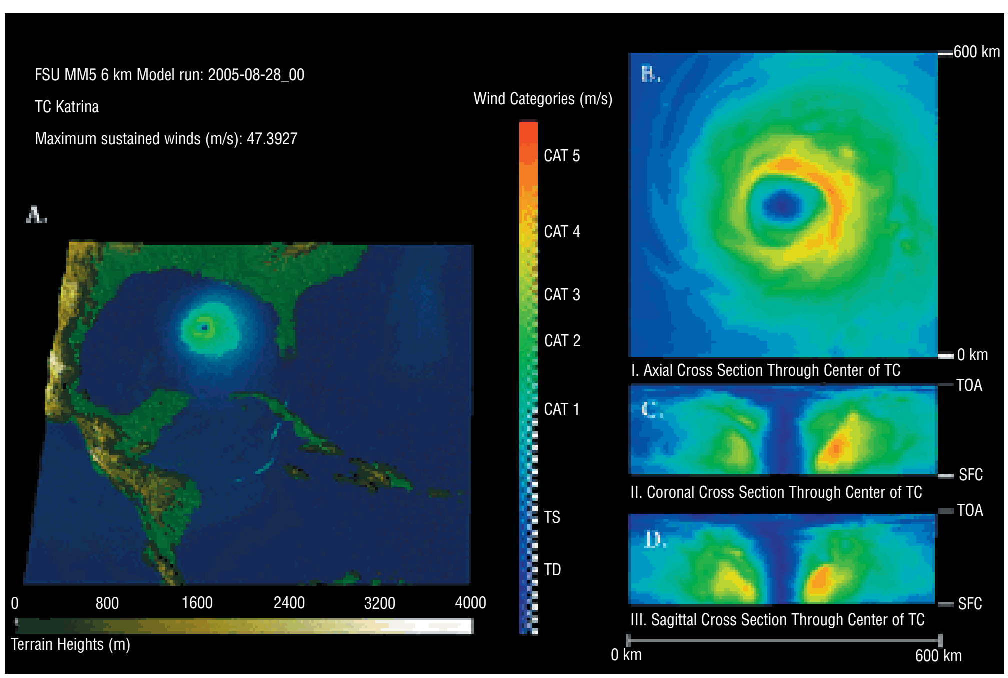
Say "weather forecast" and most people will think of the advanced animations shown on TV, illustrating moving fronts or hurricanes. While some images are actually photos or films of weather phenomena that have already passed, most are computer made visualizations of predicted weather changes, created from measurements and model data.

The visualizations are important not only to TV viewers, but also to meteorologists. With escalating public demand for forecast accuracy, along with increasing amounts of data and more powerful computer models, scientists need different tools to gain insight into the mind-boggling amounts of numbers that they need to deal with – quickly – to provide reliable forecasts.

Recently, a collaboration between the Department of Meteorology and SCS has resulted in the development of a real-time hurricane visualization system. Graduate student Henry Winterbottom, under the supervision of Xiaolei Zou, Meteorology and Gordon Erlebacher, SCS, is creating 3-dimensional animations of developing hurricanes.

VISUALIZATION SOFTWARE

To do so, he is using the Amira software, a more advanced visualization package than is normally used. Henry



A 3-D perspective of Hurricane Katrina (2005) using a MM5 6 km resolution forecast valid at August 28, 1500 UTC. An overview of the region in which Katrina is embedded is provided in A. A horizontal cross section through the center of Katrina is provided in B. An west to east cross section through Katrina is provided in C. while a south to north perspective is provided in D. The color bar provides the magnitudes of the 3-D wind field color coded according to the Saffir-Simpson wind intensity.

continued on page 2

We have passed the final step in the approval process for our new Ph.D. degree program in Computational Science. Many contributed to the effort needed to get us to this point. Special thanks go to Janet Peterson for the preparation of our proposal. We also very much appreciate the support of Provost Larry Abele and Dean Joe Travis throughout the approval process.

We now move to the implementation phase of the Ph.D. degree program. We have a good head start with the M.S. program that began last September, but a lot of work lies ahead. Our faculty are busy with the development of the courses we need to support both the M.S. and Ph.D. programs, and they will be actively involved in the recruitment of students. We all look forward to next fall when we will welcome the first students into our new Ph.D. program.

One of the major events in spring is the SCS workshop on Quantitative Computational Bio-Physics, which will take place in February, starting February 18. Leading the organizational efforts for the workshop is Professor Wei Yang. Outstanding scientists from universities across the nation have already confirmed their participation, and we look forward to this exciting event. More information can be found on page 7.

In the upcoming months we will also be recruiting new faculty and hosting several visitors. Future newsletters will provide more news about these and other activities.

Max Gunzburger,
Director, SCS

and his professors hope to contribute to the understanding of why hurricanes behave as they do, and how their genesis can be identified.

TWO FORECASTS A DAY

The forecast data in the project is provided twice daily via a real-time atmospheric model (MM5), provided by Robert E. Hart in the Department of Meteorology. Henry works with three different degrees of detail, also called forecast domains, with grid resolutions of 54 km, 18 km, and 6 km, respectively.

Immediately after the mathematical completion of a forecast for each domain, the visualization software begins producing visual animations. These give a large scale understanding of regions where future hurricane activity is possible, mainly based on the sea surface temperature. At the 54 km level, Henry also studies the vorticity, or the spin of the air, above the warm water in the areas of interest, to picture the potential intensity development of the budding hurricane.

REMOVING THE CYCLONE

At the next grid level, 18 km, individual features of a hurricane emerge. At this resolution, one observes how the hurricane is affected and steered by the surrounding environment – by moisture fields, wind speeds, etc.

Even more intriguing is the opposite phenomenon – how the hurricane itself affects its surroundings. Henry studies this by removing the cyclone from the data, and comparing the features of the surrounding air with and without the hurricane.

Finally, upon completion of the 6 km forecast domain, storm-centered visualizations for 3D variable fields within the hurricane are created. These fields allow us to understand how certain variables behave as a hurricane strengthens or weakens or as the hurricane is directly impacted by its environment. An example of this are the vertical cross-sections showing the temperature gradient through a hurricane, starting at the sea surface.

LOOK AT THE ANIMATIONS

Henry's animations can be found at http://moe.met.fsu.edu/~hrw22

hwinter@met.fsu.edu
erlebach@scs.fsu.edu

Face to Face with Scientific Data in the SCS Visualization Lab

One often hears that "A picture is worth a thousand words". How true. A scientist can gain much better understanding of a large dataset through visualization than from long lists of numbers. Besides displaying data as images and animations, scientific visualization provides scientists with algorithms that help them extract features and correlate information within datasets.

NEW QUESTIONS ASKED

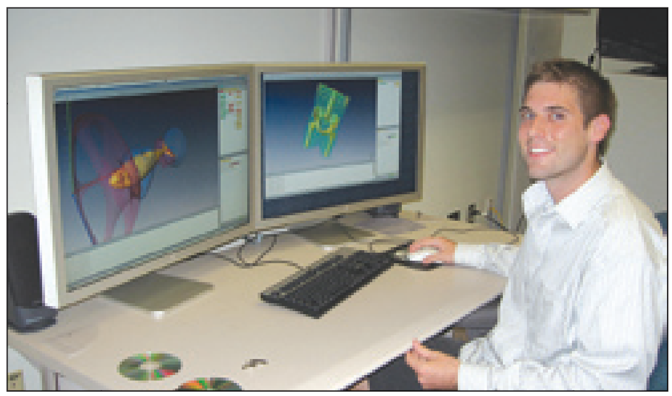
Application areas that handle large-scale datasets include, among others, fluid dynamics, oceanography, geophysics, meteorology and evolutionary biology. Scientific visualization brings researchers in these and other fields face to face with their data, a first step towards better understanding. Real time exploration also encourages scientists to ask questions, which, in many cases, lead to the initiation of new research directions.

The user can examine the data in many different ways, for instance by making 3D images of variables like pressure or density or by creating graphs of complex structures such as proteins. Animations of vector fields, which model for example the speed and direction of wind, are also indispensable.

Increasingly, the application data is three-dimensional and time-dependent. While our current machines are quite capable of manipulating on the order of 30 million data points interactively (corresponding to a 3D grid of 300 points to a side), the same cannot be said if time is added as a fourth dimension. Much research is being devoted to developing the advanced algorithms needed for this task.

SCS VIS LAB RESOURCES

The School of Computational Science runs a visualization lab open to researchers across the FSU Campus with a need to visualize their data. We have installed advanced software such as Matlab, Mathematica and Maple, along with visualization software such as Amira, VTK, Pymol, Chimera, and MeVisLab (for medical data). Additional software is installed upon request.



The lab has recently been equipped with new HP work-stations (two dual core Woodcrest processors), connected to dual wide screen displays (23" or 30"), demonstrated by SCS graduate student and Vis Lab assistant Evan Bollig. One of the workstations has two Quadro FX4500 cards.

Users are welcome to run the visualization workstations after transferring their data to the file server. This gives them the advantages of speed and interactivity, as well as access to an extensive library of books that cover analysis and visualization techniques.

We are also working to provide the means to enable efficient access to lab software from remote locations. Finally, users will soon be able to run background jobs on Vis Lab workstations through the Condor scheduler.

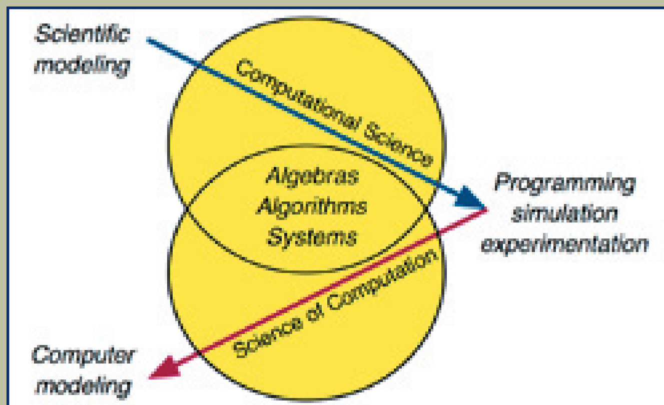
In addition to serving research and faculty, the Vis Lab supports education and research. An SCS course on scientific visualization will be offered in fall 2007. We also encourage FSU faculty to utilize the lab in their classes.

The Vis Lab has existed within SCS for several years, directed by Dr. David Banks. In July 2006, Gordon Erlebacher assumed its management. Since then, the lab has been equipped with a new generation of HP workstations and wide screen displays.

For more information, please see www.scs.fsu.edu/computeresources.php.

erlebach@scs.fsu.edu

Where Computational Science Meets Science of Computation



The point where Computational Science meets the Science of Computation is not surprisingly both human and technical. From a technical point of view, algebras, algorithms, and systems are powerful tools for the Computational Scientist to bring a model (that describes a natural phenomenon) into action through programming, simulation, and experimentation.

Computer scientists, on the other hand, use algebras and other modeling techniques to implement better algorithms which can improve computational processes overall. Working together, scientists in both disciplines have achieved significant results with multi-disciplinary research. The cross-pollination of ideas and techniques has led to scientific discoveries.

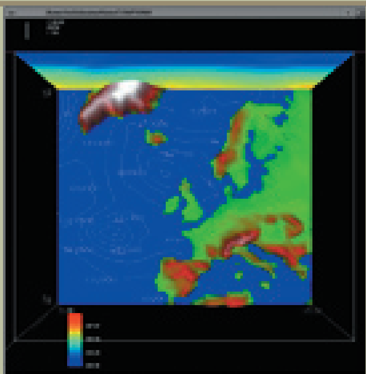
The following projects illustrate what our group has learned from experiences at this intersection.

AUTOMATIC CODE GENERATION FOR ATMOSPHERIC MODELS

In this project we developed a computer algebra system for symbolic manipulation of computational models by encapsulating many of the common discretization techniques and programming techniques used in the area of atmospheric modeling.

This system, named "Ctadel", takes the governing PDEs (Partial Differential Equations) formulated in a high-level specification language, discretizes them, and generates optimized Fortran code with MPI/PVM message passing primitives. Input to the system includes the choice of discretization operators and a machine architecture specification to let the system automatically implement the model efficiently in code. The computer algebra techniques are based on so-called algebraic "term rewriting" methods with rewrite rules that cover basic

The **Advanced Computation and Information Systems (ACIS) laboratory group** in SCS.
From left to right: Kyle Gallivan; Haohai Yu; Subhajit Datta; Wei Zhang; Wei Zhang; Johnnie Birch; Yixin Shou; Robert van Engelen and Ke Chen. The group develops algorithms, techniques, and software tools for high-performance computing and networking. It is led by **Robert van Engelen and Kyle Gallivan,** professors of Computer Science at SCS, and includes six Ph.D. students in Computer Science. **Haohai Yu** investigates the role of causal dependence strength between statistical variables in Bayesian networks to analyze the convergence rate of Markov Chain Monte Carlo (MCMC) techniques for Bayesian inference. **Subhajit Datta** works on techniques to capture changes in software requirements to improve software development practices. **Wei Zhang** develops faster networking methods for data-intensive Web services and Grid computing. **Johnnie Birch** works on new algorithms based on the Chains of Recurrences algebra to improve the effectiveness of automatic parallelizing compilers. **Yixin Shou** works on compiler algorithms to enhance the accuracy of nonlinear variable analysis. **Ke Chen** is analyzing the performance of optimizing compilers for numerical computations.



Limited area model weather forecasting using HIRLAM with code generated by Ctadel

calculus, PDEs, Boolean algebra (for boundary conditions), and Fortran statements (for code optimization). We use theorem proving techniques to effectively convert continuous PDEs to finite difference forms, by searching for the best matching combinations of difference and quadrature operators on staggered grids. The Ctadel system was used to parallelize the "dynamics" of the European HIRLAM weather forecast system. A snapshot of the output is shown in the figure above. Advanced techniques that we have also explored are automatic adjoint model generation and the mixing of forward and reverse models into a single numerical code resulting in the elimination of redundant computations.

OPTIMIZING COMPILERS FOR HIGH-PERFORMANCE COMPUTING

Automatic parallelizing compilers are powerful tools to convert serial program code to parallel code, but they often lack sufficient analysis capabilities to handle more complicated programs with compute-intensive loops that contain nonlinear induction variables, control flow, and C/C++ pointers. Parallelizing compilers transform sequential loops to parallel loops by first normalizing loops into forms in which all memory accesses via array operations are determined to be linear. A system of Diophantine equations is set up to model the read-write dependences between the linear array accesses in the loop iteration space. The solution to this system tells us if the loop can be safely transformed into a parallel version. In this project we use the "Chains of Recurrences" (CR) algebra to model the behavior of variables in a loop. The CR algebra originates from a formulation to improve function evaluations on discrete grids using differences, an approach that was also historically used by Babbage for his Analytical engine, which is considered the first mechanical computer. The CR algebra extends the notion of differences to product domains, i.e. exponential and trigonometric functions. Our extensions of the CR algebra improve compiler analysis of loops and to solve systems of nonlinear equations that model the nonlinear and symbolic cross-iteration loop dependences. We used our solver in the Polaris compiler to automatically parallelize more complicated code than the state-of-the-art compilers can currently handle. A nice result is that the GNU GCC 4.x compilers recently started using our technique for loop autovectorization.

SIMPLIFYING SOFTWARE DEVELOPMENT

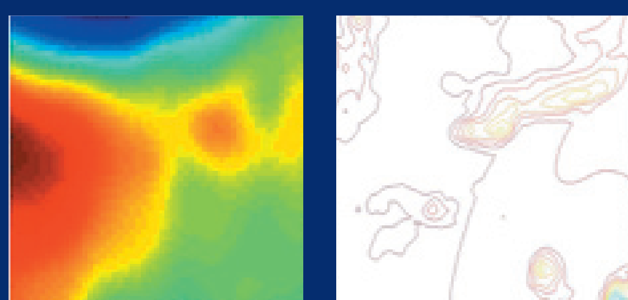
Software development in larger projects often gets out of control when requirements change frequently. In this project we developed metrics to analyze the effect of changing requirements on the software development project timeline and cost. The metrics model the effects of changing requirements on software using linear methods. Parametric optimization is considered as a means to organize code to minimize the effect of future changes.

engelen@scs.fsu.edu
gallivan@scs.fsu.edu

Application Interoperability

Applications developed in different programming languages do not easily communicate with each other due to differences in data representations. Object-request broker systems that are intended to support object exchange between applications, such as CORBA, are heavy weight and require a significant level of expertise to use. These systems may not be usable at all with certain programming languages and applications. Message passing libraries such as MPI and PVM only support arrays of select data types.

In this project we developed an automatic code generation system, named gSOAP, to produce data communications algorithms that utilize the widely used XML format to achieve interoperability between applications. The gSOAP system models the application data and decides on the best XML format based on the data characteristics, such as matrix sparsity and the presence of co-referenced data in trees and graphs. The system currently supports C, C++, Fortran (via C), and Matlab (other XML tools can be used to support other programming languages). The figure shows a rendition of the surface temperature and pressure fields with data produced by the HIRLAM weather forecast system and displayed in Matlab. The two-way communications with XML Web services also allow data modified in Matlab to be processed by the forecast system without having to copy data files.



HIRLAM temperature and pressure fields visualized in Matlab using real-time XML-based messaging between Matlab and HIRLAM using communications code generated with gSOAP.

SCS Welcomes New Faculty Members

SCS welcomes four new faculty members this semester. Three of them introduce themselves below. The fourth new faculty member, Dr. Robert van Engelen, has been with us for four years as an affiliated faculty member, so he is new to SCS only in a formal sense. He and his group are presented on page 4–5 in this issue.

Dr. Xiaoqiang Wang, Applied Mathematics:

"I graduated from the Pennsylvania State University with my Ph.D. degree in the field of Applied Mathematics in August 2005. My research is in the area of numerical analysis and applied partial differential equations with applications to biology, scientific visualization, data mining, fluid mechanics and other related areas.

My recent work focuses on the simulation of bio-membranes using phase field techniques.

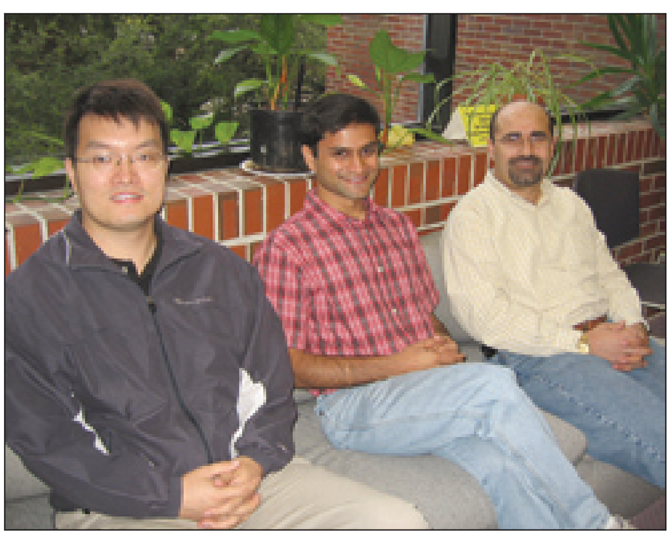
I am very happy that I can be a member of SCS, a big family with scientists coming from all kinds of disciplines."

Dr. Sachin Shanbhag, Chemical and Biomedical Engineering:

"I got my bachelors degree from IIT Bombay, and my Ph.D. (both in Chemical Engineering) from the University of Michigan, Ann Arbor in 2004. I worked for a couple of years as a postdoc before joining the faculty here (jointly with Chemical and Biomedical Engineering) in August 2006.

My primary area of research lies in modeling the structure and rheology of polymer solutions and melts using theory and simulation.

My wife Priya is finishing her Master's in Ann Arbor and will join me in January 2007, just as the winter there begins to turn nasty. We dumped our TV three years ago, which has possibly been the best decision of my life since it gives us much more time to do what we like to do. I enjoy the outdoors and like to play ultimate frisbee, bike to work, and go camping."



The new SCS faculty members, from left to right: Xiaoqiang Wang, Sachin Shanbhag, and Anter El-Azab.

Dr. Anter El-Azab, Mechanical Engineering

"I obtained my B.S. and M.S. degrees at the University of Alexandria, Egypt, and my Ph.D. in Nuclear Engineering at UCLA in 1994. I worked for four years as a lecturer and research engineer at UCLA before joining Pacific Northwest National Laboratory (PNNL) in 1998. In 2004, I joined the Mechanical Engineering Department at FSU, and I came to the School of Computational Science in August 2006.

My research interests are in the areas of theoretical and computational materials science and mechanics. My current research includes computational modeling of the morphology and structure of nanoscale materials, model reduction in electronic and atomic structure, statistical mechanics of dislocations and mesoscale deformation of metals, multiscale modeling of microstructure evolution in irradiated materials, and hydrogen storage materials.

I also enjoy reading in history, political science and philosophy."

Director Gave Invited Talk at the ICM in Madrid

The International Congress of Mathematicians (ICM) held its 2006 meeting in Madrid, Spain. The ICM, held every four years since 1897, honors past mathematical accomplishments, and announces new ones.

The meeting is regarded as the premier opportunity for mathematicians to communicate. It was at such a meeting in 1900 that David Hilbert announced his famous list of problems to challenge the new century. Again, in 1912, Edmund Landau used the ICM to pose four fundamental problems in the theory of prime numbers.

The meeting opened with the awarding of the Fields Medals, the Gauss Prize and the Nevanlinna Prize. The Gauss prize honors advances that directly affect technology and daily life. The Nevanlinna Prize recognizes achievements in information technology.

The prestigious Fields Medal is regarded as the mathematical analog of the Nobel Prize. This award recognizes both past accomplishments and future promise, and so is only given to individuals under forty. One of this year's recipients was Terence Tao of UCLA, who has done great work in partial differential equations, combinatorics, harmonic analysis and number theory. Another Fields medal was declined by the reclusive St Petersburg researcher, Grigory Perelman, who seems to have solved a century old problem called the Poincaré Conjecture.

The invited talks at the 2006 ICM were divided into twenty categories, ranging from logic to probability. Dr. Gunzburger gave one of seven invited talks in the category of Numerical Analysis and Scientific Computing. His talk, "Least-squares finite element methods" surveyed the theory and practice of these important methods, and presented some intriguing open problems. Dr. Gunzburger's years of work in this field will be presented in a book, to be published in 2007.

The social highlight of the conference was a reception at the American embassy in honor of the invited speakers.

gunzburg@scs.fsu.edu

Quantitative Computational Biophysics Workshop in February

Computational biophysics is a growing area. Quantitative descriptions of biomolecular processes will soon start to revolutionize many aspects of the biosciences. Improved algorithms and more powerful computers are used to understand biophysical processes and to design biopolymers and drugs.

FSU has a cluster of research groups in computational biophysics, especially in the School of Computational Science (SCS) and at the Institute of Molecular Biophysics (IMB). The groups are now arranging a four day workshop, hosted by SCS, and starting February 18th of 2007.

Several leading scientists in computational biophysics have confirmed participation, and it is anticipated that the workshop will be the most important event in the field for the next years. A meeting by world-class experts in these areas is timely and will trigger stimulating discussions and, hopefully, a consensus about the main challenges ahead.

The organizers of the workshop are: Max Gunzburger (SCS/Math), Tim Logan (IMB/Chem), Wei Yang (SCS/IMB/Chem), Bernd Berg (SCS/Phys), Rafael Bruschweiler (Chem), Huanxiang Zhou (SCS/IMB/Phys) and Hugh Nymeyer (SCS/IMB/Chem).

For information and updates, please see http://qcbp2007.scs.fsu.edu

School of Computational Science at Florida State University

INTEGRATING ADVANCED COMPUTING WITH SCIENCE, ENGINEERING AND LIBERAL ARTS

KTH, the Royal Institute of Technology in Stockholm, Sweden, was founded in 1827 and is the largest of Sweden's universities of technology. KTH is located in central Stockholm and housed in buildings which have historical monument status. Photo courtesy Håkan Lindgren.

Swedish Mathematics Fellowship Awarded to Raul Tempone

Assistant Professor Raul Tempone at SCS is the first recipient of a new Swedish mathematics prize, the "Dahlquist Research Fellowship". The prize, intended for a "young, promising numerical analyst", will cover one year of full time research at KTH, the Royal Institute of Technology, in Stockholm, Sweden. Raul Tempone plans to move to Stockholm in early 2007 with his family. He is well acquainted with Stockholm and KTH, where he earned his Ph.D. in 2002. He even speaks fluent Swedish.

The prize has been established by the School of Computer Science and Communication at KTH, in honor of the late Germund Dahlquist, professor at KTH. The fellowship is financed by COMSOL, Inc.

Germund Dahlquist (1925–2005) was a Swedish mathematician and numerical analyst who did pioneering work in numerical computing. He was especially known as an international expert in the numerical solution of ordinary differential equations. His famous paper on A-stability is one of the most frequently cited papers in numerical analysis.

More information about the award is available at http://www.csc.kth.se/om/priser/fellowship/

The committee states that "*Raul Tempone has been awarded the first Dahlquist Research Fellowship for his important contributions to the field of numerical approximation of deterministic and stochastic differential equations. In particular his innovative results on a posteriori error estimates and adaptive techniques for stochastic differential equations are leading the international development. This is a relatively new field with an increasing number of applications in, for example, biology, geophysics and finance. Tempone's research is mainly analytical but he is also considering various applications.*"

SCS — School of Computational Science

The mission of SCS is to be the focal point of computational science at 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. Max Gunzburger
850 644-7024

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

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