



Last summer, Peter Reichert came to Durham, NC with his wife and family for his year-long sabbatical at SAMSI. His interest in modeling of aquatic environmental systems and use of these models for scientific discovery and societal decision support brought him to the 2006-07 Program on Development, Assessment and Utilization of Complex Computer Models.

Underlying his mission at SAMSI was Peter's interest in Systems Analysis and Decision Sciences. The close proximity of Duke University's Nicholas School of the Environment & Earth Sciences, The Fuqua School of Business and experts in the Institute of Statistics and Decision Sciences at Duke was an added advantage.

Dr. Reichert holds a PhD. in Theoretical Solid State Physics and has worked at the Swiss Federal Institute of Aquatic Science and Technology (Eawag) in Zurich, Switzerland for more than 20 years. In addition to his duties at Eawag, he is Professor in the Department of Environmental Sciences at the Swiss Federal Institute of Technology (ETH) where he teaches Modeling of Aquatic Ecosystems, and Environmental Systems Analysis.

Dr. Reichert's research fields include:

- * Identification of models for technical and natural aquatic

systems, together with assessment of the identifiability of model parameters and the uncertainty of model predictions using frequentist and Bayesian techniques; primary application areas are rivers, lakes, and watersheds.

* Integration of knowledge from various sources (literature, data, output of more detailed models, expert opinions) in the form of probability network models, and use of such models to support environmental decision making.

* Design and implementation of software that supports environmental scientists in model-based evaluation of their data.

According to Dr. Reichert, "SAMSI's ability to bring researchers from different disciplines together to exchange experience and knowledge about techniques at the interface between statistics and applied modeling is very successful". This helps improving the quality of inference and uncertainty analysis techniques used in the applied sciences.

The most difficult part of Peter's year at SAMSI was trying to find time for new projects despite the burden of work brought from his home institution. However, this improved over the year; and he is finishing his stay with 6 projects in progress involving new perspectives, ideas and collaborations in modeling bias of deterministic simulation models, improving their structure, adding stochasticity, and using emulators to make Bayesian analysis feasible for computationally demanding models. These projects will continue when he returns to Switzerland.

Upon completing Peter's commitment at SAMSI, the Reicherts are planning a month long family vacation in the western United States. Plans are in progress for an after program workshop sometime next year.

samsi alumni: Do you have news you want to share? E-mail us at: alumni-news@samsi.info

samsi

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Development, Assessment and Utilization of Complex Computer Models

Computer models, or simulators, are numerical (computer) implementations of complex mathematical models intended as surrogates of reality; they are becoming ubiquitous in science and in everyday life, so this ambitious SAMSI year long program is timeless.

The program, which just held a Transition Workshop, involved a large number of national and international scientists. Due to its extension and complexity, it was articulated in 5 Subprograms: Environmental/Ecological Models (with working groups on Air Quality, Climate and Weather, Hydrological, and Terrestrial models); Models of Granular Materials (with working groups on Engineering Applications, and Statistical Mechanics of Granular Flow); Biological Modeling (with working groups in Cerebral Blood Flow, Systems Biology and Dynamics of Infectious Diseases); and the Engineering and Methodology Subprograms, with one working group each.

The program attracted many prestigious leaders. The close collaboration among scientists, applied mathematicians, physicists, and statisticians was a phenomenal success. Indeed, this is an area where significant advances are not possible without this type of close interaction, and SAMSI provided a perfect umbrella for it. There have also been extensive interactions with national and international research groups with similar interests, such as the Managing Uncertainty in Complex Models group (U.K.), Sandia and Los Alamos Laboratories and the National Center for Atmospheric Research (USA), the National Program for Complex Data Structures (Canada), among others. The activity was very exciting and can be explored through the Program Webpage (www.samsi.info/programs/2006compmodprogram.shtml); we opt here to exemplify the type of research undertaken through one example.

One of the projects getting a crucial push from this program has an ultimate goal of producing informed hazard risk maps for areas menaced from a certain kind of volcano avalanches (pyroclastic flows.) The social and economical impact derived from decisions based on such maps is enormous.

The volcanic pyroclastic mass flows involve the transport of volcanic ash, sand, soil, rocks and miscellaneous debris, often very hot, in a liquid or gas matrix. The flow deposits can be tens of meters deep and several kilometers long. Attention focused on the Soufrière Hills Volcano on Montserrat, which began its current eruption episode in July, 1995, and continues to this day; in fact, as we speak, it is building a big dome, anticipating a noticeable eruption and avalanche in the immediate future. (Because of the large and recurring eruptions, the southern half of Montserrat, including the capital Plymouth, was permanently evacuated in 1997.)

The computer model used is part of the TITAN suite of computer

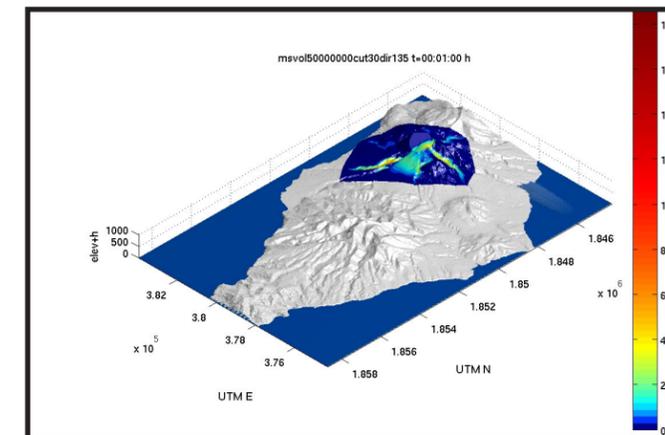


photo by Keith Dalbey

Results of a simulation of a 50 million cubic meter debris flow from the Soufrière Hills Volcano on Montserrat. The northern part of the island is toward the lower left. Pictured is the depth of the flow after 60 seconds, where dark blue is a flow depth of 10 cm, and the yellow is 40 cm. The flow reaches the ocean on the eastern side of the island, about 3 km. from the volcano.

models, developed at the University of Buffalo; the working group involves the modelers, thus guaranteeing access to state of the art simulators. Simultaneously, there has been intense collaboration with geophysicists working on site, and providing the best available (but yet unavoidably imprecise) data about eruptions of Soufrière Hills from early 1996 through late 2006. This is an impressive (and rarely available) data set.

There are many uncertainties in this challenging enterprise. First, it is obviously difficult to describe all the physics active across all the scales of a volcanic mass flow. The mathematical models have weaknesses that are partially understood, but for which there is no readily available fix. The ultimate analysis, however, needs to take this into account.

Also, there is large inherent uncertainty of the data in the model. For example, data about frequency of eruptions of any given size is not typically available. Topographical maps can also have large errors, the frictional dissipation of the mass as it flows over the terrain, and the internal dissipation of the flowing mass are very crudely measured, and materials that appear to be similar – for example, sand – may vary by 20% in this friction measurement. These uncertainties should be carried over and reflected in the final predictions.

The integrated group is further perfecting the simulator, deriving needed fast emulators, identifying high risk subsets of inputs, developing new probabilistic models for flow-frequency of eruption, which also samples from catastrophic volumes (in the risk subset.) This effort results in predictions of likely destructive flow scenarios, along with uncertainty bands, which will provide geoscientists and those entrusted with civil protection better tools to evaluate hazard potential.

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From the director...

We have just had the transition (closing) workshops of our principal annual programs, and it is a great time to look back on the year. I was personally at the transition workshop of the program highlighted in this newsletter – Development, Assessment and Utilization of Complex Computer Models (CompMod.) It was a great experience, not only hearing of the wonderful research that has been done over the year at SAMSI, but also seeing the enthusiasm of so many of the participants for continuing the work they started here.

I heard great things about the other transition workshops, but was unable to attend because they were held elsewhere. The transition workshop for the program on High Dimensional Inference and Random Matrices was held at the American Institute of Mathematics in California, and the transition workshop for the climate modeling group of the CompMod program was held at the National Center for Atmospheric Research in Colorado. Collaborative efforts such as these, and those documented on the next page, have proven to be remarkably successful and will be a staple of future SAMSI programs.

An update on the SAMSI renewal: the Division of Mathematical Sciences at the National Science Foundation has recommended that SAMSI's funding be renewed for another five years. We are working with the National Science Foundation and SAMSI's other partners to refine the budget and finalize our plans for the future. The official announcement (and all the exciting details!) should be ready for our next newsletter.

This summer we are seeing some transitions in the SAMSI family. Chris Jones has been an inspirational member of the directorate for two years, but will be leaving to pursue an exciting opportunity in England. Jim Damon has served admirably on the directorate during Chris' leave-of-absence. Finally, anyone who has had any association with SAMSI knows our administrative assistant, Nicole Scott, as someone who has been extremely helpful and effective. Nikki has left SAMSI but, luckily, has not gone far; she is now an administrative assistant at Duke University, in a role that still oversees some SAMSI functions, so we will continue to have the benefit of her expertise if not her daily presence. Chris, Jim and Nikki will all be missed.

I'm excited to announce that Michael Minion will be joining the directorate, as the representative from the University of North Carolina at Chapel Hill. Michael is an applied mathematician whose research has focused on numerical methods in fluid flow, and we look forward to having his expertise and enthusiasm on the directorate.



James O. Berger

James O. Berger
Director

NCAR/MUCM

SAMSI's "Development, Assessment and Utilization of Complex Computer Models" year-long program happened to coincide with the National Center for Atmospheric Research (NCAR) IMAGE Theme-of-the-Year "Statistics for Numerical Models." Five joint SAMSI/NCAR projects were initiated, each combining the expertise of the two institutions.

If there has been a common theme, it is the interaction of statisticians and modelers in a dialogue. The collaboration began by discovering, often empirically, things that should be 'obvious'; for example, 'phase' is a periodic input into a tidal module of an atmospheric model. But, it is never clear at the start what aspects of the physics are both important and amenable to statistical representation, and it is only by going backwards and forwards that we can explore the opportunities for tailoring the statistics to the physics, or vice versa.

Of the five projects, two are based on a 1D version of the WRF atmospheric model, one is based on the TIEGCM atmospheric model, another one looks at variations in predictions attributable to differences in boundary conditions and regional models (this is crucial for studying climate change impacts), and one studies turbulence. The balance between math and statistics varies in the projects, with turbulence at the mathematical end, the two WRF projects in the middle, and TIEGCM and the regional

study being applied statistics.

An emerging theme in the statistical field of computer experiments has been the incorporation of structural errors (model imperfection) into the calibration of physical models, and also dissatisfaction with current statistical approaches, which comprise no more than adding on some uncertainty at the end of the model evaluation. Several presentations in the SAMSI/MUCM (Managing Uncertainty in Complex Models) workshop explored better ways to do this. One possibility is dynamic emulators, where the model is still deterministic (e.g. a solver for a PDE system) but uncertainty is added bit-by-bit at each time-step, rather than a lump at the end.

More promising is to generalize the models to be stochastic; another SAMSI program theme, particularly in biological applications. One of the WRF projects concerns the development of stochastic representations for clouds. In this case, our uncertainty about the role of clouds is not limited to the values of two or three high-level model parameters, but shows up in the modeled clouds themselves which, will be different from run to run of the model. This type of development can only take place with the direct collaboration of statisticians and modelers,



Left to Right:
Susie Bayari, Universitat de València;
Anthony O'Hagan, University of Sheffield;
Thomas Loreda, Cornell University

because the representation of physically-meaningful yet tunable spatial-temporal stochastic processes is technical and subtle.

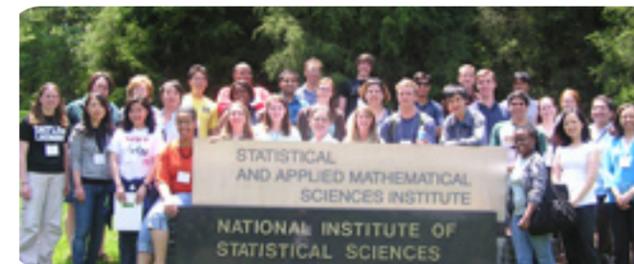
The TIEGCM model (which is deterministic) is full of interesting quirks, including spatial-temporal functional outputs, and periodicity in both inputs and outputs. Tackling these statistically has been rewarding in itself, and has generated ideas that will be transferable to other projects. But, it has also made us think more deeply about our ability to construct generic approaches to analyzing models of physical processes, both in terms of how we construct a statistical framework, and how we write computer code that can take care of the very demanding numerical issues, while at the same time offering the flexibility to incorporate as directly as possible the insights of the modelers.

SAMSI/CRSC undergraduate workshop

In May, 18 undergraduate students from 16 colleges and universities attended the fifth SAMSI/CRSC Undergraduate Workshop at North Carolina State University (NCSU.) Through a combination of lectures, tutorials and physical experiments, the attendees were introduced to a range of mathematical and statistical topics pertaining to model development, parameter estimation and analysis of experimental data.

A unique and highly effective aspect of the workshop is the fact that all tutorials and lectures were prepared and given by SAMSI Graduate and Postdoctoral Fellows.

On the first day, students met at SAMSI to attend overview lectures by Guillaume Vernieres, Elaine Spiller and Cari Kaufman regarding the 2006-2007 programs on *High Dimensional Inference and Random Matrices*, and *Development, Assessment and*



Utilization of Complex Computer Models.

Following lectures and tutorials by SAMSI graduate students and post-docs, the undergraduate attendees met at the NCSU Centennial Campus to collect experimental data at the Center for Research in Scientific Computation (CRSC) Math Instructional and Research Laboratory. During this time, they also participated in a Graduate School Panel, led by Jennifer Joyce (Mathematics Department, University of North Carolina – Chapel Hill), Ernie Stitzinger (Mathematics Department, NCSU) and Kim Weems

(Statistics Department, NCSU), and Career Panel, led by Gordon Brown (Research Triangle Institute), Kristen Foley (Environmental Protection Agency) and Julie Kimbell (Hamner Institutes for Health Sciences.) The panel sessions provided students with a wide range of information and perspectives regarding educational and career opportunities involving the mathematical and statistical sciences.

During the fourth day, attendees employed least squares optimization techniques to estimate parameters and obtain model fits to their experimental data. Each team then gave an oral presentation summarizing their analysis and results. Details regarding the workshop can be found at the website <http://www.ncsu.edu/crsc/events/ugw07/index.php>.

summer programs

Challenges in Dynamic Treatment Regimes and Multistage Decision-Making
June 18-29, 2007
(at SAMSI and Radisson)

Geometry and Statistics of Shape Spaces
July 7-13, 2007
(at SAMSI and Radisson)

CRSC/SAMSI Workshop for Graduate Students
July 23-31, 2007 (N.C. State University)

program workshops

Risk Analysis, Extreme Events and Decision Theory
September 16-19, 2007
(at SAMSI and Radisson)

Random Media
September 23-26, 2007
(at SAMSI and Radisson)

Environmental Sensor Networks
January 14-17, 2008
(at SAMSI and Radisson)

For more information about SAMSI programs and workshops, visit SAMSI's Web site at <http://www.samsi.info> or call 919-685-9350.