

SCS

Integrating Advanced
Computing with
Science, Engineering
and Liberal Arts

School of
Computational Science
at Florida State University

High Pressure over the Arctic Increases Flooding in Venice

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If you go to see the unique city of Venice, Italy in the fall, make sure to pack your rubber boots. You will appreciate them if you visit when the city is flooded by the high tide and you have to wade across the famous Piazza San Marco. The high tide, "Acqua alta", hits the city more than 60 times each year, mainly in the fall, posing an increasing threat to the priceless cultural treasures of Venice.

The flooding is caused by a combination of high astronomic tide, low atmospheric pressure,

and powerful winds from the Southeast pushing water from the Southern part of the Mediterranean Sea into the Venetian Lagoon. The sea level has to rise over 80 cm, or 32 inches, in order to flood the lowest parts of the city.

For tourists, the high tide is merely an inconvenience. If you forget to bring boots, you can buy a pair from a souvenir stand. Citizens and shop owners have learned to live with the increasing burden of the high tide by listening to the forecasts and

taking precautions. Many have simply abandoned the first floor of their houses to avoid having their belongings and merchandise soaked.

ENDANGERED VALUES

Obviously, though, the flooding is a serious long-term threat to the city and its monuments. Much effort is spent understanding, predicting and in the long run maybe even preventing the high tide from threatening Venice.

One reason for growing concern is global warming and



Photo courtesy: Comune di Venezia





These are exciting times at the SCS. We are in the midst of a very active faculty hiring season, trying to fill several positions. We are also actively recruiting students for our recently approved M.S. in Computational Science degree program, which will feed into our hopefully soon to be approved Ph.D. program.

In February and March, two very successful workshops took place under SCS sponsorship. These workshops brought to the SCS and FSU noted scientists from all over the world.

In April, we held our annual Computational Xposition at which graduate students

advised by SCS faculty present their research results to the FSU community. Additional details about all of these activities can be found elsewhere in this or the next issue of the newsletter.

During the upcoming months, we will be concentrating on the implementation of our new degree programs, including new core and advanced courses.

All together, all these activities point to the vibrance of the SCS and to its promising future.



Max Gunzburger,
Director, SCS

its effects on the sea level and the flooding.

Sergio Fagherazzi, born and raised on an island in the Venetian lagoon, now an SCS professor, has studied the sea level fluctuations together with large-scale climatic patterns, looking for correlations. He and his students have found correlation between the daily sea level and a known climatic phenomenon called the Arctic Oscillation, or AO. This is a pattern of air pressure changes over the Arctic Ocean, known to have effects on rainfall and temperature in both North America and Northern Europe. For the first time, Sergio Fagherazzi has been able to show that the AO also affects the high tides of Venice.

LOW PRESSURE, HIGH TIDE

Low air pressure causes more storms which in turn raise water levels, while high pressure lowers the sea level. Sergio Fagherazzi found that when the Arctic Oscillation is in its negative phase, it is associated with high pressure over the Arctic and low pressure over Southern Europe. This phase induces rising sea levels in the Mediterranean Sea and more severe floods in Venice.

On the average, a negative phase brings up the sea level two or three inches compared to

a positive phase. For a flat and low-lying city like Venice, that means a much larger area will be flooded.

GLOBAL WARMING

The findings of Sergio Fagherazzi and his students also suggest that global warming has two distinct, sometimes conflicting, effects on the high tide. The general increase in sea level caused by global warming presents an obvious threat. However, since the 1970's the Arctic Oscillation has tended to stay in its positive phase, which has the opposite effect on the water level. In reality this might have led to an underestimation of Venice's exposure to high tides.

While the problem is not new, the frequency of the flooding has increased from fewer than ten times a year a hundred years ago to over 60 times a year. During that time, the sea level has risen 8 cm, and the ground level of Venice has sunk by 23 cm.

Contrary to popular belief, the sinking does not continue. It was stopped in the 1960s, when Venetians realized that it happened because too much ground water was pumped out from under the city.

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Master's Program in Computational Science Approved

The School of Computational Science has received final approval for a new Master's degree program in Computational Science.

Moreover, the School's proposed Ph.D. program in Computational Science was supported at the University level and only requires approval by the Board of Governors before it will become official.

SCS also submitted proposals this year for ten new graduate courses. These were accepted by the University in April 2006 and will be officially listed for the 2006-2007 academic year. All of these courses were assigned a prefix of ISC (Interdisciplinary Sciences).

INTERDISCIPLINARY STUDIES

The new graduate programs in Computational Science will offer students interested in computational science the opportunity to train in an interdisciplinary environment and, if desired, to concentrate their research in a

specific application area.

Over the past years, it has become widely accepted that computations have joined theory and experimentation to form the three pillars of scientific discovery and technological design. The new programs allow students to be on the forefront of education and research in this growing area.

TWO STUDENT GROUPS

The new master's program will serve two types of students. The first type consists of students who are ultimately seeking a Ph.D. in Computational Science but decide to also complete the requirements for a master's degree.

The second type of student is one who wants to terminate

his/her graduate studies with an M.S. and seek employment in the non-academic sector. For these students we have implemented a Professional Science Master's track within the master's program.

The goal of this terminal M.S. is to train students in computational science and give the student the opportunity to acquire professional skills such as communication or management skills. This track strives to prepare students for leadership roles in industry or government agencies.

ACCEPTING APPLICATIONS

The School is currently recruiting graduate students in Computational Science for Fall 2006. To apply, please follow the instructions to the left.

For any questions concerning the program, please contact Professor Peterson or Eva Ronquist.
peterston@scs.fsu.edu
evaron@scs.fsu.edu

Welcome to apply for Fall 2006
– here is what you need to do:

- apply online to SCS
www.scs.fsu.edu/application.htm
- send three letters of recommendation to Professor Janet Peterson at
peterston@scs.fsu.edu
- apply officially to FSU (as for all graduate programs at FSU), and provide FSU with official transcripts, GRE scores and an application fee.
<https://admissions.fsu.edu/gradapp/>

International students also need to take the TOEFL language test and fill in score and date taken on their online application form.
<http://www.toefl.org/>

The Color of Quarks

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Bernd Berg earned his PhD in 1977 at the Free University of Berlin, Germany. He became assistant professor at Hamburg University in 1978, a position which he kept until 1984. During that time he was awarded a CERN Fellowship and spent two years at CERN, the European particle physics lab at Geneva. He became an associate professor at FSU in 1985, and was promoted to full professor in 1988. While he has kept his position at FSU since then, he has also kept close contact with many overseas research institutions through extended stays in Germany, France, Austria and Japan.

Bernd Berg has written about 150 papers, of which the 46 most well known ones have more than 3000 citations. He recently published a textbook on Markov Chain Monte Carlo (MCMC) methods. Among other honors, Bernd Berg was elected APS fellow in 2004, Leibniz Professor in 2005, and he became a named professor at FSU in 2006. Initially Berg's research at FSU focused on Lattice Gauge Theory simulations, which are relevant for investigating the properties of elementary particles. Since about 1990 it broadened into developing MCMC methods further and including applications to Statistical Physics and, more recently, Biophysics. The photo shows Bernd Berg with his two present students, **Robin Robin**, left, and **Alexei Bazavov**.

The atom contains the smallest particles of the universe. It might seem like a paradox that the study of this miniscule world requires the largest computers, but at FSU and elsewhere, particle physicists were among the first enthusiastic users of supercomputers. In fact, the

world's first electronic, digital computer was built in 1939 by a physics professor, who was driven by his need to perform faster calculations.

Ever since, physicists have gravitated towards powerful computers. The career of SCS professor Bernd Berg is a telling example. In the early 1980s,

he was an assistant professor of physics in Hamburg, Germany, developing Markov Chain Monte Carlo (MCMC) simulations in particle physics at a time when punch cards were still in use. Without much hesitation, he gave up the position and his native Germany after a telephone call from Dennis Duke at FSU. The attractions were FSU's first supercomputer, a Cyber 205, a promised powerful new system, called ETA 10, and the Supercomputer Computations Research Institute, SCRI, the ancestor of the SCS.

Bernd Berg arrived at FSU in 1985, only months after the Cyber 205 became operational. By today's measures, the Cyber 205 was not impressive – it had far less power than a modern PC. The subsequent ETA 10 never featured a fully functional operating system, so many researchers could not figure out how to use it. Bernd Berg was one of the lucky few who did, and he happily recalls having almost exclusive access to the computing power of several CPUs for his research alone.

QUANTUM THEORY

Professor Berg is a researcher in the field of quantum theory, whose laws were first uncovered during the early 20th century. Early pioneers were Max Planck, Albert Einstein, Erwin Schrödinger, Werner Heisenberg and Paul Dirac.

Dirac, a Nobel laureate at 31, has a special connection with FSU, because he joined the FSU faculty in 1970 and taught at the university for more than a decade. Bernd Berg never met Paul Dirac, who died in 1984, but the Dirac equation for the behavior of the electron is fundamental to Berg's work.

COLOR CHARGE

Quantum theory has revealed that a very strong force operates over the extremely short distances within the nucleus of an atom. This "Strong Force" overcomes the tendency of the positively charged protons in the nucleus to fly apart.

The Strong Force acts between quarks, the constituent particles of a proton. While electrons and protons carry an electric charge, the quarks carry a different type of charge called "color charge", which can be red, green and blue. This has nothing to do with the visual perception of color, it's an analogy. Just like red, blue and green light add up to white light, three quarks of different "color" bond together to form a color-neutral particle.

The color force does not fall off with the distance between the quarks. As a result the quarks within a nucleus cannot be separated. They are glued together by the color force, transmitted by particles called gluons.

The quantum field theory of quarks and gluons is called Quantum Chromodynamics (QCD). One of the problems occupying Bernd Berg concerns the calculation of masses of so called “boundstates”, particles which are temporary aggregates of quarks or gluons.

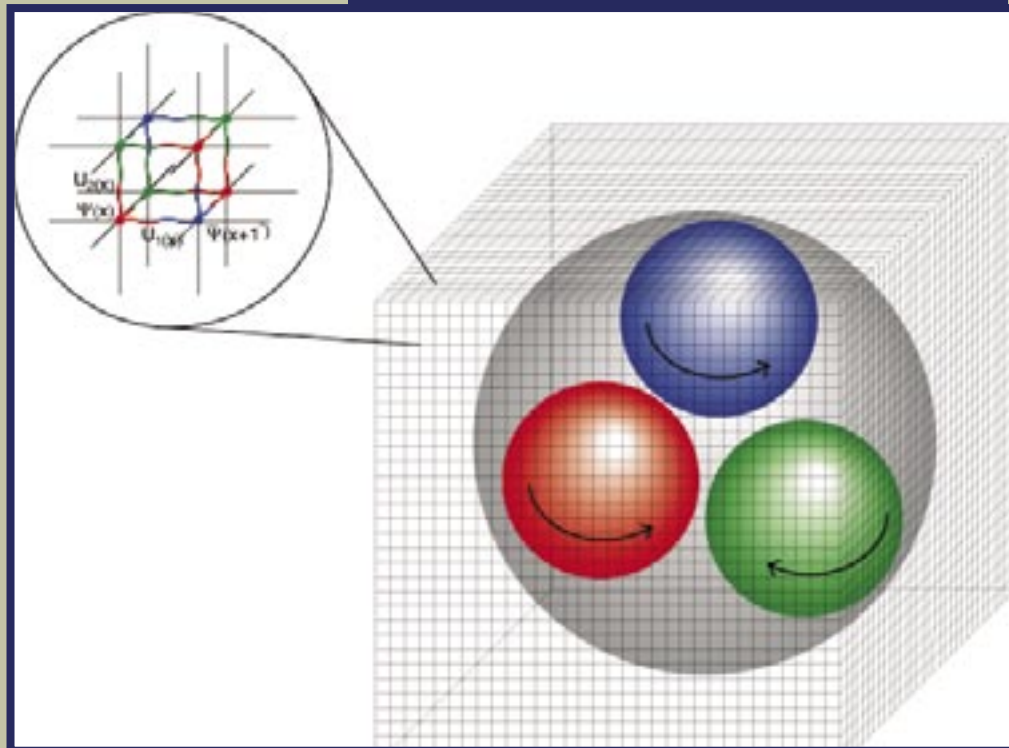
In the 1980s, Bernd Berg and his collaborator Alain Billoire, France, were able to provide estimates of masses of “glueballs”, boundstates of gluons. This work rendered them international recognition.

MONTE CARLO METHODS

The Markov Chain Monte Carlo methodology for stochastic calculations was introduced in 1953 by a group at Los Alamos. It has since been used in a wide range of scientific applications, from particle physics to ecology.

Bernd Berg has worked with MCMC calculations since the early 1980s, when his glueball mass calculations were made. More recently, he used MCMC methods for studying the “Deconfining Phase Transition”. This is a prediction that at an astronomically high temperature of about 2.3×10^{13} Kelvin, the quark and gluon boundstates dissolve into a plasma of quarks and gluons.

In 1991, Bernd Berg and former SCRI postdoc Thomas Neuhaus proposed a new approach for simulations of a statistical ensemble, called the “multicanonical” method. A statistical ensemble can be



imagined as a collection of all results of an experiment run over and over again. By averaging and analyzing these results the behavior of physical models can be studied.

NEW RESEARCH AREAS

The multicanonical ensemble allowed the physics calculations which Berg and Neuhaus were interested in. Furthermore, the method’s success attracted the attention of scientists in other disciplines, and it was soon being used in other fields, including biophysics, optics and engineering.

Berg’s three key papers on the method (two written with Thomas Neuhaus and one with Tarik Celik, Turkey) score more

The image illustrates quarks within a proton. Masses of particles which are “boundstates” of quarks or gluons can be estimated by large scale computer simulations. These are done within a framework called “Lattice Gauge Theory” (LGT). In this framework, introduced by Ken Wilson, who was awarded the 1982 Nobel Prize in physics, one discretizes Quantum Chromo Dynamics in a way quite similar to the definition of the Riemann integral in mathematics. The time direction is rotated into the Euclidean. One ends up with a four-dimensional Statistical Mechanics, where the quark fields are located on the sites and the gluon fields on the links of the lattice. This formulation allows for MCMC simulations in a way similar to classical statistical mechanics systems, for instance Ising ferromagnets.

than one thousand citations.

Ulrich Hansmann and Wolfgang Janke, two of Bernd Berg’s former postdocs, contributed significantly to introducing the methods to statistical physics and biophysics. Both are now internationally well recognized professors.

Bernd Berg has diversified his research in recent years,

but keeps one foot in particle physics. He devotes about half of his research time to investigating the dynamics of the QCD deconfining phase transition. During the other half, he collaborates with Professor Wei Yang of SCS to develop MCMC methods for simulations of biologically relevant molecules.

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Ivo Babuška at SCS

Professor Ivo M. Babuška, a legendary scientist in the field of Computational Mathematics, visited the School of Computational Science in the spring, to work with his former post doc, SCS Professor Raul Tempone. Ivo Babuška also gave a seminar called “Meshless & Generalized FEM. Theory & Application”.

Ivo Babuška and Raul Tempone are collaborating on a report for an upcoming workshop in Albuquerque, New Mexico. In addition, they are planning a new project on numerical methods for non-linear PDE's (partial differential equations) with stochastic coefficients. This project will involve SCS graduate student Clayton Webster.

Ivo Babuška was born and raised in Czechoslovakia, where he started his exceptionally successful career. In 1968 he moved to the US with his family to become a professor at University of Maryland, College Park. After his retirement in 1996 he moved to Austin, Texas, where he is a professor at Institute for Computational Engineering and Sciences.

Professor Babuška has received numerous recognitions, among them four doctorates honoris causa in Europe. He has also been elected to the National Academy of Engineering and the Academy of Medicine, Engineering, and Sciences of Texas. In 2003 he even had an asteroid named after him, the asteroid 36060 Babuška.



*Ivo M. Babuška, Raul Tempone
and Clayton Webster.*

SCS Welcomes New Members

Professor Yousuff Hussaini's group has been reinforced with administrator **Kathy Stone**. Kathy has been employed by Florida State University since 1981. Prior to her appointment with SCS, she was employed with the FSU Purchasing Department, Police Department, Computer Science Department and also at the Dean's Office at the College of Social Sciences.

In addition, Dr. Hussaini has two new postdocs in his research group. **Dr. Dilek Dustegor**, who works with Dr. Poroseva, received her Ph.D. in Automatic Control and Systems from the Université des Sciences et Technologie de Lille in France.

Dr. Dimitrios Kondaxakis from Athens, Greece, earned his Ph.D. in Computational Fluid Dynamics from the National Technical University of Athens. His main research interest lies in the area of computational mathematics, particularly the development and application of spectral element methods in problems of computational physics.

Dr. Hyung-Chun Lee is a visiting professor from Agou University, South Korea, working with Max Gunzburger. Dr. Lee is a computational mathematician with research interests including numerical analysis, applied mathematics and computational science.

Karolina Maneva-Jakimkoska, has been hired by MorphBank as a computer research specialist. The project has also employed two new assistants: **Debbie Paul** and **Katja Seltman**.

Welcome to all of you!



Kathy Stone



Dilek Dustegor



Dimitrios Kondaxakis



Hyung-Chun Lee



**Karolina
Maneva-Jakimkoska**

The Tech Support Group Shrinks – and Grows



Tom Green



Jeff McDonald

Over the last months the SCS has seen a number of changes to the personnel who make up the Technical Support Group. In December, Tim Nguyen-Pham left to be with his fiancée in Baton Rouge and in January Elaine Dennison left to help with her family in central Florida. Tim and Elaine did a great job helping to maintain the SCS computing infrastructure and we wish them the best in their future endeavors.

Soon after these departures, the SCS had the good fortune to welcome two talented individuals to the group; Tom Green and Jeff McDonald. Tom and Jeff are no strangers to the FSU campus. Tom managed the technical support group and the

application development group back when SCS was known as SCRI. Jeff comes to us from the Physics Department, where he was a research scientist in High Energy Physics (HEP) group and was also responsible for

the administration of the HEP computational resources.

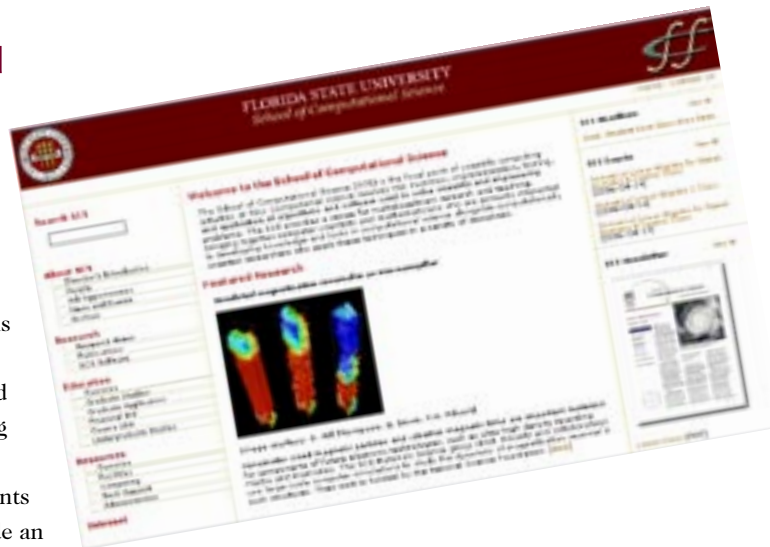
While at FSU, Tom was co-PI and project manager on a number of software development projects. In fact, Tom authored a package called DQS (the Distributed Queuing System), which was ultimately purchased by Sun Micro Systems and is now incorporated into the Sun Grid Engine.

Tom left the University in 2000 to establish his own consulting company, which focused on database design, programming, and application

development. Jeff holds a Ph.D. in physics, has published numerous scientific papers and is a collaborator on several high-profile physics projects (e.g., NuTeV, MINOS, ATLAS, and D/E). Jeff combines his research, technical, and hardware expertise to develop and implement turnkey solutions for High Performance Computing. Jeff's experience mentoring students will also be an important asset as the SCS begins to incorporate students for both infrastructure and research support activities. jjwilgenb@scs.fsu.edu

www.scs.fsu.edu

The Web site of the School of Computational Science has undergone a facelift, with added features for both internal and external users. Information for prospective students has been greatly expanded; an SCS publications database has been added; a user-friendly directory has been set up and the information about SCS computing resources and facilities has been rewritten and re-organized. Improvements to be expected during the year include an expanded section on the SCS research.



Tallahassee Workshops for Applied Mathematicians



The “Workshop for Stochastic Differential Equations with Applications” attracted mathematicians from all over the US and from several European countries. Here, they gather around the statue of Paul Dirac on the FSU campus. Raul Tempone, SCS professor and organizer of the workshop, is number four from the left in the middle row.

In early spring, SCS hosted two international workshops on applied mathematics.

The first one, “Numerics for Stochastic differential Equations with Applications” was centered around the development and analysis of efficient numerical methods for stochastic differential

equations, arising in traffic flow, molecular dynamics, materials science, and other relevant applications.

The other workshop, “Predictability, Observations, and Uncertainties in Geosciences” was supported by the National Science Foundation, and co-organized by Dr. Michael Navon at

SCS and Dr. Milija Zupanski from CIRA, Colorado. This multidisciplinary workshop focused on estimations uncertainties in modeling, such as in hurricane prediction.

For abstracts and info:
www.scs.fsu.edu/~cheng/wkFeb06/index.htm
www.scs.fsu.edu/workshop.php

Professor Ed Lorenz from MIT, pioneer in chaos theory, inspired the younger scientists at the SCS workshop on Geosciences. Here, he is talking to Dr. Arif Albayrak from Colorado State university. In the 1960s, Lorenz discovered that very small changes in the initial conditions may produce large changes in the long-term outcome of meteorological predictions. He even suggested that a flap of butterfly wings in Brazil might affect tornados in Texas.



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.scs.fsu.edu.

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