

# Preface

Computational Science is the scientific discipline that aims at the development and understanding of new computational methods and techniques to model and simulate complex systems.

The area of application includes natural systems – such as biology, environmental and geo-sciences, physics, and chemistry – and synthetic systems such as electronics and financial and economic systems. The discipline is a bridge between ‘classical’ computer science – logic, complexity, architecture, algorithms – mathematics, and the use of computers in the aforementioned areas.

The relevance for society stems from the numerous challenges that exist in the various science and engineering disciplines, which can be tackled by advances made in this field. For instance new models and methods to study environmental issues like the quality of air, water, and soil, and weather and climate predictions through simulations, as well as the simulation-supported development of cars, airplanes, and medical and transport systems etc.

Paraphrasing R. Kenway (R.D. Kenway, Contemporary Physics. 1994): ‘There is an important message to scientists, politicians, and industrialists: in the future science, the best industrial design and manufacture, the greatest medical progress, and the most accurate environmental monitoring and forecasting will be done by countries that most rapidly exploit the full potential of *computational science*’.

Nowadays we have access to high-end computer architectures and a large range of computing environments, mainly as a consequence of the enormous stimulus from the various international programs on advanced computing, e.g. HPCC (USA), HPCN (Europe), Real-World Computing (Japan), and ASCI (USA: Advanced Strategic Computing Initiative). The sequel to this, known as ‘grid-systems’ and ‘grid-computing’, will boost the computer, processing, and storage power even further. Today’s supercomputing application may be tomorrow’s desktop computing application.

The societal and industrial pulls have given a significant impulse to the rewriting of existing models and software. This has resulted among other things in a big ‘clean-up’ of often outdated software and new programming paradigms and verification techniques. With this make-up of arrears the road is paved for the study of real complex systems through computer simulations, and large scale problems that have long been intractable can now be tackled. However, the development of complexity reducing algorithms, numerical algorithms for large data sets, formal methods and associated modeling, as well as representation (i.e. visualization) techniques are still in their infancy. Deep understanding of the approaches required to model and simulate problems with increasing complexity and to efficiently exploit high performance computational techniques is still a big scientific challenge.

The International Conference on Computational Science (ICCS) series of conferences was started in May 2001 in San Francisco. The success of that meeting motivated the organization of the meeting held in Amsterdam from April 21–24, 2002.

These three volumes (Lecture Notes in Computer Science volumes 2329, 2330, and 2321) contain the proceedings of the ICCS 2002 meeting. The volumes consist of over 350 – peer reviewed – contributed and invited papers presented at the conference in the Science and Technology Center Watergraafsmeer (WTCW), in Amsterdam. The papers presented reflect the aims of the program committee to bring together major role players in the emerging field of computational science.

The conference was organized by The University of Amsterdam, Section Computational Science (<http://www.science.uva.nl/research/scs/>), SHARCNET, Canada (<http://www.sharcnet.com>), and the Innovative Computing Laboratory at The University of Tennessee.

The conference included 22 workshops, 7 keynote addresses, and over 350 contributed papers selected for oral presentation. Each paper was refereed by at least two referees.

We are deeply indebted to the members of the program committee, the workshop organizers, and all those in the community who helped us to organize a successful conference. Special thanks go to Alexander Bogdanov, Jerzy Wasniewski, and Marian Bubak for their help in the final phases of the review process. The invaluable administrative support of Manfred Stienstra, Alain Dankers, and Erik Hitipeuw is also acknowledged. Lodewijk Bos and his team were responsible for the local logistics and as always did a great job.

ICCS 2002 would not have been possible without the support of our sponsors: The University of Amsterdam, The Netherlands; Power Computing and Communication BV, The Netherlands; Elsevier Science Publishers, The Netherlands; Springer-Verlag, Germany; HPCN Foundation, The Netherlands; National Supercomputer Facilities (NCF), The Netherlands; Sun Microsystems, Inc., USA; SHARCNET, Canada; The Department of Computer Science, University of Calgary, Canada; and The School of Computer Science, The Queens University, Belfast, UK.

Amsterdam, April 2002

Peter M.A. Sloot,  
Scientific Chair 2002,

on behalf of the co-editors:  
C.J. Kenneth Tan  
Jack J. Dongarra  
Alfons G. Hoekstra

# Organization

The 2002 International Conference on Computational Science was organized jointly by The University of Amsterdam, Section Computational Science, SHARCNET, Canada, and the University of Tennessee, Department of Computer Science.

## Conference Chairs

Peter M.A. Sloot, Scientific and Overall Chair ICCS 2002 (University of Amsterdam, The Netherlands)

C.J. Kenneth Tan (SHARCNET, Canada)

Jack J. Dongarra (University of Tennessee, Knoxville, USA)

## Workshops Organizing Chair

Alfons G. Hoekstra (University of Amsterdam, The Netherlands)

## International Steering Committee

Vassil N. Alexandrov (University of Reading, UK)

J. A. Rod Blais (University of Calgary, Canada)

Alexander V. Bogdanov (Institute for High Performance Computing and Data Bases, Russia)

Marian Bubak (AGH, Poland)

Geoffrey Fox (Florida State University, USA)

Marina L. Gavrilova (University of Calgary, Canada)

Bob Hertzberger (University of Amsterdam, The Netherlands)

Anthony Hey (University of Southampton, UK)

Benjoe A. Juliano (California State University at Chico, USA)

James S. Pascoe (University of Reading, UK)

Rene S. Renner (California State University at Chico, USA)

Kokichi Sugihara (University of Tokyo, Japan)

Jerzy Wasniewski (Danish Computing Center for Research and Education, Denmark)

Albert Zomaya (University of Western Australia, Australia)

## **Local Organizing Committee**

Alfons Hoekstra (University of Amsterdam, The Netherlands)

Alexander V. Bogdanov (Institute for High Performance Computing and Data Bases, Russia)

Marian Bubak (AGH, Poland)

Jerzy Wasniewski (Danish Computing Center for Research and Education, Denmark)

## **Local Advisory Committee**

Patrick Aerts (National Computing Facilities (NCF), The Netherlands Organization for Scientific Research (NWO), The Netherlands)

Jos Engelen (NIKHEF, The Netherlands)

Daan Frenkel (Amolf, The Netherlands)

Walter Hoogland (University of Amsterdam, The Netherlands)

Anwar Osseyran (SARA, The Netherlands)

Rik Maes (Faculty of Economics, University of Amsterdam, The Netherlands)

Gerard van Oortmerssen (CWI, The Netherlands)

## **Program Committee**

Vassil N. Alexandrov (University of Reading, UK)

Hamid Arabnia (University of Georgia, USA)

J. A. Rod Blais (University of Calgary, Canada)

Alexander V. Bogdanov (Institute for High Performance Computing and Data Bases, Russia)

Marian Bubak (AGH, Poland)

Toni Cortes (University of Catalonia, Barcelona, Spain)

Brian J. d'Auriol (University of Texas at El Paso, USA)

Clint Dawson (University of Texas at Austin, USA)

Geoffrey Fox (Florida State University, USA)

Marina L. Gavrilova (University of Calgary, Canada)

James Glimm (SUNY Stony Brook, USA)

Paul Gray (University of Northern Iowa, USA)

Piet Hemker (CWI, The Netherlands)

Bob Hertzberger (University of Amsterdam, The Netherlands)

Chris Johnson (University of Utah, USA)

Dieter Kranzlmüller (Johannes Kepler University of Linz, Austria)

Antonio Lagana (University of Perugia, Italy)

Michael Mascagni (Florida State University, USA)

Jiri Nedoma (Academy of Sciences of the Czech Republic, Czech Republic)

Roman Neruda (Academy of Sciences of the Czech Republic, Czech Republic)

Jose M. Laginha M. Palma (University of Porto, Portugal)

James Pascoe (University of Reading, UK)  
 Ron Perrott (The Queen's University of Belfast, UK)  
 Andy Pimentel (The University of Amsterdam, The Netherlands)  
 William R. Pulleyblank (IBM T. J. Watson Research Center, USA)  
 Rene S. Renner (California State University at Chico, USA)  
 Laura A. Salter (University of New Mexico, USA)  
 Dale Shires (Army Research Laboratory, USA)  
 Vaidy Sunderam (Emory University, USA)  
 Jesus Vigo-Aguiar (University of Salamanca, Spain)  
 Koichi Wada (University of Tsukuba, Japan)  
 Jerzy Wasniewski (Danish Computing Center for Research and Education, Denmark)  
 Roy Williams (California Institute of Technology, USA)  
 Elena Zudilova (Corning Scientific, Russia)

## Workshop Organizers

### Computer Graphics and Geometric Modeling

Andres Iglesias (University of Cantabria, Spain)

### Modern Numerical Algorithms

Jerzy Wasniewski (Danish Computing Center for Research and Education, Denmark)

### Network Support and Services for Computational Grids

C. Pham (University of Lyon, France)  
 N. Rao (Oak Ridge National Labs, USA)

### Stochastic Computation: From Parallel Random Number Generators to Monte Carlo Simulation and Applications

Vasil Alexandrov (University of Reading, UK)  
 Michael Mascagni (Florida State University, USA)

### Global and Collaborative Computing

James Pascoe (The University of Reading, UK)  
 Peter Kacsuk (MTA SZTAKI, Hungary)  
 Vassil Alexandrov (The University of Reading, UK)  
 Vaidy Sunderam (Emory University, USA)  
 Roger Loader (The University of Reading, UK)

### Climate Systems Modeling

J. Taylor (Argonne National Laboratory, USA)

### Parallel Computational Mechanics for Complex Systems

Mark Cross (University of Greenwich, UK)

### Tools for Program Development and Analysis

Dieter Kranzlmüller (Joh. Kepler University of Linz, Austria)  
 Jens Volkert (Joh. Kepler University of Linz, Austria)

### 3G Medicine

Andy Marsh (VMW Solutions Ltd, UK)  
 Andreas Lymberis (European Commission, Belgium)  
 Ad Emmen (Genias Benelux bv, The Netherlands)

**Automatic Differentiation and Applications**

H. Martin Buecker (Aachen University of Technology, Germany)  
Christian H. Bischof (Aachen University of Technology, Germany)

**Computational Geometry and Applications**

Marina Gavrilova (University of Calgary, Canada)

**Computing in Medicine**

Hans Reiber (Leiden University Medical Center, The Netherlands)  
Rosemary Renaut (Arizona State University, USA)

**High Performance Computing in Particle Accelerator Science and Technology**

Andreas Adelman (Paul Scherrer Institute, Switzerland)  
Robert D. Ryne (Lawrence Berkeley National Laboratory, USA)

**Geometric Numerical Algorithms: Theoretical Aspects and Applications**

Nicoletta Del Buono (University of Bari, Italy)  
Tiziano Politi (Politecnico-Bari, Italy)

**Soft Computing: Systems and Applications**

Renee Renner (California State University, USA)

**PDE Software**

Hans Petter Langtangen (University of Oslo, Norway)  
Christoph Pflaum (University of Würzburg, Germany)  
Ulrich Ruede (University of Erlangen-Nürnberg, Germany)  
Stefan Turek (University of Dortmund, Germany)

**Numerical Models in Geomechanics**

R. Blaheta (Academy of Science, Czech Republic)  
J. Nedoma (Academy of Science, Czech Republic)

**Education in Computational Sciences**

Rosie Renaut (Arizona State University, USA)

**Computational Chemistry and Molecular Dynamics**

Antonio Lagana (University of Perugia, Italy)

**Geocomputation and Evolutionary Computation**

Yong Xue (CAS, UK)  
Narayana Jayaram (University of North London, UK)

**Modeling and Simulation in Supercomputing and Telecommunications**

Youngsong Mun (Korea)

**Determinism, Randomness, Irreversibility, and Predictability**

Guenri E. Norman (Russian Academy of Sciences, Russia)  
Alexander V. Bogdanov (Institute of High Performance Computing and Information Systems, Russia)  
Harald A. Pasch (University of Vienna, Austria)  
Konstantin Korotenko (Shirshov Institute of Oceanology, Russia)

## **Sponsoring Organizations**

The University of Amsterdam, The Netherlands  
Power Computing and Communication BV, The Netherlands  
Elsevier Science Publishers, The Netherlands  
Springer-Verlag, Germany  
HPCN Foundation, The Netherlands  
National Supercomputer Facilities (NCF), The Netherlands  
Sun Microsystems, Inc., USA  
SHARCNET, Canada  
Department of Computer Science, University of Calgary, Canada  
School of Computer Science, The Queens University, Belfast, UK.

## **Local Organization and Logistics**

Lodewijk Bos, MC-Consultancy  
Jeanine Mulders, Registration Office, LGCE  
Alain Dankers, University of Amsterdam  
Manfred Stienstra, University of Amsterdam

Computational Science — ICCS 2002

International Conference Amsterdam, The Netherlands,

April 21–24, 2002 Proceedings, Part III

Sloot, P.M.A.; Tan, C.J.K.; Dongarra, J.J.; Hoekstra, A.G.

(Eds.)

2002, LXXXII, 1230 p. 757 illus. In 2 volumes, not

available separately., Softcover

ISBN: 978-3-540-43594-5