ifip

Working Conference on

Uncertainty Quantification in Scientific Computing

August 1-4, 2011

Boulder, Colorado, USA

siam

NIST
National Institute of Standards and Technology
U.S. Department of Commerce

Conference Schedule at a Glance

	Sun 7/31/2011	Mon 8/1/2011	Tue 8/2/2011	Wed 8/3/2011	Thu 8/4/2011
7:30		Registration Opening			
8:30		Pascual	Goldstein	Kahan	Cox
9:30		Cunningham	Hatton	Welch	Possolo
10:15		Break	Break	Break	Break
10:45		Pasanisi	Eldred	Challenor	Glimm
11:30		Gaffney	Doostan	Smith	Johnson
12:15		Lunch	Lunch	Lunch	Lunch
13:15		Helton	Ferson	Tour of NIST and NOAA	Sandu
14:00		Nychka	Matthies		Heroux
14:45		Oberkampf	Break		Muhanna
15:30		Break	Hot Topics		Break
16:00	Registration	Panel		Visit Chautauqua Park	Enright Wrap up
17:30				Reception and Banquet (Chataugua Dining Hall)	
18:00		Reception (Hotel Courtyard)			
19:30					

Welcome to the IFIP Working Conference on Uncertainty Quantification in Scientific Computing

August 1 – 4, 2011

Activities, Resources and Logistics

Registration
The Registration and Conference Information Desk will be located in the Sunshine Room on the second floor across the hall from the Ballroom.

Technical Sessions
All technical sessions will take place in the Ballroom on the hotel's second floor.

Messages and Fax
If your office needs to reach you, there will be someone available to take messages at 303-497-4242.

Food Breaks
At check-in hotel guests will be given vouchers for a full breakfast each day in the hotel restaurant. The conference will provide all paid participants with mid - morning and afternoon refreshments each day.

Lunch Breaks
Lunch will be provided for all paid participants in the hotel's outdoor garden area. In case of inclement weather lunch will be served in the Coach's Corner.

Internet Access
For your convenience, a wireless network is available in the conference rooms. If you have a wireless card for your computer and wish to make use of this service please check at the registration desk for access information.

Social Events
The conference will host a reception at the Millennium Hotel Fire Pit area on Monday evening, August 1 from 6 -7:30 pm. The event will include appetizers and a cash bar. In case of inclement weather, the reception will take place in the Ballroom.

On Wednesday, August 3rd, the conference will host a reception and banquet at Chautauqua Dining Hall from 5:15 – 7:30pm. All paid participants are welcome to attend both events. If you are interested in bringing a guest and have not previously registered them, please register and pay for them at the conference registration desk. Buses will leave the hotel for this event at 4:30. (Those attending the tour below will be transported directly from NIST to this event.)

NIST Tour
Optional tours of the NIST and NOAA laboratory facilities will be provided on the afternoon of Wednesday, August 3. Buses will depart the hotel for the tour at 1 pm. If you are interested in participating in the tours, please notify the conference registration desk no later than Monday, August 1. Following the tour buses will transport participants either back to the hotel or directly to the conference banquet (above).

Security at NIST/NOAA
To ensure site security, visitor badges must be worn and photo identification should be at hand at all times. Please do not attempt to enter any secured areas without an escort.

Airport Transportation
Super Shuttle provides transfer service from the hotel to Denver International Airport hourly between 4:45 am and 10:45 pm. Call 303-227-0000 for reservations.

WG 2.5 Business Meeting
IFIP Working Group 2.5 will hold its yearly business meeting in the Millennium Conference Room on Friday August 5 beginning at 9:00 am.

Useful Links
Conference Website:
http://www.nist.gov/itl/math/ifip-woco-10.cfm

NIST Gaithersburg: www.nist.gov

NIST Boulder: http://www.boulder.nist.gov

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IFIP Working Conference on
Uncertainty Quantification in Scientific Computing

Millennium Harvest House
Boulder, Colorado, USA
August 1-4, 2011

All sessions will be held in the Ballroom unless otherwise noted.

Sunday July 31

16:00 – 18:00 **Registration**
Hotel Lobby

Monday August 1

Opening Session

08:15 Welcoming Remarks
Ronald Boisvert, National Institute of Standards and Technology, US
Andrew Dienstfrey, National Institute of Standards and Technology, US

Session I: Uncertainty Quantification Need: Risk, Policy, and Decision Making (Part 1)

Chair: Andrew Dienstfrey, NIST, US
Discussant: Bo Einarsson, Linköping University, Sweden

08:30 **Keynote Address**
Uncertainties in Using Genomic Information to Make Regulatory Decisions
Pasky Pascual, Environmental Protection Agency, US

09:30 Considerations of Uncertainties in Regulatory Decision Making
Mark Cunningham, Nuclear Regulatory Commission, US

10:15 **Break**

10:45 An Industrial Viewpoint on Uncertainty Quantification in Simulation: Stakes, Methods, Tools, Examples
Alberto Pasanisi, Electricité de France, France

11:30 Living with Uncertainty
Patrick Gaffney, Bergen Software Services International, Norway

12:15 **Lunch**
Outdoor patio (Coach's Corner in bad weather)

Session II: Uncertainty Quantification Need: Risk, Policy, and Decision Making (Part 2)

Chair: Tony O'Hagan, University of Sheffield, UK
Discussant: Tim Hopkins, University of Kent, UK

13:15 Uncertainty and Sensitivity Analysis: From Regulatory Requirements to Conceptual Structure and Computational Implementation
Jon Helton, Sandia National Laboratories, US

14:00 Interpreting Regional Climate Predictions
Doug Nychka, National Center for Atmospheric Research, US

14:45 Weaknesses and Failures of Risk Assessment
William Oberkampf, Sandia National Laboratories, US (retired)

15:30 **Break**

16:00 **Panel Discussion:** UQ and Decision Making
Mac Hyman, Tulane University, US (Moderator)
Sandy Landsberg, Department of Energy, US
Larry Winter, University of Arizona, US
Charles Romine, NIST, US

17:30 **Adjourn**

18:00-19:30 **Reception**
Outdoor patio, Fire pit area (Ballroom in bad weather)

Tuesday August 2

Session III: Uncertainty Quantification Theory (Part 1)

Chair: Richard Hanson, Rogue Wave Software, US
Discussant: Peter Tang, The D.E. Shaw Group, USA

08:30 **Keynote Address**
Bayesian Analysis for Complex Physical Systems Modeled by Computer Simulators: Current Status and Future Challenges
Michael Goldstein, Durham University, UK

09:30 Scientific Computation and the Scientific Method: A Tentative Road Map for Convergence
Les Hatton, Kingston University, UK

10:15 **Break**

10:45 Overview of Uncertainty Quantification Algorithm R&D in the DAKOTA Project
Michael Eldred, Sandia National Laboratories, US

11:30 A Compressive Sampling Approach to Uncertainty Propagation
Alireza Doostan, University of Colorado

12:15 **Lunch**
Outdoor patio (Coach's Corner in bad weather)

Session IV: Uncertainty Quantification Theory (Part 2)

Chair: Ronald Cools, Katholieke Universiteit Leuven, Belgium
Discussant: Shigeo Kawata, Utsunomiya University, Japan

13:15 **Keynote Address**
Verified Computation with Probability Distributions and Uncertain Numbers
Scott Ferson, Applied Biomathematics, US

14:15 Parametric Uncertainty Computations with Tensor Product Representations
Hermann Matthies, Technische Universität Braunschweig, Germany

15:00 **Break**

15:30 **Hot Topics Session**
Those wishing to speak should contact the moderator by 13:00 on Tuesday.
Brian Ford, NAG Ltd., UK (Moderator)

17:30 **Adjourn**

Wednesday August 3

Session V: Uncertainty Quantification Tools

Chair: Bo Einarsson, Linköping University, Sweden
Discussant: Van Snyder, NASA Jet Propulsion Laboratory, US

08:30 **Keynote Address**
Desperately Needed Remedies for the Undebugability of Large-scale Floating-point Computations in Science and Engineering
William Kahan, University of California at Berkeley, US

09:30 Accurate Prediction of Complex Computer Codes via Adaptive Designs
William Welch, University of British Columbia, Canada

10:15 **Break**

10:45 Using Emulators to Estimate Uncertainty in Complex Models
Peter Challenor, National Oceanography Centre, UK

11:30 Measuring Uncertainty in Scientific Computations Using the Test Harness
Brian Smith, Numerica 21 Inc., US

12:15 **Lunch**
Outdoor patio (Coach's Corner in bad weather)

13:00 **Tour of NIST and NOAA Laboratories**
Bus pickup outside hotel lobby

16:15 **Chatauqua Excursion/Banquet**
Bus pickup outside hotel lobby
(Those on NOST/NOAA tour will be transported directly from NIST to Chatauqua)

16:30 **Walk in Chautaqua Meadows**

17:15 **Reception and Banquet**
Chautauqua Dining Hall

19:30 **Buses Depart for Hotel**

Thursday August 4

Session VI: Uncertainty Quantification Practice (Part 1)

Chair: Michael Thuné, University of Uppsala, Sweden
Discussant: Wilfried Gansterer, University of Vienna, Austria

08:30 **Keynote Address**
Numerical Aspects of Evaluating Uncertainty in Measurement
Maurice Cox, National Physical Laboratory, UK

09:30 Model-based Interpolation, Approximation, and Prediction
Antonio Possolo, NIST, US

10:15 **Break**

10:45 Uncertainty Quantification for Turbulent Reacting Flows
James Glimm, State University of New York at Stony Brook, US

11:30 Visualization of Error and Uncertainty
Chris Johnson, University of Utah, US

12:15 **Lunch**
Outdoor patio (Coach's Corner in bad weather)

Session VII: Uncertainty Quantification Practice (Part 2)

Chair: Ronald Boisvert, NIST
Discussant: Jennifer Scott, Rutherford Appleton Laboratory, UK

13:15 Uncertainty Reduction in Atmospheric Composition Models by Chemical Data Assimilation
Adrian Sandu, Virginia Tech, US

14:00 Emerging Architectures and UQ: Implications and Opportunities
Michael Heroux, Sandia National Laboratory, US

14:45 Interval Based Finite Elements for Uncertainty Quantification in Engineering Mechanics
Rafi Muhanna, Georgia Tech Savannah, US

15:30 **Break**

16:00 Reducing the Uncertainty When Approximating the Solution of ODEs
Wayne Enright, University of Toronto, Canada

16:45 **Closing Remarks**
Andrew Dienstfrey, NIST, US

17:00 **Conference Adjourns**

Peter Challenor (National Oceanography Centre, UK)

Using Emulators to Estimate Uncertainty in Complex Models

The Managing Uncertainty in Complex Models project has been developing methods for estimating uncertainty in complex models using emulators. Emulators are statistical descriptions of our beliefs about the models (or simulators). They can also be thought of as interpolators of simulator outputs between previous runs. Because they are quick to run, emulators can be used to carry out calculations that would otherwise require large numbers of simulator runs, for example Monte Carlo uncertainty calculations. Both Gaussian and Bayes Linear emulators will be explained and examples given. One of the outputs of the MUCM project is the MUCM toolkit, an on-line "recipe book" for emulator based methods. Using the toolkit as our basis we will illustrate the breadth of applications that can be addressed by emulator methodology and detail some of the methodology. We will cover sensitivity and uncertainty analysis and describe in less detail other aspects such as how emulators can also be used to calibrate complex computer simulators and how they can be modified for use with stochastic simulators.

Peter Challenor is a principal scientist in the Marine System Modelling research group at the National Oceanography Centre. Originally trained as a statistician, he has worked in ocean and climate related science for over 30 years. He has had an interest in the interaction of statistics and numerical models for a number of years, and has considerable expertise in the use of complex models in oceanography and climate research. He is a co-investigator on the Managing Uncertainty in Complex Models (MUCM) consortium investigating the use of emulators to analyze complex numerical codes. He is principal investigator for a project looking at the risk of the abrupt changes in the climate. In recent years he was a Distinguished Research Fellow at the Institute of Advanced Studies in Durham and has been a research fellow at the Isaac Newton Institute for Mathematical Sciences on programmes concerned with statistics and climate and experimental design. Peter is a member of the council of the Royal Statistical Society.

Maurice Cox (National Physical Laboratory, UK)

Numerical Aspects of Evaluating Uncertainty in Measurement

We examine aspects of quantifying the numerical accuracy in results from a measurement uncertainty computation in terms of the inputs to that computation.

The primary output from such a computation is often an approximation to the PDF (probability density function) for the measurand (the quantity intended to be measured), which may be a scalar or vector quantity. From this PDF all results of interest can be derived. The following aspects are considered:

1. The numerical quality of the PDF obtained by using Monte Carlo or Monte Carlo Markov Chain methods in terms of (a) the random number generators used, (b) the (stochastic) convergence rate, and its possible acceleration, and (c) adaptive schemes to achieve a (nominal) prescribed accuracy.
2. The production of a smooth and possibly compact representation of the approximate PDF so obtained, for purposes such as when the PDF is used as input to a further uncertainty evaluation, or when visualization is required.
3. The sensitivities of the numerical results with respect to the inputs to the computation.

We speculate as to future requirements in the area and how they might be addressed.

Maurice Cox is a Consultant Mathematician and a Senior Fellow at the National Physical Laboratory (NPL) in the UK. Maurice is a Visiting Professor in Computational Mathematics at Kingston University. He obtained a BSc in Applied Mathematics from City University, London, and a PhD in Numerical Analysis (spline functions), also from City University. After several years working for GEC, he has been with NPL since 1968, and has current research interests in measurement uncertainty evaluation, and the application of mathematics, statistics and numerical analysis to all branches of science.

Maurice is a Chartered Mathematician and a Fellow of the Institute of Mathematics and its Applications. He is a founder member of Working Group 1 of the Joint Committee for Guides in Metrology, leading a number of projects including editorial responsibility for revision of the "GUM" (the Guide to the expression of uncertainty in measurement), a document that is used exceedingly widely. He is chair of a number of national and international Committees and Groups concerned with the application of statistics, statistical software, uncertainty evaluation, and international measurement comparisons. He has over 250 publications, mainly in the application of mathematics and statistics to measurement science.

Mark Cunningham (Nuclear Regulatory Commission, US)

Considerations of Uncertainties in Regulatory Decision Making

In early 2011, a task force was established within the Nuclear Regulatory Commission (NRC) to develop proposals for a long-term vision on using risk information in its regulatory processes. This task force, established by NRC's Chairman Jaczko, is being led by Commissioner Apostolakis, and has a charter to "develop a strategic vision and options for adopting a more comprehensive and holistic risk-informed, performance-based regulatory approach for reactors, materials, waste, fuel cycle, and transportation that would continue to ensure the safe and secure use of nuclear material." This presentation will discuss some of the issues being considered by the task force in the context of how to manage the uncertainties associated with unlikely but potentially high consequence accident scenarios.

Mr. Cunningham's involvement in U.S. Nuclear Regulatory Commission (NRC) risk assessment program began in 1975, when he joined the agency as a Project Engineer in the Office of Nuclear Regulatory Research's (RES) Probabilistic Risk Analysis Branch. In 1979 and 1980, he served on NRC's Special Inquiry Group on the accident at Three Mile Island. In 1989, Mr. Cunningham was selected for the position of Chief, Probabilistic Risk Analysis Branch, RES. Subsequent to that, he held a number of management positions in RES, including Deputy Director, Division of Risk Analysis and Applications, Director, Division of Engineering Technology, and Director, Division of Fuel, Engineering, and Radiological Research. Between June 2007 and his retirement in February 2011, Mr. Cunningham served as Director, Division of Risk Assessment in the Office of Nuclear Reactor Regulation. Mr. Cunningham is currently supporting NRC's effort on assessing options for more holistic risk-informed and performance-based regulatory approach. Mr. Cunningham received a B.S. degree in Nuclear Engineering from the University of Florida and an M.S. degree in Nuclear Engineering from the Massachusetts Institute of Technology.

Michael Eldred (Sandia National Laboratories, US)

Overview of Uncertainty Quantification Algorithm R&D in the DAKOTA Project

Uncertainty quantification (UQ) is a key enabling technology for assessing the predictive accuracy of computational models and for enabling risk-informed decision making. This presentation will provide an overview of algorithms for UQ, including sampling methods such as Latin Hypercube sampling, local and global reliability methods such as AMV2+ and EGRA, stochastic expansion methods including polynomial chaos and stochastic collocation, and epistemic methods such as interval-valued probability, second-order probability, and evidence theory. Strengths and weaknesses of these different algorithms will be summarized and example applications will be described. Time permitting, I will also provide a short overview of DAKOTA, an open source software toolkit that provides a delivery vehicle for much of the UQ research at the DOE defense laboratories.

Mike Eldred received his B.S. in Aerospace Engineering from Virginia Tech in 1989 and his M.S.E. and Ph.D. in Aerospace Engineering from the University of Michigan in 1990 and 1993. Mike joined Sandia National Laboratories in 1994 and is currently a Distinguished Member of the Technical Staff in the Optimization and Uncertainty Quantification Department within the Computation, Computers, Information, and Mathematics Center. Mike initiated the DAKOTA effort shortly after joining Sandia in 1994 and led the project's R&D activities for 15 years. Having recently turned over project leadership to an energetic newcomer, Mike can now devote more time to algorithm R&D. Mike's research activities have focused on the areas of uncertainty quantification, design under uncertainty, surrogate-based optimization, and high performance computing. Mike is an Associate Fellow of the AIAA and member of SIAM, ISSMO, and USACM

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Wayne Enright (University of Toronto, Canada)

Reducing the Uncertainty when Approximating the Solution of ODEs

In the numerical solution of ODEs, it is now possible to develop efficient techniques that compute approximate solutions that are more convenient to interpret and understand when used by practitioners who are interested in accurate and reliable simulations of their mathematical models. We have developed a class of ODE methods and associated software tools that will deliver a piecewise polynomial as the approximate solution and facilitate the investigation of various aspects of the problem that are often of as much interest as the approximate solution itself.

These methods are designed so that the resulting piecewise polynomial will satisfy a perturbed ODE with an associated defect (or residual) that is *reliably* controlled. We will introduce measures that can be used to quantify the reliability of an approximate solution and how one can implement methods that, at some extra cost, can produce very reliable approximate solutions. We show how the ODE methods we have developed can be the basis for implementing effective tools for visualizing an approximate solution, and for performing key tasks such as sensitivity analysis, global error estimation and investigation of problems which are parameter-dependent. Software implementing this approach will be described for systems of IVPs, BVPs, DDEs, and VIEs.

Some numerical results will be presented for mathematical models arising in application areas such as computational medicine or the modeling of predator-prey systems in ecology.

Wayne Enright was born and raised in British Columbia. He received a BSc from UBC in 1968, an MSc in Mathematics from the University of Toronto in 1969 and a PhD in Computer Science from the University of Toronto in 1972. He was Chair of the department from 1993 to 1998. His research interests are in the general area of numerical analysis and scientific computation with a particular focus on the analysis and development of reliable numerical methods for ordinary differential equations and the design and evaluation of numerical software. Much of his research has been concerned with the development of more reliable and robust error control techniques for continuous numerical ODE methods. He and his students have developed general purpose reliable software packages for simulations in important application areas such as computational medicine, computational biology and population dynamics. He is also interested in the visualization of solutions of partial differential equations and scientific visualization in general.

Professor Enright is a past president of the Canadian Applied and Industrial Mathematics Society (CAIMS) and a current executive member of IFIP WG2.5 on Numerical Software. He has organized several international and national conferences and served on research evaluation panels in Canada, the US and the UK. He is also on the editorial boards of ACM Transactions on Mathematical Software and Advances in Computational Mathematics and on the Advisory Board of COMPUTING.

Scott Ferson (Applied Biomathematics, US)

Verified Uncertainty Projection for Probabilistic Models

Interval analysis is often offered as the method for verified computation, but the pessimism in the old saw that "interval analysis is the mathematics of the future, and always will be" is perhaps justified by the impracticality of interval bounding as an approach to projecting uncertainty in real-world problems. Intervals cannot account for dependence among variables, so propagations commonly explode to triviality. Likewise, the dream of a workable 'probabilistic arithmetic', which has been imagined by many people, seems similarly unachievable. Even in sophisticated applications such as nuclear power plant risk analyses, whenever probability theory has been used to make calculations, analysts have routinely assumed (i) probabilities and probability distributions can be precisely specified, (ii) most or all variables are independent of one another, and (iii) model structure is known without error. For the most part, these assumptions have been made for the sake of mathematical convenience, rather than with any empirical justification. And, until recently, these or essentially similar assumptions were pretty much necessary in order to get any answer at all. New methods now allow us to compute bounds on estimates of probabilities and probability distributions that are guaranteed to be correct even when one or more of the assumptions is relaxed or removed. In many cases, the results obtained are the best possible bounds, which means that tightening them would require additional empirical information. This talk will present an overview of probability bounds analysis, as a computationally practical implementation of imprecise probabilities, that combines ideas from both interval analysis and probability theory to sidestep the limitations of each.

Scott Ferson is a senior scientist at Applied Biomathematics, a small-business research firm on Long Island, New York, and has an adjunct appointment at the School of Marine and Atmospheric Sciences. He holds a Ph.D. in ecology and evolution from Stony Brook University and has over 100 papers and 5 books on risk analysis and related topics. His recent work, funded primarily by NIH and NASA, has focused on developing statistical methods and software to solve quantitative assessment problems when data are poor or lacking and structural knowledge is severely limited.

Patrick Gaffney (Bergen Software Services International, Norway)

Living with Uncertainty

This talk describes 12 years of experience in developing simulation software for automotive companies. By building software from scratch, using boundary integral methods and other techniques, it has been possible to tailor the software to address specific issues that arise in painting processes applied to vehicles and to provide engineers with results for real-time optimization and manufacturing analysis. The talk will focus on one particular simulator for predicting electrocoat deposition on a vehicle and will address the topics of verification, validation, and uncertainty quantification as they relate to the development and use of the simulator in operational situations.

The general theme throughout the talk is the author's belief of an almost total disconnection between engineers and the requirements of computational scientists. This belief is quite scary, and was certainly unexpected when starting the work 12 years ago. However, through several examples, the talk demonstrates the problems in attempting to extract from engineers the high quality input required to produce accurate simulation results.

The title provides the focus and the talk describes how living under the shadow of uncertainty has made us more innovative and more resourceful in solving problems that we never really expected to encounter when we started on this journey in 1999.

Patrick Gaffney's education in computing began in 1971 at the Thames Polytechnic in South East London. It continued during a sandwich year at the Royal Aircraft Establishment in Bedford England, and culminated at Oxford University where he acquired a M.Sc. in Mathematics, under the tutelage of Professor Leslie Fox and later a D.Phil. in Mathematics, under the supervision of Professor M.J.D. Powell.

Gaffney's career in computing began in 1975, at the Atomic Energy Research Establishment in Harwell England, and continued from 1977 until 1984 as a numerical analyst consultant with the Fusion Energy Division of the Oak Ridge National Laboratory in the USA. In 1984, he returned to Europe, first to set up a Computer Science department at the Christian Michelsen's Institute in Bergen Norway and then to IBM as the Director of their Scientific Centre in Bergen (in 1989, converted to IBM's European Environmental Sciences Centre). In 1994, Patrick Gaffney left IBM and founded Bergen Software Services International (BSSI).

BSSI designs, develops, and sells software systems and services applied to industrial manufacturing and assembly processes - especially for the automotive and other manufacturing industries. In particular, BSSI's software systems minimize or replace trial and error testing on physical prototypes by using mathematically valid computer simulations.

James Glimm, (SUNY Stonybrook, US)

Uncertainty Quantification for Turbulent Reacting Flows.

Uncertainty Quantification (UQ) for fluid mixing depends on the lengths scales for observation: macro, meso and micro, each with its own UQ requirements. New results are presented for each. For the micro observables, recent theories argue that convergence of numerical simulations in the Large Eddy Simulation (LES) should be governed by probability distribution functions (pdfs, or in the present context, Young measures) which satisfy the Euler equation. From a single deterministic simulation in the LES, or inertial regime, we extract a pdf by binning results from a space time neighborhood of the convergence point. The binned state values constitute a discrete set of solution values which define an approximate pdf.

Such a step coarsens the resolution, but not more than standard LES simulation methods, which typically employ an extended spatial filter in the definition of the filtered equations and associated subgrid scale (SGS) terms. The convergence of the resulting pdfs is assessed by standard function space metrics applied to the associated probability distribution function, i.e. the indefinite integral of the pdf. Such a metric is needed to reduce noise inherent in the pdf itself.

V&V/UQ results for mixing and reacting flows are presented to support this point of view.

James Glimm received his PhD from Columbia University in 1959. He has held academic positions at MIT, Courant Institute, NYU, Rockafeller University and Stony Brook University, where he is the Head of the Department of Applied Mathematics and Statistics. He is a member of the National Academy of Sciences and the American Academy of Science and a recipient of the National Medal of Science. He is noted for research in a broad range of areas, including mathematical analysis, partial differential equations, quantum field theory, statistical physics, numerical analysis and turbulence modeling.

Michael Goldstein (Durham University, UK)

Bayesian Analysis for Complex Physical Systems Modeled by Computer Simulators: Current Status and Future Challenges

Most large and complex physical systems are studied by mathematical models, implemented as high dimensional computer simulators. While all such cases differ in physical description, each analysis of a physical system based on a computer simulator involves the same underlying sources of uncertainty. These are: condition uncertainty (unknown initial conditions, boundary conditions and forcing functions), parametric uncertainty (as the appropriate choices for the model parameters are not known), functional uncertainty (as models are typically expensive to evaluate for any choice of parameters), structural uncertainty (as the model is different from the physical system), measurement uncertainty (in the data used to calibrate the model), stochastic uncertainty (arising from intrinsic randomness in the system equations), solution uncertainty (as solutions to the system equations can only be assessed approximately) and multi-model uncertainty (as there often is a family of models, at different levels of resolution, possibly with different representations of the underlying physics).

There is a growing field of study which aims to quantify and synthesize all of the uncertainties involved in relating models to physical systems, within the framework of Bayesian statistics, and to use the resultant uncertainty specification to address problems of forecasting and decision making based on the application of these methods. Examples of areas in which such methodology is being applied include asset management for oil reservoirs, galaxy modeling, and rapid climate change. In this talk, we shall give an overview of the current status and future challenges in this emerging methodology, illustrating with examples of current areas of application.

Michael Goldstein has worked throughout his career on the foundations, methodology and applications of Bayesian statistics (which concerns the development of informed uncertainty assessments based on the combination of expert judgment, probabilistic modeling and observational data). In particular, he has developed a general approach termed Bayes linear analysis, similar in spirit to the usual Bayesian approach, but which concerns the appropriate treatment of problems which are too complicated for full probabilistic specification. Over the last eighteen years, he has applied this approach to the analysis of all of the sources of uncertainty arising when studying large scale physical systems via complex mathematical models. This work has been well supported by research council and commercial funding, and he is currently developing methodology to address basic problems arising in areas such as climate change, systems biology, energy science and cosmology, as part of the Basic Technology MUCM consortium, the NERC Rapid consortium, the Leverhume Tipping Points consortium, and the oil company funded JIBA consortium.

Les Hatton (Kingston University, UK)

Scientific Computation and the Scientific Method: A Tentative Road Map for Convergence

For the last couple of centuries, the scientific method whereby we have followed Karl Popper's model of endlessly seeking to refute new and existing discoveries, forcing them to submit to repeatability and detailed peer review of both the theory and the experimental methods employed to flush out insecure conclusions, has served us extremely well. Much progress has been made. For the last 40 years or so however, there has been an increasing reliance on computation in the pursuit of scientific discovery. Computation is an entirely different animal. Its repeatability has proved unreliable, we have been unable to eliminate defect or even to quantify its effects, and there has been a rash of unconstrained creativity making it very difficult to make systematic progress to align it with the philosophy of the scientific method. At the same time, computation has become the dominant partner in many scientific areas.

This paper will address a number of issues. Through a series of very large experiments involving millions of lines of code in several languages along with an underpinning theory, it will put forward the viewpoint that defect is both inevitable and essentially a statistical phenomenon. In other words looking for purely technical computational solutions is unlikely to help much - there very likely is no silver bullet. Instead we must urgently promote the viewpoint that for any results which depend on computation, the computational method employed must be subject to the same scrutiny as has served us well in the years preceding computation. Baldly, that means that if the program source, the method of making and running the system, the test results and the data are not openly available, then it is not science. Even then we face an enormous challenge when digitally lubricated media can distort evidence to undermine the strongest of scientific cases.

Les Hatton is part-time Professor of Forensic Software Engineering at Kingston University, London. He graduated with an MA in mathematics from Kings College Cambridge in 1970, and an MSc and PhD in computational fluid dynamics from the University of Manchester in 1971 and 1973.

He started his career in numerical weather prediction and then became a geophysicist, for which he was awarded the Conrad Schlumberger prize in 1987 before becoming interested in software reliability and switching careers again in the 1990s. Although he has spent most of his working life in industry, he was formerly a Professor of Geophysics at TU Delft and later Professor of Software Reliability at Kent.

He has published several books and many technical papers and his 1995 book "Safer C" helped promote the use of safer language subsets in embedded control systems. His latest book "Email Forensics: eliminating Spam, Scams and Phishing" will appear in 2011. He has designed and implemented a number of commercial IT systems, including The Safer C toolset, a toolset for detecting defect in C-based systems and Gundalf a marine seismic source modelling package, both in use in many countries.

Jon Helton (Sandia National Laboratories, US)

Uncertainty and Sensitivity Analysis: From Regulatory Requirements to Conceptual Structure and Computational Implementation

The importance of an appropriate treatment of uncertainty in an analysis of a complex system is now almost universally recognized. As consequence, requirements for complex systems (e.g., nuclear power plants, radioactive waste disposal facilities, nuclear weapons) now typically call for some form of uncertainty analysis. However, these requirements are usually expressed at a high level and lack the detail needed to unambiguously define the intent, structure and outcomes of an analysis that provides a meaningful representation of the effects and implications of uncertainty. Consequently, it is necessary for the individuals performing an analysis to show compliance with a set of requirements to define a conceptual structure for the analysis that (i) is consistent with the intent of the requirements and (ii) also provides the basis for a meaningful uncertainty and sensitivity analysis. In many, if not most analysis situations, a core consideration is maintaining an appropriate distinction between aleatory uncertainty (i.e., inherent randomness in possible future behaviors of the system under study) and epistemic uncertainty (i.e., lack of knowledge with respect to the appropriate values to use for quantities that have fixed but poorly known values in the context of the particular study being performed). Conceptually, this leads to an analysis involving three basic entities: a probability space (A, Σ_A, p_A) characterizing aleatory uncertainty, a probability space (E, Σ_E, p_E) characterizing epistemic uncertainty, and a model that predicts system behavior (i.e., a function $f(t|\mathbf{a},\mathbf{e})$ that defines system behavior at time t conditional on elements $\mathbf{a}$ and $\mathbf{e}$ of the sample spaces A and E for aleatory and epistemic uncertainty). In turn, this conceptual structure leads to an analysis in which (i) uncertainty analysis results are defined by integrals involving the function $f(t|\mathbf{a},\mathbf{e})$ and the two indicated probability spaces and (ii) sensitivity analysis results are defined by the relationships between epistemically uncertain analysis inputs (i.e., elements $\mathbf{e}_j$ of $\mathbf{e}$) and analysis results defined by the function $f(t|\mathbf{a},\mathbf{e})$ and also by various integrals of this function. Computationally, this leads to an analysis in which (i) high-dimensional integrals must be evaluated to obtain uncertainty analysis results and (ii) mappings between high-dimensional spaces must be generated and explored to obtain sensitivity analysis results. The preceding ideas and concepts are illustrated with an analysis carried out in support of a license application for the proposed repository for high-level radioactive waste at Yucca Mountain, Nevada.

Jon Helton is a Professor Emeritus of Mathematics at Arizona State University. He has over 30 years experience in uncertainty and sensitivity analysis of models for complex systems and in the design of performance assessments and probabilistic risk assessments for engineered systems. He participated in the NRC's original program to develop an analysis capability to assess the geologic disposal of high-level radioactive waste, the NRC's MELCOR program to develop a new suite of models for nuclear power plant accidents, the NRC's NUREG-1150 analyses to reassess the risk from accidents at commercial nuclear power plants, the DOE's performance assessments for the Waste Isolation Power Plant and the proposed repository for high-level radioactive waste at Yucca Mountain, and the NNSA's ASCI and ASC programs to develop advanced computing capabilities to assess the reliability of the nation's nuclear stockpile.

Michael Heroux (Sandia National Laboratories, US)

Emerging Architectures and UQ: Implications and Opportunities

Computer architecture is changing dramatically. Most noticeable is the introduction of multicore and GPU (collectively, manycore) processors. These manycore architectures promise the availability of a terascale laptop, petascale deskside and exascale compute center in the next few years. At the same time, manycore nodes will forces a universal refactoring of code in order to realize this performance potential. Furthermore, the sheer number of components in very high-end systems increases the chance that user applications will experience frequent system faults in the form of soft errors.

In this presentation we give an overview of architecture trends and their potential impact on scientific computing in general and uncertainty quantification (UQ) computations specifically. We will also discuss growing opportunities for UQ that are enabled by increasing computing capabilities, and new opportunities to help address the anticipated increase in soft errors that must be addressed at the application level.

Michael Heroux is a Distinguished Member of the Technical Staff at Sandia National Laboratories, working on new algorithm development, and robust parallel implementation of solver components for problems of interest to Sandia and the broader scientific and engineering community. He leads development of the Trilinos Project, an effort to provide state of the art solution methods in a state of the art software framework. Trilinos is a 2004 R&D 100 award-winning product, freely available as open source and actively developed by dozens of researchers.

Dr. Heroux also works on the development of scalable parallel scientific and engineering applications and maintains his interest in the interaction of scientific/engineering applications and high performance computer architectures. He leads the Mantevo project, which is focused on the development of open source, portable miniapplications and minidrivers for scientific and engineering applications.

Dr. Heroux maintains an office in rural central Minnesota and at St. John's University where he is Scientist in Residence in the Computer Science Department. He is a member of the Society for Industrial and Applied Mathematics. He is a Distinguished Scientist of the Association for Computing Machinery, and the Editor-in-Chief of the ACM Transactions on Mathematical Software.

Chris Johnson (University of Utah, US)

Visualization of Error and Uncertainty

As former English Statesmen and Nobel Laureate (Literature), Winston Churchill said, "True genius resides in the capacity for evaluation of uncertain, hazardous, and conflicting information." Churchill is echoed by Nobel Prize winning Physicist Richard Feynman, "What is not surrounded by uncertainty cannot be the truth." Yet, with few exceptions, visualization research has ignored the visual representation of errors and uncertainty for three-dimensional (and higher) visualizations. In this presentation, I will give an overview of the current state-of-the-art in uncertainty visualization and discuss future challenges.

Chris Johnson directs the Scientific Computing and Imaging (SCI) Institute at the University of Utah where he is a Distinguished Professor of Computer Science and holds faculty appointments in the Departments of Physics and Bioengineering. His research interests are in the areas of scientific computing and scientific visualization. Dr. Johnson founded the SCI research group in 1992, which has since grown to become the SCI Institute employing over 200 faculty, staff and students. Professor Johnson serves on several international journal editorial boards, as well as on advisory boards to several national and international research centers. Professor Johnson has received several awards, including the NSF Presidential Faculty Fellow (PFF) award from President Clinton in 1995 and the Governor's Medal for Science and Technology in 1999. He is a Fellow of the American Institute for Medical and Biological Engineering (AIMBE), a Fellow of the American Association for the Advancement of Science (AAAS) and a Fellow of the Society of Industrial and Applied Mathematics (SIAM). In 2009, he received the Utah Cyber Pioneer Award and in 2010 Professor Johnson received the Rosenblatt Award from the University of Utah and the IEEE Visualization Career Award. (http://www.cs.utah.edu/~crj/)

William Kahan (University of California at Berkeley, US)

Desperately Needed Remedies for the Undebuggability of Large-Scale Floating-Point Computations in Science and Engineering

If suspicions about the accuracy of a computed result arise, how long does it take to either allay or justify them? Often diagnosis has taken longer than the computing platform's service life. Software tools to speed up diagnosis by at least an order of magnitude could be provided but almost no scientists and engineers know to ask for them, though almost all these tools have existed, albeit not all together in the same place at the same time. These tools would cope with vulnerabilities peculiar to Floating-Point, namely roundoff and arithmetic exceptions. But who would pay to develop the suite of these tools? Nobody, unless he suspects that the incidence of misleadingly anomalous floating-point results rather exceeds what is generally believed. And there is ample evidence to suspect that.

This document will be posted at www.eecs.berkeley.edu/~wkahan/Boulder.pdf.

More details have already been posted at www.eecs.berkeley.edu/~wkahan/NeeDebug.pdf and www.eecs.berkeley.edu/~wkahan/Mindless.pdf

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Prof. W. Kahan (now retired) error-analyzes scientific and engineering floating-point computations on electronic computers, which he has programmed since 1953. Among his contributions are the infallible algorithms for the HP-12C financial calculator (still for sale since 1982), fast and accurate singular-value decompositions (with G.H. Golub in 1964) now very widely used, and the mathematical basis for the now near-ubiquitous IEEE Standard 754 for Binary (and later Decimal) Floating-Point. Among his trophies are the ACM Turing Award (1989) and S.I.A.M's Von Neumann Lecture (1997). Born and educated in Toronto, Canada, he has worked at the Univ. of Calif. in Berkeley since 1969.

Hermann Matthies (Technische Universität Braunschweig, Germany)

Parametric Uncertainty Computations with Tensor Product Representations

Parametric versions of state equations of some complex system – the uncertainty quantification problem with the parameter as a random quantity is a special case of this general class – lead via association to a linear operator to analogues of covariance, its spectral decomposition, and the associated Karhunen-Loève expansion. This results in a generalized tensor representation. The parameter in question may be a number, a tuple of numbers - a finite dimensional vector or function, a stochastic process, or a random tensor field.

Examples of stochastic problems, dynamic problems, and similar will be given to explain the concept. If possible, the tensor factorization may be cascaded, leading to tensors of higher degree.

In numerical approximations this cascading tensor decomposition may be repeated on the discrete level, leading to very sparse representations of the high dimensional quantities involved in such parametric problems.

This is achieved by choosing low-rank approximations, in effect an information compression. These representations allow also for very efficient computation. Updating of uncertainty for new information is an important part of uncertainty quantification. Formulated in terms or random variables instead of measures, the Bayesian update is a projection and allows the use of the tensor factorizations also in this case. This will be demonstrated on some examples.

Hermann G. Matthies was born in 1951 in Hamburg and studied Mathematics, Physics, and Computer Science at Technische Universität Berlin, finishing with a Diploma in Mathematics in 1976.

From 1976 on he was a graduate student at the MIT, obtaining his Ph. D. under the direction of Gilbert Strang there in 1978. From 1979 until 1995 he worked at Germanischer Lloyd in Hamburg in various positions, including research in computational methods and finite element technology, offshore structures and technology, and wind energy. Since 1996 he is a full professor at Technische Unversität Braunschweig and the director of the Institute of Scientific Computing. From 1996 to 2006 he was additionally the head of the university computing centre.

His research interests are currently coupled problems and multiscale problems, as well as formulation and computational methods for uncertainty quantification and Bayesian inverse problems.

Rafi Muhanna (Georgia Tech, US)

Interval Based Finite Elements for Uncertainty Quantification in Engineering Mechanics

Latest scientific and engineering advances have started to recognize the need for defining multiple types of uncertainty. The behavior of a mathematical model of any system is determined by the values of the model's parameters. These parameters, in turn, are determined by available information which may range from scarce to comprehensive. When data is scarce, analysts fall back to deterministic analysis. On the other hand, when more data is available but insufficient to distinguish between candidate probability functions, analysts supplement the available statistical data by judgmental information. In such a case, we find ourselves in the extreme either/or situation: a deterministic setting which does not reflect parameter variability, or a full probabilistic analysis conditional on the validity of the probability models describing the uncertainties. The above discussion illustrates the challenge that engineering analysis and design is facing in how to circumvent situations that do not reflect the actual state of knowledge of considered systems and are based on unjustified assumptions. Probability Bounds (PB) methods offer a resolution to this problem as they are sufficiently flexible to quantify uncertainty absent assumptions in the form of the probability density functions (PDF) of system parameters, yet they can incorporate this structure into the analysis when available. Such approach will ensure that the actual state of knowledge on the system parameters is correctly reflected in the analysis and design; hence, design reliability and robustness are achieved.

Probability bounds is built on interval analysis as its foundation. This talk will address the problem of overestimation of enclosures for target and derived quantities, a critical challenge in the formulation of Interval Finite Element Methods (IFEM). A new formulation for Interval Finite Element Methods will be introduced where both primary and derived quantities of interest are included in the original uncertain system as primary variables.

Dr. Muhanna is an associate professor in the School of Civil and Environmental Engineering at Georgia Institute of Technology. He joined Georgia Tech in 2000. Dr. Muhanna received the B.S. Eng. Degree in Civil Engineering from the University of Damascus, Syria, and his M.S. and Ph.D. degrees in the area of Solid and Structural Mechanics from the Higher Institute for Structure and Architecture, Sofia, Bulgaria. He has also served on the faculty at the University of Damascus, Case Western Reserve University, Ohio and the University of Maryland, College Park. Dr. Muhanna's research activity is in the general area of computational solid and structural mechanics that includes uncertainty modeling, structural reliability, computational reliability, and optimization of masonry building materials in structural systems. Dr. Muhanna has won a number of international prizes, among them: the Aga Khan Award for Architecture, one of the most prestigious architectural awards in the world (1992); the Golden Prize of the United Nations World Intellectual Property Organization (1988); and the Special Prize of the United Nations HABITAT (1989). Dr. Muhanna is the founder and director of the Center for Reliable Engineering Computing (REC) that has been organizing the series of biannual international conferences on Reliable Engineering Computing since 2004.

Doug Nychka (National Center for Atmospheric Research, US)

Interpreting Regional Climate Projections

As attention shifts from broad global summaries of climate change to more specific regional impacts there is a need for statistics to quantify the uncertainty in regional projections. This talk will provide an overview on interpreting regional climate experiments (physically based simulations based on coupled global and regional climate models) using statistical methods to manage the discrepancies among models, their internal variability, regridding errors, model biases and other factors. The extensive simulations being produced in the North American Regional Climate Change and Assessment Program (NARCCAP) provide a context for our statistical approaches. An emerging principle is adapting analysis of variance decompositions to test for equality of mean fields, to quantify the variability due to different components in a numerical experiment and to identify the departures from observed climate fields.

Douglas Nychka is a statistical scientist with an interest in the problems posed by geophysical data sets. His Ph. D. (1983) is from the University of Wisconsin and he subsequently spent 14 years as a faculty member at North Carolina State University. His research background in fitting curves and surfaces lead to an interest in the analysis of spatial and environmental data. Pursuing this area of application, he assumed leadership of the Geophysical Statistics Project at the National Center for Atmospheric Research (NCAR) in 1997, an NSF funded program to build collaborative research and training between statistics and the geosciences. In 2004, he became Director of the Institute of Mathematics Applied to Geosciences, an interdisciplinary component at NCAR with a focus on transferring innovative mathematical models and tools to the geosciences. His current interests are in quantifying the uncertainty of numerical experiments that simulate the Earth's present and possible future climate.

William Oberkampf (Sandia National Laboratories (retired), US)

Weaknesses and Failures of Risk Assessment

Within the technical community, it is instinctive to conduct uncertainty quantification analyses and risk assessments for use in risk-informed decision making. The value and reliability of some formal assessments, however, have been sharply criticized not only by well-known scientists, but also by the public after high-visibility failures such as the loss of two Space Shuttles, major damage at the Three-Mile Island nuclear power plant, and the disaster at the Fukushima plant. The realities of these failures, and many others, belie the predicted probabilities of failure for these systems and the credibility of risk assessments in general. The uncertainty quantification and risk assessment communities can attempt to defend and make excuses for notoriously poor (or misused) analyses, or we can learn how to improve technical aspects of analyses and to develop procedures to help guard against fraudulent analyses. This talk will take the latter route by first examining divergent goals of risk analyses; neglected sources of uncertainty in modeling the hazards or initiating events, external influences on the system of interest, and the system itself; and the importance of mathematical representations of uncertainties and their dependencies. We will also argue that risk analyses are not simply mathematical activities, but they are also human endeavors that are susceptible to a wide range of human weaknesses. As a result, we discuss how analyses can be distorted and/or biased by analysts and sponsors of the analysis, and how results of analyses can be miscommunicated and misinterpreted, either unintentionally or deliberately.

William L. Oberkampf has 41 years of experience in research and development in fluid dynamics, heat transfer, flight dynamics, solid mechanics, and uncertainty quantification. He received his PhD in 1970 from the University of Notre Dame in Aerospace Engineering. He served on the faculty of the Mechanical Engineering Department at the University of Texas at Austin from 1970 to 1979. From 1979 until 2007 he worked in both staff and management positions at Sandia National Laboratories in Albuquerque, New Mexico. During his career he has been deeply involved in both computational simulation and experimental activities. Many of these activities have been focused on verification, validation, uncertainty quantification, and risk analyses in modeling and simulation. He retired from Sandia as Distinguished Member of the Technical Staff and is a Fellow of the American Institute of Aeronautics and Astronautics. He has over 160 journal articles, book chapters, conference papers, and technical reports, and co-authored, with Christopher Roy, the book "Verification and Validation in Scientific Computing" published by Cambridge University Press.

Alberto Pasanisi (Electricité de France, France)

An Industrial Viewpoint on Uncertainty Quantification in Simulation: Stakes, Methods, Tools, Examples.

Simulation is nowadays a major tool in industrial R&D and engineering studies. In industrial practice, in both design and operating stages, the behavior of a complex system is described and forecasted by a computer model, which is, most of time, deterministic. Yet, engineers coping with quantitative predictions using deterministic models deal actually with several sources of uncertainties affecting the inputs (and eventually the model itself) which are transferred to the outputs, i.e. the outcomes of the study. Uncertainty quantification in simulation has gained more and more importance in the last years and it has now become a common practice in several industrial contexts. In this talk we will give an industrial feedback and viewpoint on this question. After a reminder of the main stakes related to uncertainty quantification and probabilistic computing, we will particularly insist on the specific methodology and software tools which have been developed for dealing with this problem. Several examples, concerning different physical framework, different initial questions and different mathematical tools, will complete this talk.

Alberto Pasanisi has a Civil Engineering degree from the University of Napoli (Italy) and a PhD in Statistics from the French National Institute for Rural Engineering, Water and Forest Management (ENGREF). He is currently project manager in uncertainty analysis at the Industrial Risk Management Department of the R&D Unit of EDF (Electricité de France). He formerly worked in several fields of engineering (hydraulics, coastal management, metering, buildings thermal simulation) in Italy and in France.

Pasky Pascual (Environmental Protection Agency, US)

Uncertainties in Using Genomic Information to Make Regulatory Decisions

In 2007, the U.S. National Academy of Sciences issued a report, "Toxicity Testing in the 21st Century: a Vision and a Strategy," which proposed a vision and a roadmap for toxicology by advocating the use of systems-oriented, data-driven predictive models to explain how toxic chemicals impact human health and the environment. The report noted the limitations of whole animal tests that have become the standard basis for risk assessments at the U.S. Environmental Protection Agency. That same year, in response to the recall of the pain-killing drug, Vioxx, Congress passed the the Food and Drug Administration Act (FDAA).Vioxx had been approved for release by the U.S. government, and only belatedly was it discovered that the drug increased the risk of heart disease.

This presentation suggests that these two events anticipate the need to build on developments in genomics, cellular biology, bioinformatics and other fields to craft predictive models that provide the rationale for regulating risks to public health and the environment. It suggests that both are a step in the right direction, but that long-standing issues of uncertainty in scientific inference must be more widely appreciated and understood, particularly within the regulatory system, if society hopes to capitalize on these scientific advances.

Pasky Pascual is an environmental scientist and lawyer who works for the U.S. Environmental Protection Agency. He served as Director for the EPA's Council for Regulatory Environmental Modeling. His primary interest is in the area of regulatory decision-making, and he has published papers on the judicial review of regulatory science. Pasky began his work at EPA with the Climate Change Division, during which he worked with non-governmental organizations to help measure the greenhouse gases avoided through projects funded by the EPA. He followed this up with work on an initiative spearheaded by the Clinton Administration, leading stakeholders from industry, government, and the NGO sector to develop approaches to facility management that combined environmental performance, regulatory flexibility, and economic efficiency. On behalf of EPA's Office of Research and Development, he currently manages a portfolio of extramural research on using genomic information and other biomarkers derived from high-throughput assays to develop models of environmental and public health risk.

Antonio Possolo (National Institute of Standards and Technology, US)

Model-Based Interpolation, Approximation, and Prediction

Model-based interpolation, approximation, and prediction are contingent on the choice of model: since multiple alternative models typically can reasonably be entertained for each of these tasks, and the results are correspondingly varied, this often is a major source of uncertainty. Several statistical methods are illustrated that can be used to assess this uncertainty component: when interpolating concentrations of greenhouse gases over Indianapolis, predicting the viral load in a patient infected with influenza A, and approximating the solution of the kinetic equations that model the progression of the infection.

Antonio Possolo, Chief of the Statistical Engineering Division (Information Technology Laboratory, NIST), holds a Ph.D. in Statistics from Yale University. Besides his current role in government (for five years now), he has sixteen years of previous experience in industry (General Electric, Boeing), and seven years of academic experience (Princeton University, and University of Washington in Seattle). He is committed to the development and application of probabilistic and statistical methods that contribute to advances in science and technology. His areas of specialty include statistical data analysis and modeling of spatio-temporal phenomena, and the characterization of measurement uncertainty.

Adrian Sandu (Virginia Tech, US)

Uncertainty Reduction in Atmospheric Composition Models by Chemical Data Assimilation

Data assimilation reduces the uncertainty with which the state of a physical system is known by combining imperfect model results with sparse and noisy observations of reality. Chemical data assimilation refers to the use of measurements of trace gases and particulates to improve our understanding of the atmospheric composition.

Two families of methods are widely used in data assimilation: the four dimensional variational (4D-Var) approach, and the ensemble Kalman filter (EnKF) approach. In the four dimensional variational (4D-Var) framework data assimilation is formulated as an optimization problem, which is solved using gradient based methods to obtain maximum likelihood estimates of the uncertain state and parameters. A central issue in 4D-Var data assimilation is the construction of the adjoint model. Kalman filters are rooted in statistical estimation theory, and seek to obtain moments of the posterior distribution that quantifies the reduced uncertainty after measurements have been considered. A central issue in Kalman filter data assimilation is to manage the size of covariance matrices by employing various computationally feasible approximations.

In this talk we review computational aspects and tools that are important for chemical data assimilation. They include the construction, analysis, and efficient implementation of discrete adjoint models in 4D-Var assimilation, optimization aspects, and the construction of background covariance matrices. State-of-the-art solvers for large scale PDEs adaptively refine the time step and the mesh in order to control the numerical errors. We discuss newly developed algorithms for variational data assimilation with adaptive models. Particular aspects of the use of ensemble Kalman filters in chemical data assimilation are highlighted. New hybrid data assimilation ideas that combine the relative strengths the variational and ensemble approaches are reviewed. Examples of chemical data assimilation studies with real data and widely used chemical transport models are given.

Adrian Sandu has received the diploma in Electrical Engineering from the Polytechnic University Bucharest, M.S. in Computer Science, and Ph.D. in Computational Sciences from the University of Iowa. Before joining Virginia Tech he held a postdoctoral research position at the Courant Institute of Mathematical Sciences and assistant professor position in the Department of Computer Science at Michigan Tech.

The overarching goal of Sandu's research is to advance the field of computational science through the development of new numerical techniques and software and through the application of these tools to solve significant scientific and engineering problems. Sandu's research interests include time integration algorithms, data assimilation and inverse problems, uncertainty quantification, and high performance computing. He co-authored over 60 peer reviewed journal articles in these areas, numerous peer reviewed conference publications, as well as several widely used software packages.

Brian Smith (University of New Mexico, US)

Measuring Uncertainty in Scientific Computations Using the Test Harness

The test harness TH is a tool developed by Numerica 21 to facilitate the testing and evaluation of scientific software during the development and maintenance phases of such software. This paper describes how the tool can be used to measure uncertainty in scientific computations. It confirms that the actual behavior of the code when subjected to changes, typically small, in the code input data reflects formal analysis of the problem's sensitivity to its input. Although motivated by studying small changes in the input data, the test harness can measure the impact of any changes, including those that go beyond the formal analysis.

Brian T. Smith received his Ph.D in Computer Science in 1969 from the University of Toronto supervised by Prof. W. Kahan. After spending a year at the Eidgenossische Technische Hochschule in Zurich, Switzerland in 1969-1970 supervised by Prof. P. Henrici, he joined the staff of the Mathematics and Computer Science Division at Argonne National Laboratory from 1970 to 1988. While at Argonne, he was co-participant in the EISPACK project, and he developed an automated reasoning tool called AURA. He used AURA to solve open mathematical questions and to validate control system circuits and codes for a critical application. Dr. Brian Smith was a member of the Fortran standards committee for 25 years and helped develop Fortran 90 and Fortran 95. He worked on many collaborative projects in numerical software and computing science, including a continuous cooperation with Numerical Algorithms Group Oxford since May 1970.

In 1989, he joined the faculty of the Computer Science Department at the University of New Mexico until his retirement as Emeritus Professor in 2003. While at UNM, he was co-founder and co-principal investigator of the Maul High Performance Computer Center Project supported by the US Air Force. After retirement, he co-founded the company Numerica 21 Inc. and is its President. He is also Chief Software Engineer for the company Accurate Solutions in Applied Physics LLC. He is the co-author of several handbooks on Fortran, including one each of Fortran 90, Fortran 95, and Fortran 2003. He is also a member of the Board of the Numerical Algorithms Group Ltd, Oxford, UK and has been a member of the IFIP WG 2.5 since its inception.

William Welch (University of British Columbia, Canada)

Accurate Prediction of Complex Computer Codes via Adaptive Designs

There are many useful classes of design for an initial computer experiment: Latin hypercubes, orthogonal array Latin hypercubes, maximin-distance designs, etc. Often, the intitial experiment has about n = 10d runs, where d is the dimensionality of the input space (Loeppky, Sacks, and Welch, "Choosing the Sample Size of a Computer Experiment," Technometrics 2009). Once the computer model has been run according to the design, a first step is usually to build a computationally inexpensive statistical surrogate for the computer model, often via a Gaussian Process / Random Function statistical model. But what if the analysis of the data from this initial design provides poor prediction accuracy?

Poor accuracy implies the underlying input-output function is complex in some sense. If the complexity is restricted to a few of the inputs or to local subregions of the parameter space, there may be opportunity to use the initial analysis to guide further experimentation. Subsequent runs of the code should take account of what has been learned. Similarly, analysis should be adaptive.

This talk will demonstrate strategies for experimenting sequentially. Difficult functions, including real computer codes, will be used to illustrate. The advantages will be assessed in terms of empirical prediction accuracy and theoretical measures.

Will Welch joined the Department of Statistics, UBC as a Professor in 2003 and was Head of the Department from 2003 until 2008. Prior to coming to UBC, he was a Professor at the University of Waterloo. He also held the honorary title of Visiting Professor in the Business School, Loughborough University, UK, 2004–2009.

Welch's research has concentrated on computer-aided design of experiments, quality improvement, the design and analysis of computer experiments, and the design and analysis of drug-discovery data from high-throughput screening. His work is highly cited: six of the publications each have 100–500 citations in the Web of Science.

Welch has served on the editorial boards of the Annals of Applied Statistics and the Canadian Journal of Statistics. He is President of the Business and Industrial Statistics Section of the Statistical Society of Canada. In 2000 he won the American Statistical Association's Statistics in Chemistry Prize.