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IFIP – The International Federation for Information Processing

IFIP was founded in 1960 under the auspices of UNESCO, following the First World Computer Congress held in Paris the previous year. An umbrella organization for societies working in information processing, IFIP's aim is two-fold: to support information processing within ist member countries and to encourage technology transfer to developing nations. As ist mission statement clearly states,

> *IFIP's mission is to be the leading, truly international, apolitical organization which encourages and assists in the development, exploitation and application of information technology for the benefit of all people.*

IFIP is a non-profitmaking organization, run almost solely by 2500 volunteers. It operates through a number of technical committees, which organize events and publications. IFIP's events range from an international congress to local seminars, but the most important are:

- The IFIP World Computer Congress, held every second year;
- Open conferences;
- Working conferences.

The flagship event is the IFIP World Computer Congress, at which both invited and contributed papers are presented. Contributed papers are rigorously refereed and the rejection rate is high.

As with the Congress, participation in the open conferences is open to all and papers may be invited or submitted. Again, submitted papers are stringently refereed.

The working conferences are structured differently. They are usually run by a working group and attendance is small and by invitation only. Their purpose is to create an atmosphere conducive to innovation and development. Refereeing is less rigorous and papers are subjected to extensive group discussion.

Publications arising from IFIP events vary. The papers presented at the IFIP World Computer Congress and at open conferences are published as conference proceedings, while the results of the working conferences are often published as collections of selected and edited papers.

Any national society whose primary activity is in information may apply to become a full member of IFIP, although full membership is restricted to one society per country. Full members are entitled to vote at the annual General Assembly, National societies preferring a less committed involvement may apply for associate or corresponding membership. Associate members enjoy the same benefits as full members, but without voting rights. Corresponding members are not represented in IFIP bodies. Affiliated membership is open to non-national societies, and individual and honorary membership schemes are also offered.

Andrew M. Dienstfrey Ronald F. Boisvert (Eds.)

Uncertainty Quantification in Scientific Computing

10th IFIP WG 2.5 Working Conference, WoCoUQ 2011
Boulder, CO, USA, August 1-4, 2011
Revised Selected Papers

Springer

Volume Editors

Andrew M. Dienstfrey
National Institute of Standards and Technology
Information Technology Laboratory
325 Broadway, Mail Stop 891, Boulder, CO 80305, USA
E-mail: andrew.dienstfrey@nist.gov

Ronald F. Boisvert
National Institute of Standards and Technology
Applied and Computational Mathematics Division
100 Bureau Drive, Mail Stop 8910, Gaithersburg, MD 20899, USA
E-mail: boisvert@nist.gov

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Preface

Computing has become an indispensable component of modern science and engineering research. As has been repeatedly observed and documented, processing speed measured in floating point operations per second has experienced exponential growth in the last few decades. These hardware efficiencies have been accompanied by innovations in mathematical algorithms, numerical software, and programming tools. The result is that, by any measure, the modern computer is many orders of magnitude more powerful than its early predecessors, capable of simulating physical problems of unprecedented complexity.

Given the success of scientific computation as a research tool, it is natural that scientists, engineers, and policy makers strive to harness this immense potential by using computational models for critical decision making. Increasingly, computers are being used to supplement experiments, to prototype engineering systems, or to predict the safety and reliability of high-consequence systems. Such use inevitably leads one to question: "How good are these simulations? Would you bet your life on them?" Unfortunately, most computational scientists today are ill equipped to address such important questions with the same scientific rigor that is routine in experimental science.

The International Federation of Information Processing (IFIP) Working Conference on Uncertainty Quantification in Scientific Computing was convened as a means to address these questions. Participants in the working conference consisted of experts in mathematical modeling, numerical analysis, numerical software engineering, and statistics, as well as policy analysts from a range of application domains to assess our current ability to quantify uncertainty in modeling and simulation (UQ), to raise awareness of this issue within the numerical software community, and to help envision a research agenda to address this critical need. The conference was held in serial plenary sessions organized around four thematic areas: needs, theory, tools, and practice. Keynote speakers introduced each thematic area in broad strokes, followed by invited speakers presenting targeted studies. An additional "Hot Topics" session was organized in real time to provide participants with a venue to expand upon discussions generated by conference presentations, and to present late-breaking material. Finally, adding another dimension, a panel consisting of high-level representatives from government agencies and academia were invited to discuss present practice and future opportunities for uncertainty quantification in scientific computing in the context of the missions of their respective organizations.

The conference Program Committee hoped to generate active engagement on a range of topics both broad and deep. From questions about floating-point compliance and exception handling to computations of 10,000-year risk assessments of nuclear waste repositories, no scale of time, space, and numerical accuracy was beyond scope. Theoretical treatments reflected the full range of uncertainty

and risk analysis from approaches recommended by international guidance documents of measurement institutes worldwide, to Bayesian analyses, to a presentation and energetic discussion of the axiomatic foundations of a relatively new theory of uncertainty quantification referred to as probabilistic bounds analysis. Finally, the applications and needs were equally diverse, covering topics of judiciary and regulatory constraints on the use of predictive computation for environmental and reactor safety models, to simulation-based engineering of the electrodeposition paint application process as used by prominent automotive manufacturers. Underlying this diversity, however, the common thread binding all participants was the shared commitment to better achieve the promise offered by numerical computation as a means not only to scientific discovery, but to reliable decision making in matters of importance for society at large.

Of the 24 talks given at the conference, 20 authors contributed papers for these proceedings. Keeping with the tradition of past IFIP Working Conferences, each conference talk was followed by a lively discussion session. During these sessions, assigned discussants presented forms to participants on which they recorded their questions for the speakers. These forms were collected and distributed to speakers with the request that they respond in writing. The resulting record of the discussions appears after each chapter.

As with any activity of this scope many acknowledgments are due. First the success of the conference can largely be attributed to an unmatched Program Committee drawn from a global network of leaders. Many thanks to them for actively participating in conference calls spanning multiple time zones. It was by these efforts that conference topics were defined and associated speakers identified. The fruits of this labor are represented in the pages that follow. Behind the scenes there were too many moving parts to thank all parties. We draw attention to the incredible logistical and planning support provided by Wendy McBride and other members of the Public and Business Affairs Office at the National Institute of Standards and Technology (NIST) in Boulder. Furthermore, numerous speakers and participants would have never made it to Boulder had it not been for the tireless efforts of Lorna Buhse and Robin Bickel of NIST in navigating the cross-cutting constraints mandated for international travel under sponsorship of the United States government. The financial support of the NIST Applied and Computational Mathematics Division is gratefully acknowledged, as is the in-kind support provided by the International Federation of Information Processing's Working Group 2.5 on Numerical Software, the Society of Industrial and Applied Mathematics, and the United States Department of Energy. Finally, we thank our wives and families for stepping in to fill the gaps created by our limitations, and remaining steadfast as we traveled the ups and downs associated with planning and executing such an event. We are happy to report that the ride is over (for now).

April 2012

Andrew Dienstfrey
Ronald F. Boisvert

Organization

The IFIP Working Conference on Uncertainty Quantification in Scientific Computing was organized by the US National Institute of Standards and Technology (NIST) on behalf of the International Federation for Information Processing (IFIP) Working Group 2.5 on Numerical Software, in cooperation with the Society for Industrial and Applied Mathematics (SIAM).

Organizing Committee

Ronald F. Boisvert	NIST, USA, *Chair*
Andrew Dienstfrey	NIST, USA
James C.T. Pool	CalTech, USA (retired)

Program Committee

Andrew Dienstfrey	NIST, USA, *Chair*
Ronald F. Boisvert	NIST, USA
Maurice Cox	National Physical Laboratory, UK
Bo Einarsson	Linköping University, Sweden (retired)
Brian Ford	Numerical Algorithms Group Ltd., UK (retired)
James (Mac) Hyman	Tulane University, US, SIAM Representative
William L. Oberkampf	W.L. Oberkampf Consulting, USA
Tony O'Hagan	University of Sheffield, UK
Michael Oberguggenberger	University of Innsbruck, Austria

Program

The IFIP Working Conference on Uncertainty Quantification in Scientific Computing was held in Boulder, Colorado, USA on August 1–4, 2011.

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: UQ Need: Risk, Policy, and Decision Making (Part 1)
Chair: Andrew Dienstfrey, NIST, US
Discussant: Bo Einarsson, Linköping University, SE

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

Session II: UQ 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, W.L. Oberkampf Consulting, US
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 Reception

Tuesday August 2

Session III: UQ Theory (Part 1)
Chair: Richard Hanson, Rogue Wave Software, US
Discussant: Peter Tang, The D.E. Shaw Group, US

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

Session IV: UQ 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 Universitt Braunschweig, Germany
15:00 Break

Hot Topics Session
Moderator: Brian Ford, NAG Ltd., UK

1. UQ for Life Cycle Assessment Indicators
Mark Campanelli, NIST, US

2. Assessing Uncertainties in Prediction of Models Validated using Experimental Data Distantly Related to Systems of Interest
   William Oberkampf, W.L. Oberkampf Consulting, and Wayne King, Lawrence Livermore National Laboratory
3. For UQ: What Software Tools, What Computing Languages, etc. are Required?
   Richard Hanson, Rogue Wave, US
4. Expert Elicitation
   Anthony O'Hagan, Sheffield University, UK
5. Software Security Attacks and Security Failures
   Mladen Vouk, North Carolina State University, US
6. What Hinders the Enjoyment of Interval Arithmetic by its Potential Beneficiaries
   William Kahan (University of California at Berkeley)
7. Choosing Between Suspects — Availability of the Human Mind to Handle Information
   Mladen Vouk, North Carolina State University, US

Wednesday August 3

Session V: UQ Tools
Chair: Bo Einarsson, Linkóping 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
13:00 Tour of NIST and NOAA Laboratories
17:15 Reception and Banquet (Chautauqua Dining Hall)

Thursday August 4

Session VI: UQ 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

Session VII: UQ Theory (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

Participants

Ron Bates	Rolls-Royce PLC	UK
Ronald Boisvert	NIST	USA
Mark Campanelli	NIST	USA
Peter Challenor	National Oceanography Centre	UK
Kevin Coakley	NIST	USA
Ronald Cools	Katholieke Universiteit Leuven	BE
Maurice Cox	National Physical Laboratory	UK
Mark Cunningham	Nuclear Regulatory Commission	USA
Andrew Dienstfrey	NIST	USA
Alireza Doostan	University of Colorado Boulder	USA
Bo Einarsson	Linköping University	SE
Michael Eldred	Sandia National Laboratories	USA
Ryan Elmore	National Renewable Energy Lab	USA
Wayne Enright	University of Toronto	CA
Jonathan Feinberg	Simula Research Laboratory	NO
Scott Ferson	Applied Biomathematics	USA
Jeffrey Fong	NIST	USA
Brian Ford	NAG/University of Oxford	UK
Patrick Gaffney	Bergen Software Services International AS	NO
Wilfried Gansterer	University of Vienna	AT
James Gattiker	Los Alamos National Laboratory	USA
James Glimm	Stony Brook University	USA
Michael Goldstein	Durham University	UK
John Hagedorn	NIST	USA
Richard Hanson	Rogue Wave	USA
Leslie Hatton	Kingston University, London	UK
Jon Helton	Arizona State University	USA
Michael Heroux	Sandia National Laboratories	USA
Kyle Hickmann	Tulane University	USA
Charles Hogg	NIST	USA
Tim Hopkins	University of Kent	UK
Shang-Rou (Henry) Hsieh	Lawrence Livermore National Laboratory	USA
Mac Hyman	Tulane University	USA
Ruth Jacobsen	NIST /University of Maryland	USA
Chris Johnson	University of Utah	USA
Russell Johnson	NIST	USA
Raghu Kacker	NIST	USA
William Kahan	University of California at Berkeley	USA
Shigeo Kawata	Utsunomiya University	JP
Peter Ketcham	NIST	USA

Wayne King	Lawrence Livermore National Laboratory	USA
Emanuel Knill	NIST	USA
Ulrich Kulisch	Universität Karlsruhe	DE
Sandy Landsberg	Department of Energy	USA
Eric Machorro	Nevada National Security Site	USA
Hermann G. Matthies	Technische Universität Braunschweig	DE
Ian Mitchell	University of British Columbia	CA
Felipe Montes	USDA Agricultural Research Service	USA
Rafi Muhanna	Georgia Institute of Technology	USA
Katherine Mullen	NIST	USA
Douglas Nychka	National Center for Atmospheric Research	USA
Abbie O'Gallagher	NIST	USA
Anthony O'Hagan	University of Sheffield	UK
William Oberkampf	W.L. Oberkampf Consulting	USA
Michal Odyniec	National Security Technologies	USA
Alberto Pasanisi	Électricité de France R&D	FR
Pasky Pascual	U.S. Environmental Protection Agency	USA
Adele Peskin	NIST	USA
Antonio Possolo	NIST	USA
John Reid	JKR Associates	UK
John Rice	Purdue University	USA
Adrian Sandu	Virginia Tech	USA
Jennifer Scott	Rutherford Appleton Laboratory	UK
David Sheen	NIST	USA
Brian Smith	Numerica 21 Inc.	USA
William Van Snyder	NASA Jet Propulsion Laboratory	USA
Jolene Splett	NIST	USA
Philip Starhill	IBM	USA
Ping Tak Peter Tang	Intel Corporation	USA
Judith Terrill	NIST	USA
Michael Thuné	Uppsala University	SE
Mladen Vouk	North Carolina State University	USA
William Wallace	NIST	USA
Jack C.M. Wang	NIST	USA
William Welch	University of British Columbia	CA
Larry Winter	University of Arizona	USA

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