

ICCS 2011 program booklet

The information in this booklet was frozen on May 23, later changes are not included

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Committees

Organisers

The Conference Chairs

Conference Co-chairs

Workshop Chair

Scientific Chair

Scientific Co-chair

Mitsuhisa Sato
Satoshi Matsuoka
Dick van Albada
Peter Sloot
Jack Dongarra

University of Tsukuba, Japan
Tokyo Inst. of Technology, Japan
University of Amsterdam, The Netherlands
University of Amsterdam, The Netherlands
University of Tennessee, USA

Local organising committee in Tsukuba

Honorable Organising committee Chair

Organising committee Vice-Chairs

Finance Chair

Local Arrangement Chair

Publicity Chair

Kimihiko Hira
Taisuke Boku
Kengo Nakajima
Takahiro Katagiri
Hiroto Tadano
Tasuku Hiraishi

Riken, Japan
University of Tsukuba, Japan
The University of Tokyo, Japan
The University of Tokyo, Japan
University of Tsukuba, Japan
Kyoto University, Japan

Local organising committee at NTU Singapore

Steve Turner
Michael Lees

Program Committee

D. Abramson *Monash University, Australia*
M. Aldinucci *University of Torino, Italy*
V.N. Alexandrov *Barcelona Supercomputing Center, Spain*
G.D. Allen *Louisiana State University, USA*
M. Antolovich *Charles Sturt University, Australia*
T. Aoki *Tokyo Inst of Technology, Japan*
D.A. Bader *Georgia Institute of Technology, USA*
E. Bagheri *University of Athabasca, Canada*
B. Balis *AGH University of Science and Technology, Krakow, Poland*
P.K. Baruah *Sri Sathya Sai University, Prasanthinilayam, India*
R.G. Belleman *University of Amsterdam, The Netherlands*
A.S.Z. Belloum *University of Amsterdam, The Netherlands*
J. Berthold *University of Copenhagen, Denmark*
I. Bethke *University of Amsterdam, The Netherlands*
A.V. Bogdanov *Institute for High-performance Computing and Information Systems, St. Petersburg, Russia*
M. Bubak *AGH Krakow PL and Universiteit van Amsterdam NL*
K. Bubendorfer *Victoria University of Wellington, New Zealand*
Q.C. Bui *University of Amsterdam, The Netherlands*
J. Buisson *UEB, Ecoles de St-Cyr Coetquidan, VALORIA, France*
J. Chen *Swinburne University of Technology, Australia*
J.C. Cunha *Univ. Nova de Lisboa, Portugal*
S. Date *Osaka University, Japan*
M. Dayde *CNRS, France*
D. Deschrijver *Ghent University, Belgium*
T. Dhaene *Ghent University, Belgium*
I.T. Dimov *IPP, Bulgarian Academy of Sciences*
J. Dongarra *University of Tennessee, USA*
J. Du The *University of Utah, USA*
V. Duarte *Universidade Nova de Lisboa, Portugal*
W. Dzwiniel *AGH University of Science and Technology, Krakow, Poland*
N. Emad *University of Versailles, France*
K. Emoto *University of Tokyo, Japan*
G. Ertaylan *University of Amsterdam, The Netherlands*
G. Fox *Indiana University, USA*
W. Funika *AGH University of Science and Technology, Krakow, Poland*
F. Gava *University Paris-East, France*
A. Gerbessiotis *NJIT, USA*

R.S.M. *Goh Institute of High Performance Computing, Singapore*
Y. Gorbachev *Geolink Systems LLC, Russia*
G.A. Gravvanis *Democritus University of Thrace, Greece*
C. Grelck *University of Amsterdam, The Netherlands*
T. Gubala *ACC CYFRONET AGH, Krakow, Poland*
M. Hardt *KIT, Germany*
A.G. Hoekstra *University of Amsterdam, The Netherlands*
H. Iwasaki *The University of Electro-communications, Japan*
T. Iwashita *Kyoto University, Japan*
H. Jin *Huazhong University of Science and Technology, China*
D. Johnson *University of Oxford, UK*
H. Kaiser *Louisiana State University, USA*
B.D. Kandhai *University of Amsterdam, The Netherlands*
T. Katagiri *University of Tokyo, Japan*
W.A. Kelly *Queensland University of Technology, Australia*
M. Koda *University of Tsukuba Japan*
S.V. Kovalchuk *ITMO, Russia*
B. Kryza *Academic Computer Centre CYFRONET-AGH, Krakow, Poland*
A.V. Larchenkov *ITMO, Russia*
R. Leshchinskiy *Standard Chartered Bank, UK*
A. Lewis *Griffith University, Australia*
F. Liu *DOE Ames Laboratory, USA*
E. Lorenz *University of Amsterdam, The Netherlands*
F. Loulergue *University of Orleans, France*
P. Lu *University of Alberta, Canada*
M. Malawski *Institute of Computer Science AGH, Poland*
M. Mascagni *Florida State University, USA*
K. Nakajima *University of Tokyo, Japan*
S. Naqvi *CETIC, Belgium*
L. Naumov *University of Amsterdam, The Netherlands*
P.O.A. Navaux *Universidade Federal do Rio Grande do Sul, Brazil*
Z. Németh *MTA SZTAKI Computer and Automation Research Institute, Hungary*
M. Paprzycki *IBS PAN and WSM, Poland*
S. Petiton *LIFL, France*
R. Quax *University of Amsterdam, The Netherlands*
M.R. Radecki *ACK CYFRONET AGH, Poland*
B. Raffin *INRIA, France*
A. Rendell *Dept Computer Science, Australian National University*
C. Ribbens *Virginia Tech, USA*
M. Riedel *Research Centre Jülich, Germany*
D. Rodríguez *García University of Alcalá, Spain*
K. Rycerz *AGH University of Science and Technology, Krakow, Poland*
M. Sato *University of Tsukuba, Japan*
H. Sato *Tokyo Institute of Technology, Japan*
M. Sekijima *Tokyo Inst of Technology, Japan*
P.M.A. Sloot *University of Amsterdam, The Netherlands*
R. Slota AGH *University of Science and Technology, Krakow, Poland*
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A. Streit *Karlsruher Institut für Technologie, Germany*
H. Sun Beihang *University, China*
R. Tadeusiewicz *AGH University of Science and Technology, Krakow, Poland*
D. Takahashi *University of Tsukuba, Japan*
C. Tedeschi *University of Rennes 1 - INRIA, France*
P. Tvrđik *Czech Technical University Prague*
S.J. van Albada *Forschungszentrum Jülich, Germany*
G.D. van Albada *University of Amsterdam, The Netherlands*
D.W. Walker *Cardiff University, UK*
K. Walkowiak *Wroclaw University of Technology, Poland*
C.L. Wang *University of Hong Kong, China*
C.T. Yang *Department of Computer Science, Tunghai University, Taiwan*
N. Zarrabi *University of Amsterdam, The Netherlands*

Program at a Glance

Wednesday, 01 June

	8:00	9:00	10:00	11:00	12:00	13:00	14:00	15:00	16:00	17:00	18:00	19:00	20:00	21:00	22:00
Lobby	8:30 - 17:00 Registration														
Audrium		9:30-10:15 Keynote3	10:00-10:45 Keynote1	11:05 - 12:45 W31a			13:45-14:30 Keynote2	14:40 - 16:20 W31b			16:40 - 18:20 W31c				
Large BO Room 1				11:05 - 12:45 M01				14:40 - 16:20 M02			16:40 - 18:20 M05				
Large BO Room 2				11:05 - 12:45 W05a				14:40 - 16:20 W05b			16:40 - 18:20 W13a				
Large BO Room 3				11:05 - 12:45 W17a				14:40 - 16:20 M04			16:40 - 18:20 M03				
Large BO Room 4				11:05 - 12:45 W18a				14:40 - 16:20 W18b			16:40 - 18:20 W18c				
Lecture Room 5				11:05 - 12:45 W02a				14:40 - 16:20 W02b			16:40 - 18:20 W02c				
Lecture Room 6				11:05 - 12:45 W27a				14:40 - 16:20 W27b			16:40 - 18:20 W22a				
Lecture Room 2				11:05 - 12:45 W33a				14:40 - 16:20 W33b			16:40 - 18:20 W33c				
Lobby															
Social Event etc.							12:45 - 13:45 Lunch								19:45 - 22:30 Reception Halla Restaurant in the Botanical Gardens

Thursday, 02 June

	8:00	9:00	10:00	11:00	12:00	13:00	14:00	15:00	16:00	17:00	18:00	19:00	20:00	21:00	22:00
Lobby	9:00 - 13:30 Registration														
Audrium		9:30-10:15 Keynote3	10:35 - 12:15 W31d			13:35-14:20 Keynote4	14:30 - 16:10 W31e			16:30 - 18:10 W31f					
Large BO Room 1			10:35 - 12:15 M06				14:30 - 16:10 M07			16:30 - 18:10 M08					
Large BO Room 2			10:35 - 12:15 W13b				14:30 - 16:10 W06a			16:30 - 18:10 W06b					
Large BO Room 3			10:35 - 12:15 W28a				14:30 - 16:10 W15a			16:30 - 18:10 W15b					
Large BO Room 4			10:35 - 12:15 W21a				14:30 - 16:10 W21b/ W23a			16:30 - 18:10 W16a					
Lecture Room 5			10:35 - 12:15 W11a				14:30 - 16:10 W11b			16:30 - 18:10 W09a					
Lecture Room 6			10:35 - 12:15 W22b				14:30 - 16:10 W10a			16:30 - 18:10 W10b					
Lecture Room 2			10:35 - 12:15 W33d				14:30 - 16:10 W03a			16:30 - 18:10 W03b					
Lobby		9:30 - 10:30 Poster Set-Up	Poster			12:15 - 13:35 W34a	Poster								
Social Event etc.						12:15 - 13:35 Lunch									19:45 - 22:30 Banquet IndoChine Waterfront Restaurant

Friday, 03 June

	8:00	9:00	10:00	11:00	12:00	13:00	14:00	15:00
Lobby		9:00 - 13:30 Registration						
Audtrium		09:30 - 11:10 M09		11:30- 12:15 Keynote5				
Large BO Room 1		09:30 - 11:10 M11						
Large BO Room 2		09:30 - 11:10 W08a				13:15 - 14:55 W08b		
Large BO Room 3		09:30 - 11:10 M10						
Large BO Room 4		09:30 - 11:10 W16b						
Lecture Room 5		09:30 - 11:10 W09b				13:15 - 14:55 W09c		
Lecture Room 6		09:30 - 11:10 W29a				13:15 - 14:55 W29b		
Lecture Room 2		09:30 - 11:10 W01a						
Lobby		9:30 - 13:30 Poster Removal						
Social Event etc.					12:15 - 13:15 Lunch			

Conference Information

Operating Hours of Registration Desk

Wed, 01 June 8:30- 17:00
Thu, 02 June 9:00- 13:30
Fri, 03 June 9:00- 13:30

Conference materials, name badges will be distributed at the Registration Desk.

Conference Name badge

Conference name badges must be worn at all times while participants are in conference venue. The badge will serve as your admission to all sessions and official functions.

Message Board

Any program changes or urgent announcements from the secretariat and private messages will be posted on the message board in the registration area. Please check the message board occasionally.

Social Program

•Welcome Reception

Date: Wed, 01 June 19:45-22:30

Venue: Halia Restaurant in the Botanical Gardens

*Shuttle Bus will be provided from Nanyang Executive Centre (NEC) to the restaurant. If you join the Reception, please be at the entrance at 18:20 with the ticket.

•Banquet

Date: Tue, 02 June 19:45-22:30

Venue: IndoChine Waterfront Restaurant

*Shuttle Bus will be provided from NEC to the restaurant. If you join the Banquet, please come the entrance at 18:10 with the ticket.

Instruction for Speakers

The allocation of time

Keynote lecture: 45 minutes

Oral Presentation: 20 minutes

Short Presentation: 10 minutes

Instruction for Poster Session (W34a)

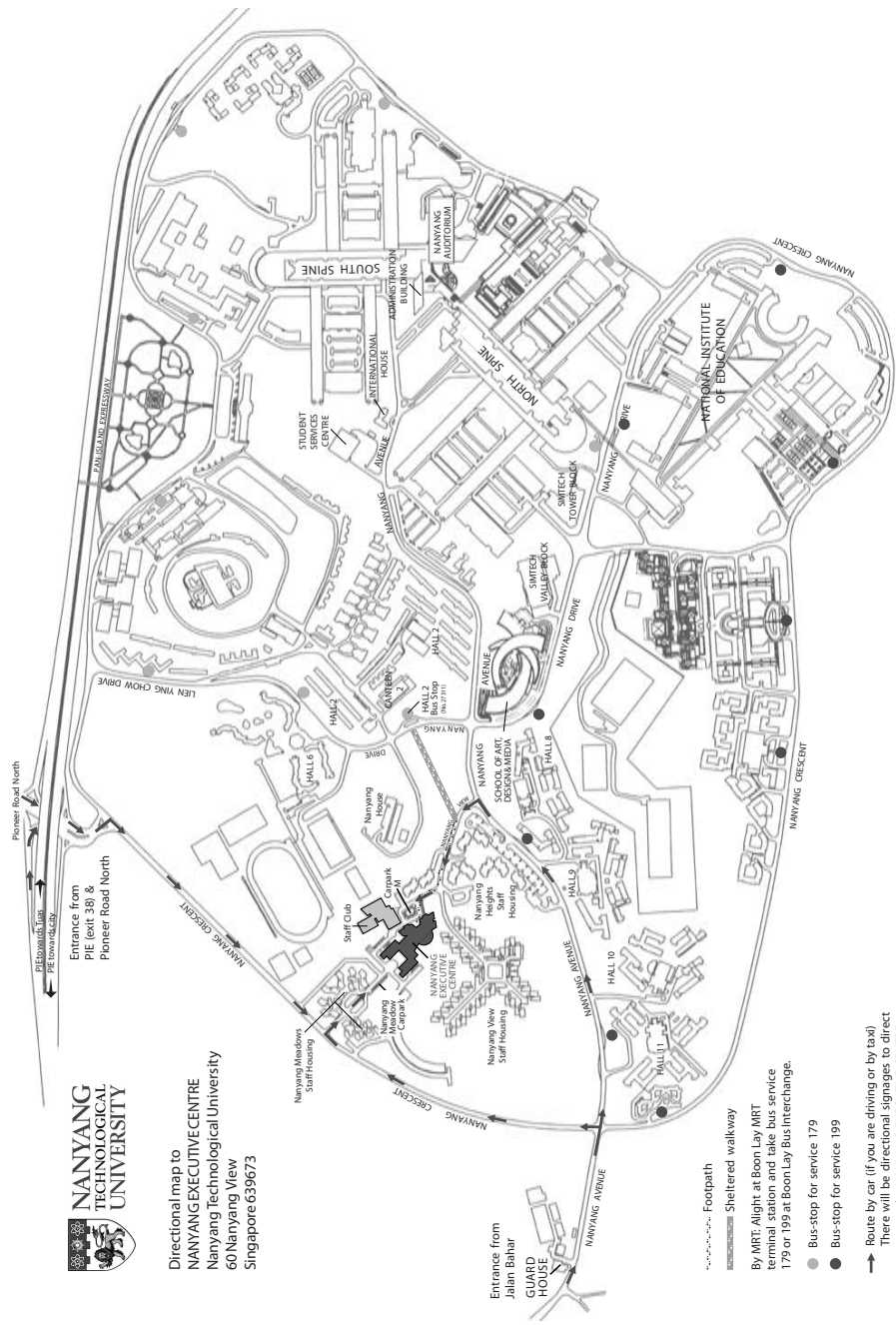
The poster presentation will take place in the 1st floor Lobby. The size of one poster board is A0 size. Posters should be displayed on the boards using pushpins that will be available from the organizers. No other adhesive method is permitted on the boards.

Presenters are asked to place their materials on the place assigned by the secretariat on the following schedule:

Set-up	Thu, 02 June	9:30-10:35
Core Time	Thu, 02 June	12:15-13:35
Removal	Fri, 03 June	9:30-13:30

During the core-time, presenters will be expected to be present in front of their posters to answer questions. Presenters are responsible for setting up and removing their exhibits. The secretariat will not be responsible for any loss after removal time.

Map



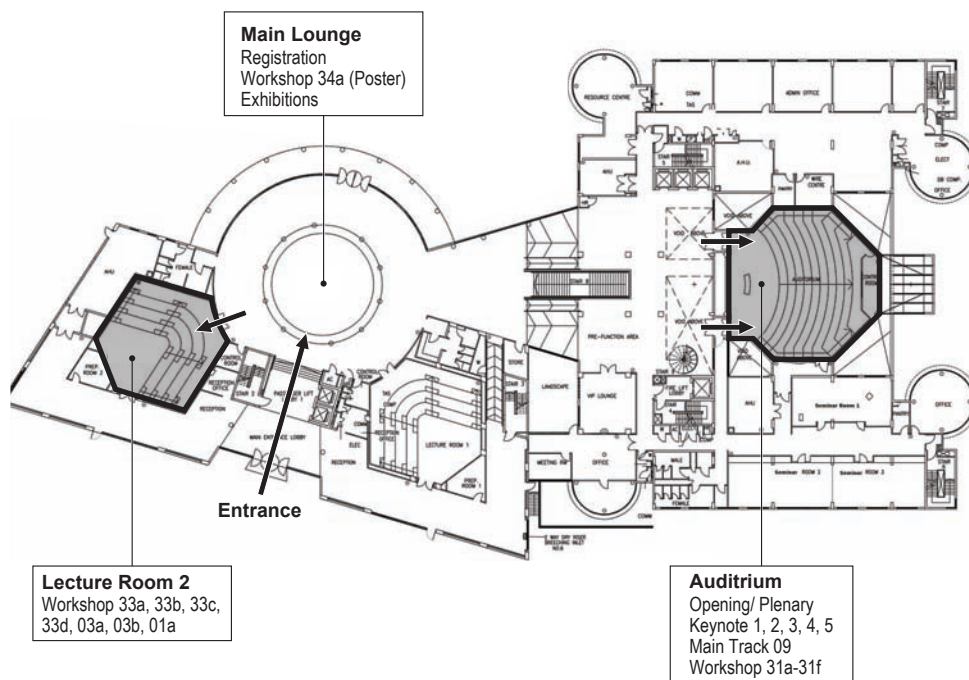
Directional map to
NANYANG EXECUTIVE CENTRE
 Nanyang Technological University
 60 Nanyang View
 Singapore 639673

- Footpath
- Sheltered walkway
- By MRT: Alight at Boon Lay MRT terminal station and take bus service 179 or 199 at Boon Lay Bus Interchange.
- Bus-stop for service 179
- Bus-stop for service 199
- Route by car (if you are driving or by taxi)
 There will be directional signages to direct you to the NANYANG EXECUTIVE CENTRE

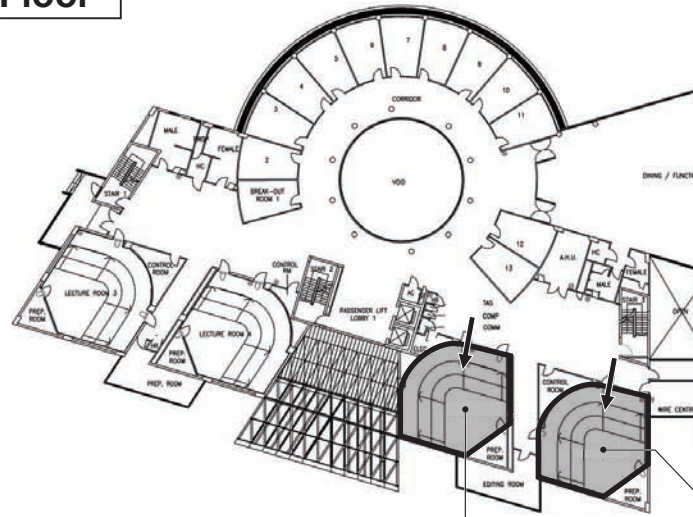
Floor Plan

Nanyang Executive Centre

2nd Floor (Ground Floor)



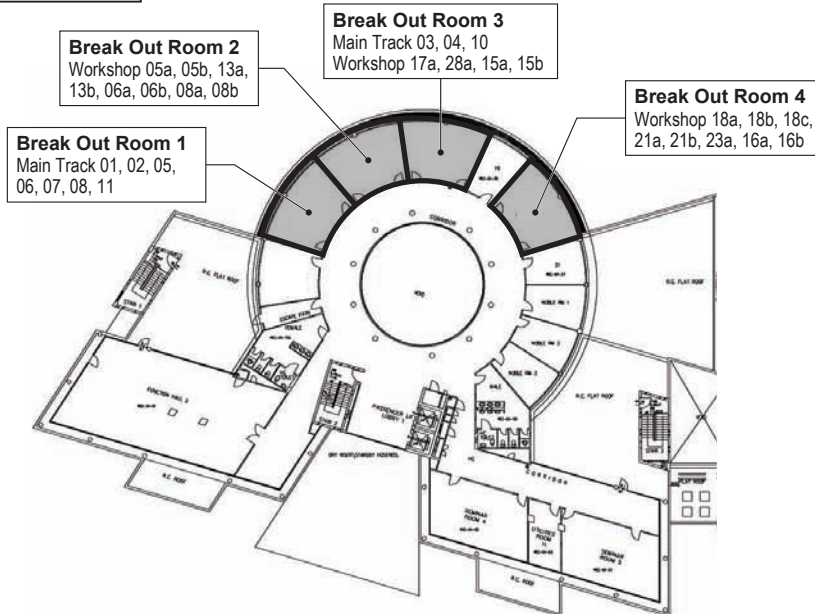
3rd Floor



Lecture Room 5
Workshop 02a, 02b, 02c,
11a, 11b, 09a, 09b, 09c

Lecture Room 6
Workshop 27a, 27b, 22a,
22b, 10a, 10b, 29a, 29b

4th Floor



Break Out Room 1
Main Track 01, 02, 05,
06, 07, 08, 11

Break Out Room 2
Workshop 05a, 05b, 13a,
13b, 06a, 06b, 08a, 08b

Break Out Room 3
Main Track 03, 04, 10
Workshop 17a, 28a, 15a, 15b

Break Out Room 4
Workshop 18a, 18b, 18c,
21a, 21b, 23a, 16a, 16b

Plenary Program

Keynote 1

Room: Auditorium
Date: Wed, 01 June 10:00 - 10:45

Computational Materials Science & Geometry: geometrical principles and microstructure evolution

Prof. David Srolovitz (*Institute of High-Performance Computing, National University of Singapore*)

Keynote 2

Room: Auditorium
Date: Wed, 01 June 13:45 - 14:30

TBA

Prof. Chris Barret (*Virginia Tech*)

Keynote 3

Room: Auditorium
Date: Thu, 02 June 09:30 - 10:15

The Well-tempered Ensemble

Prof. Michele Parrinello (*ETH Zürich*)

Keynote 4

Room: Auditorium
Date: Thu, 02 June 13:35 - 14:20

Exascale, Tablet, and Smartphone: As Energy limits Redefine Computers, how can Computational Science Benefit?

Prof. Andrew Chien (*Intel Research and University of California, San Diego*)

Keynote 5

Room: Auditorium
Date: Fri, 03 June 11:30 - 12:15

Building up Quantum Universe through Computation

Prof. Akira Ukawa (*Center for Computational Sciences and Institute of Physics, University of Tsukuba*)

Main Track

M01

Wed, 01 Jun 2011, 11:05 - 12:45 Room: Break Out 1

1. **A Practical Tree Contraction Algorithm for Parallel Skeletons on Trees of Unbounded Degree**
Author(s): A. Morihata, K. Matsuzaki
Presenter: A. Morihata, Tohoku University
2. **A measure of the local connectivity between graph vertices**
Author(s): I. Safro, J. Chen
Presenter: S.H.K. Narayanan, Argonne National Laboratory
3. **Simplifying and Improving Ant-based Clustering**
Author(s): S.C. Tan, K.M. Ting, S.W. Teng
Presenter: S.C. Tan, SIM University
4. **Improving Scalability Using Hybrid Asynchronous Methods For Non-Hermitian Eigenproblems**
Author(s): J.D. Dubois, C.C. Calvin, S.P. Petiton
Presenter: J.D. Dubois, Commissariat a l'energie atomique
5. **Dense Triangular Solvers on Multicore Clusters using UPC**
Author(s): J. González-Domínguez, M.J. Martín, G.L. Taboada, J. Touriño
Presenter: J. González-Domínguez, Computer Architecture Group, Department of Electronics and Systems, University of A Coruña, Spain

M02

Wed, 01 Jun 2011, 14:40 - 16:20 Room: Break Out 1

1. **Toward Malleable Model Coupling**
Author(s): D. Kim, J.W. Larson, K. Chiu
Presenter: J.W. Larson, Argonne National Laboratory
2. **Can models of scientific software-hardware interactions be predictive?**
Author(s): M. Frasca, A. Chatterjee, P. Raghavan
Presenter: P. Raghavan, The Pennsylvania State University
3. **Towards High-Dimensional Computational Steering of Precomputed Simulation Data using Sparse Grids**
Author(s): D. Butnaru, D. Pflüger, H.-J. Bungartz
Presenter: D. Butnaru, Technical University of Munich
4. **An Alternating Mesh Quality Metric Scheme for Efficient Mesh Quality Improvement**
Author(s): J. Park, S.M. Shontz
Presenter: S.M. Shontz, The Pennsylvania State University
5. **MDEC: MeTiS-based Domain Decomposition for Parallel 2D Mesh Generation**
Author(s): T. Panitanarak, S.M. Shontz
Presenter: S.M. Shontz, The Pennsylvania State University

M03

Wed, 01 Jun 2011, 16:40 - 18:20 Room: Break Out 3

1. **GX-Means: A model-based divide and merge algorithm for geospatial image clustering**
Author(s): R.R. Vatsavai, C.T. Symons, V. Chandola, G. Jun
Presenter: R.R. Vatsavai, Oak Ridge National Laboratory

2. **Query-driven Multiscale Data Postprocessing in Computational Fluid Dynamics**
Author(s): A.N.A. Atanasov, T.W. Weinzierl
Presenter: A.N.A. Atanasov, Technische Universität München
3. **Visualization of numerical simulations of astrophysical and fusion plasmas with the SDvision code**
Author(s): B. THOORIS, D. POMAREDE
Presenter: B. THOORIS, CEA-IRFU Saclay
4. **Cellular Microscopic Pattern Recogniser – A Distributed Computational Approach for Macroscopic Event Detection in WSN**
Author(s): W.M. Alfehaid, A.I. Khan
Presenter: W.M. Alfehaid, Clayton school of IT, Monash University, Victoria, 3800, Australia

M04

Wed, 01 Jun 2011, 14:40 - 16:20 Room: Break Out 3

1. **A Multi-Stage Blackboard Query Optimization Framework for World-Spanning Distributed Database Resources**
Author(s): P.P. Beran, W. Mach, E. Schikuta, R. Vigne
Presenter: E. Schikuta, University of Vienna
2. **A Dynamic Multi-Objective Optimization Framework for Selecting Distributed Deployments in a Heterogeneous Environment**
Author(s): E. Vinek, P.P. Beran, E. Schikuta
Presenter: E. Schikuta, University of Vienna
3. **A Scheduler based on Resource Competition for Parameter Sweep Workflow**
Author(s): S. Smachat, M. Indrawan, S. Ling, C. Enticott, D. Abramson
Presenter: S. Ling, Faculty of Information Technology, Monash University

M05

Wed, 01 Jun 2011, 16:40 - 18:20 Room: Break Out 1

1. **Multi-level Optimization of Matrix Multiplication for GPU-equipped Systems**
Author(s): K. Matsumoto, N. Nakasato, T. Sakai, H. Yahagi, S. Sedukhin
Presenter: K. Matsumoto, The University of Aizu
2. **GPU-Assisted Buffer Management**
Author(s): J.L. Zhong, B.S. He
Presenter: B.S. He, Nanyang Technological University
3. **Parallel application benchmarks and performance evaluation of the Intel Xeon 7500 family processors**
Author(s): K. Kurowski, P. Kopta, T. Piontek, P. Gepner, M. Puchalski, J. Komasa, M. Kulczewski
Presenter: P. Gepner, Intel Corporation
4. **Efficient Probabilistic Latent Semantic Indexing using Graphics Processing Unit**
Author(s): K.K.E. KOUASSI, T.A. AMAGASA, H.K. KITAGAWA
Presenter: T.A. AMAGASA, University of Tsukuba
5. **Modelling the Runtime of the Gaussian Computational Chemistry Application and Assessing the Impacts of Microarchitectural Variations**
Author(s): J. Antony, A.P. Rendell, R. Yang, G.W. Trucks, M.J. Frisch
Presenter: J. Antony, ANU Supercomputer Facility

6. **APTCC : Auto Parallelizing Translator From C To CUDA**
Author(s): T. Nawata, R. Suda
Presenter: T. Nawata, Department of Computer Science, Graduate School of Information Science, the University of Tokyo

M06

Thu, 02 Jun 2011, 10:35 - 12:15 Room: Break Out 1

1. **The UrbanFlood Common Information Space for Early Warning Systems**
Author(s): B. Balis, M. Kasztelnik, M. Bubak, T. Bartynski, T. Gubala, P. Nowakowski, J. Broekhuijsen
Presenter: B. Balis, AGH University of Science and Technology
2. **Flood early warning system: design, implementation and computational modules**
Author(s): V.V. Krzhizhanovskaya, G.S. Shirshov, N.B. Melnikova, R.G. Belleman, F.I. Rusadi, B.J. Broekhuijsen, B.P. Gouldby, J. Lhomme, B. Balis, M. Bubak, A.L. Pyayt, I.I. Mokhov, A.V. Ozhigin, B. Lang, R.J. Meijer
Presenter: V.V. Krzhizhanovskaya, University of Amsterdam, The Netherlands
3. **InSt: An Integrated Steering Framework for Critical Weather Applications**
Author(s): P. Malakar, V. Natarajan, S. Vadhiyar
Presenter: P. Malakar, Indian Institute of Science
4. **OpenMP parallelization of the SCIARA Cellular Automata lava flow model: performance analysis on shared-memory computers**
Author(s): W. Spataro, M. Oliverio, D. D'Ambrosio, R. Rongo, G. Spingola, G.A. Trunfio
Presenter: D. D'Ambrosio, University of Calabria, Italy
5. **Higher Order Numerical Discretization Methods with Sobolev Norm Minimization**
Author(s): K.R. Jayaraman, S. Chandrasekaran, J. Moffitt, M. Gu, H.N. Mhaskar
Presenter: K.R. Jayaraman, Dept. of Electrical and Computer Engineering, UC Santa Barbara, USA

M07

Thu, 02 Jun 2011, 14:30 - 16:10 Room: Break Out 1

1. **GPAW - massively parallel electronic structure calculations with Python based software**
Author(s): J. Enkovaara, N.A. Romero, J.J. Mortensen, S. Shende
Presenter: J. Enkovaara, CSC - IT Center for Science Ltd.
2. **A Verified Bulk Synchronous Parallel ML Heat Diffusion Simulation**
Author(s): F. Loulergue, J. Tesson
Presenter: F. Loulergue, University of Orleans, France
3. **Analysis Method of Influence of Potential Edge on Information Diffusion**
Author(s): K. Nagata, S. Shirayama
Presenter: K. Nagata
4. **Theoretical study of the reversible photoconversion mechanism in Dronpa**
Author(s): M. Tachikawa, J. Koseki, Y. Kita, U. Nagashima
Presenter: J. Koseki, Yokohama-city University
5. **A Multilevel Parallelism Support for Multi-Physics Coupling**
Author(s): F. Liu
Presenter: F. Liu, USDOE Ames Laboratory, Iowa State University

M08

Thu, 02 Jun 2011, 16:30 - 18:10 Room: Break Out 1

1. **High performance distributed cluster-based individual-oriented fish school simulation**
Author(s): R.S. Roberto Solar, R.S. Remo Suppi, E.L. Emilio Luque
Presenter: R.S. Roberto Solar, Universidad Autonoma de Barcelona
2. **Efficient Solution of Evolution Models for Virus Populations**
Author(s): G. Niederbrucker, W.N. Gansterer
Presenter: G. Niederbrucker, University of Vienna
3. **A Parallel Graph Sampling Algorithm for Analyzing Gene Correlation Networks**
Author(s): K. Dempsey, K. Duraisamy, H. Ali, S. Bhowmick
Presenter: S. Bhowmick, University of Nebraska at Omaha
4. **TEAM Network: Building Web-based Data Access and Analysis Environments for Ecosystem Services**
Author(s): C. Youn, C. Baru, S. Chandra, E.H. Fegraus, K. Lin
Presenter: C. Youn, San Diego Supercomputer Center, University of California, San Diego

M09

Fri, 03 Jun 2011, 09:30 - 11:10 Room: Auditorium

1. **A Web API Framework for Developing Grid Portals**
Author(s): V. De Luca, I. Epicoco, D. Lezzi, G. Aloisio
Presenter: I. Epicoco, Dep. Engineering for Innovation, University of Salento, Lecce, Italy
2. **Dynamic Multilevel Hybrid Scheduling Algorithms for Grid Computing**
Author(s): S.N.M. Shah, A.K.B. Mahmood, A. Oxley
Presenter: S.N.M. Shah, Universiti Teknologi PETRONAS, Malaysia
3. **A method for reliably managing files with RNS in multi Data Grids**
Author(s): Y. Kawai, A. Hasan, G. Iwai, T. Sasaki, Y. Watase
Presenter: Y. Kawai, KEK
4. **Distributed Speculative Parallelization using Checkpoint Restart**
Author(s): D. Ghoshal, S.R. Ramkumar, A. Chauhan
Presenter: D. Ghoshal, Indiana University
5. **Component Approach to Computational Applications on Clouds**
Author(s): M. Malawski, J. Meizner, M. Bubak, P. Gepner
Presenter: M. Bubak, Institute of Computer Science AGH, Krakow, Poland

M10

Fri, 03 Jun 2011, 09:30 - 11:10 Room: Break Out 3

1. **Node-to-set disjoint-path routing in perfect hierarchical hypercubes**
Author(s): A. Bossard, K. Kaneko, S. Peng
Presenter: A. Bossard, Tokyo University of Agriculture and Technology
2. **ASIODES - An Asynchronous and Smart I/O Delegation System**
Author(s): M.R. hugues, S.G. Petiton, M. Moretti, H. Calandra
Presenter: M.R. hugues, LIFL
3. **Computational Steering and Parallel Online Monitoring Using RMA through the HDF5 DSM Virtual File Driver**
Author(s): J. Soumagne, J. Biddiscombe
Presenter: J. Soumagne, CSCS - Swiss National Supercomputing Centre

4. **Early performance evaluation of AVX for HPC**
 Author(s): P. Gepner, V. Gamayunov, D.L. Fraser
 Presenter: P. Gepner, Platform & Technology Enabling Group Intel Corporation, Pipers Way, Swindon Wiltshire SN3 1RJ, United Kingdom
5. **Management of Non-functional Attributes of Parallel Components**
 Author(s): Y. Peng, C. Hu, C. Zhao, S. Li, S. Yao
 Presenter: Y. Peng, University of Science and Technology Beijing

M11

Fri, 03 Jun 2011, 09:30 - 11:10 Room: Break Out 1

1. **Validation of Dunbar's number in Twitter conversations**
 Author(s): B. Goncalves, N. Perra, A. Vespignani
 Presenter: B. Goncalves, Center for Complex Networks and Systems Research, School of Informatics and Computing, Indiana University, IN 47408, USA
2. **Ridge Detection with the Steepest Ascent Method**
 Author(s): S. Koka, K. Anada, K. Nomaki, K. Sugita, K. Tsuchida, T. Yaku
 Presenter: S. Koka, Nihon University
3. **Parallel And SIMD Optimization Of Image Feature Extraction**
 Author(s): M. Qi, G. Sun, G. Chen
 Presenter: M. Qi, University of Science and Technology of China
4. **QoS Support in Event Detection in WSN through Optimal k-Coverage**
 Author(s): K.M. Alam, J. Kamruzzaman, G. Karmakar, M. Murshed, A.K.M. Azad
 Presenter: K.M. Alam, Monash University, Australia
5. **Effects of Reduced Precision on Floating-Point SVM Classification Accuracy**
 Author(s): B. Lesser, M. Mücke, W.N. Gansterer
 Presenter: B. Lesser, University of Vienna

Workshop 01

Simulation of Multiphysics Multiscale Systems, 8th International Workshop

W01a: Multiphysics Multiscale Systems

Fri, 03 Jun 2011, 09:30 - 11:10 Room: Lecture Room 2

1. **Simulation of Multiphysics Multiscale Systems, 8th International Workshop**
 Author(s): V.V. Krzhizhanovskaya
 Presenter: V.V. Krzhizhanovskaya, University of Amsterdam, The Netherlands
2. **Stochastic Droplet-Fiber Collisions**
 Author(s): S. Schroeder, F. Olawsky, M. Hering-Bertram, H. Hagen
 Presenter: S. Schroeder, Computer Graphics and HCI Group, University of Kaiserslautern
3. **Virtual Dike: multiscale simulation of dike stability**
 Author(s): N.B. Melnikova, V.V. Krzhizhanovskaya, G.S. Shirshov
 Presenter: N.B. Melnikova, National Research University ITMO, St. Petersburg, Russia and University of Amsterdam, The Netherlands
4. **Pulsatile flow in model cerebral aneurysms**
 Author(s): J. Mikhal, B.J. Geurts
 Presenter: J. Mikhal, Dept. Applied Mathematics, Faculty EEMCS, University of Twente, The Netherlands

5. **Scalable parallel preconditioners for an open source cardiac electrophysiology simulation package**
Author(s): M.O. Bernabeu, D. Kay
Presenter: M.O. Bernabeu, Oxford University Computing Laboratory
6. **Visualizing Process Composition and Load Balance in Parallel Coupled Models**
Author(s): J.W. Larson
Presenter: J.W. Larson, Argonne National Laboratory

Workshop 02

2nd Workshop on Computational Optimization, Modelling and Simulation (COMS 2011)

W02a: COMS 2011

Wed, 01 Jun 2011, 11:05 - 12:45 Room: Lecture Room 5

1. **Computational Optimization, Modelling and Simulation: Recent Advances and Overview**
Author(s): X.S. Yang, S. Koziel, L. Leifsson
Presenter: X.S. Yang, National Physical Laboratory, UK
2. **Inverse Design of Transonic Airfoils Using Variable-Resolution Modeling and Pressure Distribution Alignment**
Author(s): L. Leifsson, S. Koziel, S. Ogurtsov
Presenter: L. Leifsson, Reykjavik University
3. **Real-coded Estimation of Distribution Algorithm by Using Probabilistic Models with Multiple Learning Rates**
Author(s): M. Nakao, T. Hiroyasu, M. Miki, H. Yokouchi, M. Yoshimi
Presenter: M. Nakao, Center for Computational Sciences, University of Tsukuba
4. **Simulation-Driven Design of Antennas Using Coarse-Discretization Electromagnetic Models**
Author(s): S. Koziel, S. Ogurtsov, L. Leifsson
Presenter: S. Koziel, Reykjavik University
5. **A robust approximation for setting target inventory levels in a constrained production environment**
Author(s): J. Betts
Presenter: J. Betts, Monash University

W02b: COMS 2011

Wed, 01 Jun 2011, 14:40 - 16:20 Room: Lecture Room 5

1. **Sequential Optimization of Paths in Directed Graphs Relative to Different Cost Functions**
Author(s): S. Hussain, J. AbuBeker, I. Chikalov, M. Moshlov
Presenter: S. Hussain, King Abdullah University of Science and Technology
2. **PACC: A Path Associativity Congestion Control and Throughput Model For Multi-path TCP**
Author(s): Y. Liu, K. Xu, Z. Ma, B.J. Wang
Presenter: Z. Ma, Computer Science & Technology, University of Tsinghua, Beijing, China

3. **An Efficient Algorithm for Computing the K overlapping Maximum Convex Sum Problem**
Author(s): M. Thaher, T. Takaoka
Presenter: M. Thaher, University of Canterbury
4. **Nearest Neighbor For Histogram-based Feature Extraction**
Author(s): F.S. Mohamad, A.A. Manaf, S. Chuprat
Presenter: F.S. Mohamad, University of Technology Malaysia
5. **3D Off-Line Path Planning For Aerial Vehicle Using Distance Transform Technique**
Author(s): S. Jaishankar, R.N. Pralhad
Presenter: S. Jaishankar, Defence Institute of Advanced Technology, Pune India

W02c: COMS 2011

Wed, 01 Jun 2011, 16:40 - 18:20 Room: Lecture Room 5

1. **Integrating the fault detection method and run-to-run control for improving the semiconductor process control**
Author(s): C.H. Jen, J.M. Wang
Presenter: C.H. Jen
2. **Applying an approximate T_w (the weakest t-norm) fuzzy GERT to evaluate two-unit standby redundant system reliability**
Author(s): K.-P. Lin, K.-C. Hung, S.-P. Lai, Y.-T. Yu, P.-T. Wu
Presenter: K.-P. Lin, Department of Information Management, Lunghwa University of Science and Technology
3. **Personalized Translation Listening System for Age Groups**
Author(s): D.W. Jang, D.J. Kim, K.S. Hong
Presenter: D.W. Jang, Sungkyunkwan University
4. **An overlapping domain decomposition method for a polymer exchange membrane fuel cell model**
Author(s): P.T. Sun, M.Y. He, Z.P. Huang, C. Wang, S. Zhai
Presenter: M.Y. He, Tongji University

Workshop 03

6th Workshop on Computational Chemistry and Its Applications

W03a: Computational Chemistry

Thu, 02 Jun 2011, 14:30 - 16:10 Room: Lecture Room 2

Chair: H. Abou-Rachid

1. **Theory of molecular recognition and its application to drug design**
Author(s): F. Hirata
Presenter: F. Hirata, Institute for Molecular Science, Japan
2. **Chemically accurate and computationally-efficient time-dependent density functional theory (TD-DFT) modeling of the UV/Vis spectra of Pechmann dyes and related compounds**
Author(s): E.A.B. Kantchev, T.B. Norsten, M.B. Sullivan
Presenter: E.A.B. Kantchev, Institute of Materials Research and Engineering
3. **DFT Study on mechanochemical bond breaking in COGEF and Molecular Dynamics simulations**
Author(s): B.M. Szyja, E.A. Pidko, R. Groote, E.J.M. Hensen, R. Sijbesma
Presenter: B.M. Szyja, Eindhoven University of Technology

4. **Atomistic studies of RDX and FOX-7 -Based Plastic-Bonded explosives: molecular dynamics simulation**
 Author(s): M. Jaidann, H. Abou-Rachid, X. Lafleurs-Lambert, J. Brisson
 Presenter: H. Abou-Rachid, Defence Research and Development Canada
5. **Solvation structure and gelation ability of polyelectrolytes: predictions by quantum chemistry methods and integral equation theory of molecular liquids**
 Author(s): O. Lyubimova, X. Liu, S. Gusarov, A.E. Kobrin, A. Kovalenko
 Presenter: X. Liu, Department of Mechanical Engineering, University of Alberta, Edmonton, Alberta, T6G2G8, Canada

W03b: Computational Chemistry

Thu, 02 Jun 2011, 16:30 - 18:10 Room: Lecture Room 2

Chair: H. Abou-Rachid

1. **Understanding Adsorption and Separation behavior of shorter chain alkane mixtures in Zeolitic Imidazolate Frameworks by molecular simulations**
 Author(s): L. Zhang, Q. Li, Z. Lu, X. Wang
 Presenter: L. Zhang, Department of chemistry, Zhejiang Sci-Tech university, China
2. **Tungsten Imido-Catalysed Dimerisation of alpha-Olefins: Insight into the Lewis Acid's Function Revealed from Computational Studies**
 Author(s): S. Tobisch
 Presenter: S. Tobisch
3. **Molecular Ornstein-Zernike self-consistent-field approach to hydrated electron**
 Author(s): N. Yoshida
 Presenter: N. Yoshida, Institute for Molecular Science
4. **Deactivation of Ru-benzylidene Grubbs catalysts active in olefin metathesis**
 Author(s): A. Poater, F. Ragone, M. Garrido, S. Pérez, M. Poch, A. Correa, L. Cavallo
 Presenter: A. Poater, Catalan Institute for Water Research, H2O Building, Scientific and Technological Park of the University of Girona, Giron

Workshop 05

Tools for Program Development and Analysis in Computational Science

W05a: Tools

Wed, 01 Jun 2011, 11:05 - 12:45 Room: Break Out 2

1. **Workshop on tools for program development and analysis in computational science**
 Author(s): J. Tao
 Presenter: J. Tao, Karlsruhe Institute of Technology
2. **An Intuitive Framework for Accessing Computing Clouds**
 Author(s): J. Tao, H. Marten, D. Kramer, W. Karl
 Presenter: J. Tao, Karlsruhe Institute of Technology
3. **Gleipnir: A Memory Analysis Tool**
 Author(s): T. Janjusic
 Presenter: K.K. Kavi, University of North Texas
4. **Developing an Automated Mechanism for Cluster Computing in Computerized Classroom**
 Author(s): S.T. Wang, C.H. Li, H.Y. Chang, Y.C. Chen, C.H. Hsu
 Presenter: S.T. Wang, National Center for High-Performance Computing

5. **A Multitier System for the Verification, Visualization and Management of CHIMERA**
Author(s): E.J. Lingerfelt, O.E.B. Messer, J.A. Osborne, R.D. Budiardja, A. Mezzacappa
Presenter: E.J. Lingerfelt, Oak Ridge National Laboratory

W05b: Tools

Wed, 01 Jun 2011, 14:40 - 16:20 Room: Break Out 2

1. **ALPS: A Methodology for Application-Level Communication Characterization of Parsec 2.1**
Author(s): D. Hillenbrand, J. Tao, M. Balzer
Presenter: D. Hillenbrand, Karlsruhe Institute of Technology
2. **User-defined Events for Hardware Performance Monitoring**
Author(s): S. Moore, J. Ralph
Presenter: S. Moore, EECS Dept., University of Tennessee, Knoxville, TN, USA
3. **Design and Implementation of a Runtime System for Parallel Numeric Simulations on Large-Scale Systems**
Author(s): M. Schliephake, X. Aguilar, E. Laure
4. **Presenter: M. Schliephake, PDC, KTH Royal Institute of Technology**
Sparse Jacobian Computation Using ADIC2 and ColPack
Author(s): S.H.K. Narayanan, B. Norris, P.D. Hovland, D. Nguyen, A.H. Gebremedhin
Presenter: S.H.K. Narayanan, Argonne National Laboratory

Workshop 06

Third Workshop on Emerging Parallel Architectures

W06a: Emerging Parallel Architectures

Thu, 02 Jun 2011, 14:30 - 16:10 Room: Break Out 2

1. **Third Workshop on using Emerging Parallel Architectures**
Author(s): B. Schmidt, D. Maskell
Presenter: B. Schmidt, Nanyang Technological University
2. **Massively parallel FPGA-based implementation of BLASTp with the two-hit method**
Author(s): L. Wienbrandt, S. Baumgart, J. Bissel, F. Schatz, M. Schimmler
Presenter: L. Wienbrandt, Department of Computer Science,
Christian-Albrechts-University of Kiel, Germany
3. **Coarse Grained Parallelized Scientific Applications on a Cost Efficient Intel Atom Based Cluster**
Author(s): R.G. Geyer, A.G. Georgi, W.E.N. Nagel
Presenter: R.G. Geyer, Student at TU Dresden ZIH
4. **10x10: A General-purpose Architectural Approach to Heterogeneity and Energy Efficiency**
Author(s): A.A. Chien, A.E. Snaveley, M. Gahagan
Presenter: A.A. Chien, University of California, San Diego
5. **A single processor approach for loosely synchronized execution of parallel flows on heterogeneous multicore**
Author(s): S.R. Louise, V. David, F. Calcado
Presenter: S.R. Louise, CEA, LIST

W06b: Emerging Parallel Architectures

Thu, 02 Jun 2011, 16:30 - 18:10 Room: Break Out 2

1. **GPU-accelerated Chemical Similarity Assessment for Large Scale Databases**
Author(s): M. Maggioni, M.D. Santambrogio, J. Liang
Presenter: M. Maggioni, University of Illinois at Chicago
2. **A Framework for Running the ADCIRC Discontinuous Galerkin Storm Surge Model on a GPU**
Author(s): M.J. Duchene, A.M. Spagnuolo, E.J. Kubatko, J.J. Westerink, C. Dawson
Presenter: M.J. Duchene, Department of Computer Science and Engineering, University of Notre Dame, Notre Dame, IN 46556, USA
3. **High Performance Stencil Code Algorithms for GPGPUs**
Author(s): A. Schäfer, D. Fey
Presenter: A. Schäfer, Friedrich-Alexander-Universität Erlangen-Nürnberg
4. **Performance comparison of designated preprocessing white light interferometry algorithms on emerging multi- and many-core architectures**
Author(s): M. Schneider, D. Fey, D. Kapusi, T. Machleidt
Presenter: M. Schneider, Friedrich-Alexander-University Erlangen-Nuremberg

Workshop 08

Dynamic Data Driven Application Systems - DDDAS 2011

W08a: Dynamic Data Driven Application Systems

Fri, 03 Jun 2011, 09:30 - 11:10 Room: Break Out 2

1. **Intelligent fracture creation for shale gas development**
Author(s): C.C. Douglas, G. Qin, N. Collier, B. Gong
Presenter: C.C. Douglas, University of Wyoming
2. **A Data-Driven Framework for Dynamic Trust Management**
Author(s): O.O. Onolaja, G.K. Theodoropoulos, R. Bahsoon
Presenter: O.O. Onolaja, University of Birmingham
3. **Prediction Time Assessment in a DDDAS for Natural Hazard Management: Forest Fire Study Case**
Author(s): A. Cencerrado, A. Cortés, T. Margalef
Presenter: A. Cencerrado, Universitat Autònoma de Barcelona
4. **On the adaptive solution of space-time inverse problems with the adjoint method**
Author(s): M. Alexe, A. Sandu
Presenter: A. Sandu, Virginia Tech

W08b: Dynamic Data Driven Application Systems

Fri, 03 Jun 2011, 13:15 - 14:55 Room: Break Out 2

1. **InfoSymbiotics/DDDAS and SuperGrids**
Author(s): F. Darema
Presenter: F. Darema, Air Force Office of Scientific Research
2. **Memristor as an Archetype of DDDAS and its Applications to Sensor Networks**
Author(s): G.-E. Paziienza, R. Kozma
Presenter: R. Kozma, University of Memphis, TN

Workshop 09

Agent-Based Simulations, Adaptive Algorithms and Solvers

W09a: Agent-Based Simulations

Thu, 02 Jun 2011, 16:30 - 18:10 Room: Lecture Room 5

1. **Out-of-core multi-frontal solver for multi-physics hp adaptive problems**
Author(s): A. Paszynska, M. Paszynski, D. Pardo, L. Demkowicz
Presenter: A. Paszynska, Jagiellonian University, Krakow, Poland
2. **A Simulation Framework to Investigate in vitro Viral Infection Dynamics**
Author(s): A. Bankhead, E. Mancini, A.C. Sims, R.S. Baric, S. McWeeney, P.M.A. Slood
Presenter: A. Bankhead, Oregon Health and Science University
3. **Application of Hierarchical Chromosome Based Genetic Algorithm to the problem of finding optimal initial three dimensional meshes for the self adaptive hp-Finite Element Method**
Author(s): A. Paszynska, M. Stozek
Presenter: A. Paszynska, Jagiellonian University, Krakow, Poland
4. **Anisotropic 2D mesh adaptation in hp-adaptive FEM**
Author(s): M. Paszynski, A. Szymczak, A. Paszynska, D. Pardo
Presenter: M. Paszynski, AGH University of Science and Technology

W09b: Agent-Based Simulations

Fri, 03 Jun 2011, 09:30 - 11:10 Room: Lecture Room 5

1. **Diffusive Wave Approximation to the Shallow Water Equations: Computational Approach**
Author(s): N.O.C. Collier, H.R. Radwan, L.D. Dalcin, V.M.C. Calo
Presenter: V.M.C. Calo, King Abdullah University of Science and Technology
2. **Computational method for agent-based E-commerce negotiations with adaptive negotiation behaviors**
Author(s): G. Wang, T.N. Wong, C.X. Yu
Presenter: G. Wang, The University of Hong Kong
3. **Agent-oriented image processing with the hp-adaptive projection-based interpolation method**
Author(s): M.T. Sieniek, P. Gurgul, M.J. Skotniczny, K. Magiera, M. Paszynski
Presenter: P. Gurgul, Department of Computer Science, AGH University of Science and Technology
4. **Computational complexity and memory usage for multi-frontal direct solver used in p finite element analysis**
Author(s): V.M. Calo, N.O. Collier, D. Pardo, M.R. Paszynski
Presenter: N.O. Collier

W09c: Agent-Based Simulations

Fri, 03 Jun 2011, 13:15 - 14:55 Room: Lecture Room 5

1. **Discontinuous Petrov-Galerkin method based on the optimal test space norm for one-dimensional transport problems**
Author(s): A.H. Niemi, N.O. Collier, V.M. Calo
Presenter: A.H. Niemi, King Abdullah University of Science and Technology

2. **An Agent-Based Decision Support System for Hospitals Emergency Departments**
 Author(s): M. Taboada, E. Cabrera, M.L. Iglesias, F. Epelde, E. Luque
 Presenter: E. Luque, Computer Architecture and Operating Systems Department , UAB, Spain
3. **Optimization of Healthcare Emergency Departments by Agent-Based Simulation**
 Author(s): E.C. CABRERA, M. Taboada, E. Luque, M.L. Iglesias, F. Epelde
 Presenter: E.C. CABRERA, Computer Architecture and Operating Systems Department, UNIVERSITY AUTONOMA OF BARCELONA, UAB
4. **Farmer-Pest Problem: A Multidimensional Problem Domain for Comparison of Agent Learning Methods**
 Author(s): B. Sniezynski, J. Dajda, M. Mlostek, M. Pulchny
 Presenter: B. Sniezynski, AGH University of Science and Technology

Workshop 10

Computational Science of Mesoscopic Methods for Fluid Dynamics

W10a: Mesoscopic Methods for Fluid Dynamics

Thu, 02 Jun 2011, 14:30 - 16:10 Room: Lecture Room 6

1. **Free-Surface Lattice-Boltzmann Simulation on Many-Core Architectures**
 Author(s): M. Schreiber, P. Neumann, S. Zimmer, H.-J. Bungartz
 Presenter: M. Schreiber, SCCS, Technische Universitaet Muenchen, Germany
2. **Optimization of Multi-Phase Compressible Lattice Boltzmann Codes on Massively Parallel Multi-Core Systems**
 Author(s): S.F. SCHIFANO, L. BIFERALE, F. MANTOVANI, M. PIVANTI, F. POZZATI, M. Sbragaglia, A. Scagliarini, F. TOSCHI, R. Tripiccione
 Presenter: S.F. SCHIFANO, University and INFN Ferrara, Italy
3. **Lattice Boltzmann Simulation Code Optimization Based on Constant-time Circular Array Shifting**
 Author(s): G. Dethier, P.-A. de Marneffe, P. Marchot
 Presenter: G. Dethier, EECS Department, University of Liège, Belgium
4. **Two Complementary Approaches for Integrating Lattice Boltzmann Flow Solvers into Simulation Frameworks**
 Author(s): J. Bernsdorf, D. Wang, G. Berti
 Presenter: J. Bernsdorf, German Research School for Simulation Sciences

W10b: Mesoscopic Methods for Fluid Dynamics

Thu, 02 Jun 2011, 16:30 - 18:10 Room: Lecture Room 6

1. **Incorporating Chemical Reactions in Dissipative Particle Dynamics Simulations**
 Author(s): Z.-Y. Lu, H. Liu, H. Li
 Presenter: H. Liu, Jilin University
2. **Mesoscopic study of dynamics and gelation ability of oligomeric electrolyte gelator with dissipative particle dynamics**
 Author(s): X. Liu, O. Lyubimova, A.E. Kobryn, S. Gusarov, A. Kovalenko
 Presenter: X. Liu, National Institute for Nanotechnology, National Research Council of Canada, 11421 Saskatchewan Drive, Edmonton, Alberta,

3. **Effect of divalent cations on cell adhesion between human neutrophil and endothelial ligand VCAM-1: a lattice Boltzmann analysis**
 Author(s): Y. Liu, W.W. Yan, B.M. Fu
 Presenter: Y. Liu, Department of Mechanical Engineering, The Hong Kong Polytechnic University
4. **Lattice Boltzmann Simulation of non-Darcy Flow in Porous Media**
 Author(s): M. Hasert, J. Bernsdorf, S. Roller
 Presenter: M. Hasert, German Research School of Simulation Sciences

Workshop 11

Fifth Workshop on Teaching Computational Science (WTCS 2011)

W11a: WTCS 2011

Thu, 02 Jun 2011, 10:35 - 12:15 Room: Lecture Room 5

1. **The Fifth Workshop on Teaching Computational Science (WTCS 2011)**
 Author(s): A. Tirado-Ramos, A.B. Shiflet
 Presenter: A.B. Shiflet, Wofford College
2. **Making Connections: Modeling Epidemiological Networks in Mathematical Modeling and HPC Courses**
 Author(s): A.B. Shiflet, G.W. Shiflet
 Presenter: A.B. Shiflet, Wofford College
3. **An Innovative Teaching Tool based on Semantic Tableaux for Verification and Debugging of Imperative Programs**
 Author(s): R. del Vado Virseda, F. Perez Morente
 Presenter: R. del Vado Virseda, Universidad Complutense de Madrid. Departamento de Sistemas Informaticos y Computacion
4. **Linux Cluster in Theory and Practice: A Novel Approach for Teaching Cluster Computing Based on the Intel Atom Platform**
 Author(s): A. Georgi, S. Höhlig, R. Geyer, W.E. Nagel
 Presenter: A. Georgi, Center for Information Services and High Performance Computing, Faculty of Computer Science, Technische Universität Dres

W11b: WTCS 2011

Thu, 02 Jun 2011, 14:30 - 16:10 Room: Lecture Room 5

1. **A practical and comprehensive graduate course preparing students for research involving scientific computing**
 Author(s): G. Allen, W. Benger, A. Hutanu, S. Jha, F. Loeffler, E. Schnetter
 Presenter: G. Allen, Louisiana State University
2. **Teaching Computing to STEM Students via Visualization Tools**
 Author(s): H. Chi, H. Jain
 Presenter: H. Chi, Florida A&M University
3. **A Game-based Learning System for Theory of Computation Using Lego NXT Robot**
 Author(s): M. Hamada, S. Sato
 Presenter: M. Hamada
4. **eScience: Building our Body of Knowledge**
 Author(s): V. Maxville
 Presenter: V. Maxville, iVEC, Kensington WA, Australia

Workshop 13

Sixth international Workshop on Automatic Performance Tuning (iWAPT2011)

W13a: Automatic Performance Tuning

Wed, 01 Jun 2011, 16:40 - 18:20 Room: Break Out 2

1. **The Sixth International Workshop on Automatic Performance Tuning (iWAPT2011)**
Author(s): T.K. Katagiri
Presenter: T.K. Katagiri, The University of Tokyo
2. **The Future of Auto-Tuning**
Author(s): V. Pankratius
Presenter: V. Pankratius, Karlsruhe Institute of Technology, Germany
3. **Autotuning in an Array Processing Language using High-level Program Transformations**
Author(s): Y. Shirota, J. Segawa, M. Tarui, T. Kanai
Presenter: Y. Shirota, Toshiba Corporation
4. **Can search algorithms save large-scale automatic performance tuning?**
Author(s): P. Balaprakash, S.M. Wild, P. Hovland
Presenter: P. Balaprakash, Argonne National Lab
5. **Towards a Multi-Level Cache Performance Model for 3D Stencil Computation**
Author(s): R. de la Cruz, M. Araya-Polo
Presenter: R. de la Cruz, Barcelona Supercomputing Center

W13b: Automatic Performance Tuning

Thu, 02 Jun 2011, 10:35 - 12:15 Room: Break Out 2

1. **Towards Automating Black Belt Programming**
Author(s): F. Franchetti
Presenter: F. Franchetti, Carnegie Mellon University, USA
2. **Extensive Parameteirzation And Tuning of Architecture-Sensitive Optimizations**
Author(s): Q. Yi, J. Guo
Presenter: Q. Yi, University of Texas at San Antonio
3. **I/O-Performance Prediction Method for Mission-critical Grid-batch Processing**
Author(s): T. Kashiyama, T. Hanai, Y. Suzuki, K. Naono
Presenter: T. Kashiyama, Hitachi, Ltd., Central Research Laboratory
4. **Autotuning a Random Walk Boolean Satisfiability Solver**
Author(s): T. Cui, F. Franchetti
Presenter: F. Franchetti, Carnegie Mellon University
5. **Performance prediction of ocean color Monte Carlo simulations using multi-layer perceptron neural networks**
Author(s): T. Kajiyama, D. D'Alimonte, J.C. Cunha
Presenter: T. Kajiyama, CITI, Departamento de Informática, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa

Workshop 15

Fourth Workshop on Biomedical and Bioinformatics Challenges to Computer Science

W15a: Biomedical & Bioinformatics

Thu, 02 Jun 2011, 14:30 - 16:10 Room: Break Out 3

1. **Biomedical and Bioinformatics Challenges to Computer Science: Bioinformatics, Modeling of Biomedical Systems and Clinical Applications**
Author(s): M. Cannataro, J. Sundnes, R. Weber dos Santos
Presenter: M. Cannataro, University of Catanzaro
2. **The Exact Closest String Problem as a Constraint Satisfaction Problem**
Author(s): T.W. Kelsey, L. Kotthoff
Presenter: T.W. Kelsey, University of St Andrews
3. **Improved prediction of protein interaction from microarray data using asymmetric correlation**
Author(s): K. Yano
Presenter: K. Yano, Osaka Institute of Technology
4. **Bio Search Computing: Bioinformatics web service integration for data-driven answering of complex Life Science questions**
Author(s): M.M. Masseroli, G.G. Ghisalberti, S.C. Ceri
Presenter: M.M. Masseroli, Politecnico di Milano

W15b: Biomedical & Bioinformatics

Thu, 02 Jun 2011, 16:30 - 18:10 Room: Break Out 3

1. **Adaptive Time Step for Cardiac Computational Models**
Author(s): R.S. Campos, M. Lobosco, R.W.D. Santos
Presenter: R.S. Campos, Universidade Federal de Juiz de Fora, Brazil
2. **A System for the Analysis of Snore Signals**
Author(s): M. Cannataro, B. Calabrese, P. Veltri, P.H. Guzzi, F. Pucci, M. Sturniolo, A. Gambardella
Presenter: M. Cannataro, University of Catanzaro
3. **Towards a Virtual Research Environment for International Adrenal Cancer Research**
Author(s): R.O. Sinnott, A.J. Stell
Presenter: R.O. Sinnott, University of Melbourne
4. **The ACGT project in retrospect: Lessons learned and future outlook**
Author(s): A. Bucur, S. Rüping, T. Sengstag, S. Sfakianakis, M. Tsiknakis, D. Wegener
Presenter: T. Sengstag, RIKEN Yokohama Institute, Japan

Workshop 16

Second International Workshop on Computational Stochastics

W16a: Computational Stochastics

Thu, 02 Jun 2011, 16:30 - 18:10 Room: Break Out 4

1. **Meso-GSHMC: A stochastic algorithm for meso-scale constant temperature simulations**
Author(s): E. Akhmatskaya, S. Reich
Presenter: E. Akhmatskaya, Basque Center for Applied Mathematics, Derio, Spain
2. **The value of information in multi-armed bandits with exponentially distributed rewards**
Author(s): I.O. Ryzhov, W.B. Powell
Presenter: I.O. Ryzhov, Princeton University
3. **Management of dam systems via optimal price control**
Author(s): D.J. McInnes, B.M. Miller
Presenter: D.J. McInnes, School of Mathematical Sciences, Monash University
4. **Algorithm for waiting time distribution of a discrete-time multiserver queue with deterministic service times and multi-threshold service polic**
Author(s): W. Feng
Presenter: W. Feng, Nagoya Institute of Technology
5. **A flat Dirichlet process switching model for Bayesian estimation of hybrid systems**
Author(s): H. Wu, F. Noe
Presenter: H. Wu, Department of Mathematics and Computer Science, Free University of Berlin, Germany

W16b: Computational Stochastics

Fri, 03 Jun 2011, 09:30 - 11:10 Room : Break Out 4

1. **A Monte Carlo Method for High-Dimensional Volume Estimation and Application to Polytopes**
Author(s): U. Jaekel
Presenter: U. Jaekel, Department of Mathematics and Technology, University of Applied Sciences Koblenz, Germany
2. **A new approximate CVA of interest rate swap in the SABR/LIBOR market model : an asymptotic expansion approach**
Author(s): M. Nishiba
Presenter: M. Nishiba, Tokyo Institute of Technology
3. **A Trust-Region Algorithm for Bi-Objective Stochastic Optimization**
Author(s): S. Kim, J. Ryu
Presenter: J. RYU, National University of Singapore
4. **Two Dimensional Hull-White Model of Stochastic Volatility and Its Nonlinear Filtering Estimation**
Author(s): B.A. Surya
Presenter: B.A. Surya, School of Business and Management, Bandung Institute of Technology, Indonesia

Workshop 17

Dynamic Network Analysis

W17a: Dynamic Network Analysis

Wed, 01 Jun 2011, 11:05 - 12:45 Room: Break Out 3

1. **Dynamic Rewiring Processes in Binary Decision Networks**
Author(s): K.E. Kürten
Presenter: K.E. Kürten, Faculty of Physics, Universität Wien, Austria
2. **Effects of Sample Duration on Network Statistics in Elementary Models of Dynamic Networks**
Author(s): G. László
Presenter: G. László, AITIA International, Inc., Hungary
3. **Evolution of Betweenness Centrality in Dynamic Networks with Changing Density**
Author(s): T. Cséri
Presenter: T. Cséri, Collegium Budapest, Institute for Advanced Study, Budapest, Hungary
4. **Node Resilience versus Structural Change: Limits to Information Spreading in Dynamic Networks**
Author(s): G. Kampis
Presenter: G. Kampis, Collegium Budapest, Institute for Advanced Study, Budapest, Hungary

Workshop 18

First International Workshop on Advances in High-Performance Computational Earth Sciences: Applications and Frameworks (IHPCES)

W18a: High-Performance Computational Earth Sciences

Wed, 01 Jun 2011, 11:05 - 12:45 Room: Break Out 4

1. **First International Workshop on Advances in High-Performance Computational Earth Sciences: Applications and Frameworks (IHPCES)**
Author(s): T. Furumura, K. Nakajima, M. Satoh
Presenter: K. Nakajima, The University of Tokyo, Japan
2. **Fast Computation of Quasi-Dynamic Earthquake Cycle Simulation with Hierarchical Matrices**
Author(s): M. Ohtani, K. Hirahara, Y. Takahashi, T. Hori, M. Hyodo, H. Nakashima, T. Iwashita
Presenter: M. Ohtani, Graduate School of Science, Kyoto University, Japan
3. **Interior Point Methods for the Inverse Medium Problem on Massively Parallel Architectures**
Author(s): M.J. Grote, J. Huber, O. Schenk
Presenter: M.J. Grote, Department of Mathematics and Computer Science, University of Basel, Switzerland
4. **Goal-Oriented Self-Adaptive hp Finite Element Simulation of 3D DC Borehole Resistivity Simulations**
Author(s): V.M. Calo, D. Pardo, M.R. Paszynski
Presenter: N.O. Collier

5. **MPI-OpenMP hybrid simulations using boundary integral equation and finite difference methods for earthquake dynamics and wave propagation: Application to the 2007 Niigata Chuetsu-Oki earthquake (Mw6.6)**
Author(s): H. Aochi, F. Dupros
Presenter: F. Dupros, BRGM

W18b: High-Performance Computational Earth Sciences

Wed, 01 Jun 2011, 14:40 - 16:20 Room: Break Out 4

1. **An OpenMP-enabled parallel simulator for particle transport in fluid flows**
Author(s): W. Wei, O. Al-Khayat, X. Cai
Presenter: W. Wei, Simula Research Laboratory
2. **Numerical modeling of three dimensional self-gravitating Stokes flow problem with free surface**
Author(s): M. Furuichi
Presenter: M. Furuichi, IFREE JAMSTEC
3. **Ascent of Bubbles in Magma Conduits Using Boundary Elements and Particles**
Author(s): G. Morra, L. Quevedo, D.A. Yuen, P. Chatelain
Presenter: D.A. Yuen, Minnesota Supercomputer Institute, University of Minnesota, Minneapolis, MN 55415-1227, USA
4. **Numerical Investigation of Melt Segregation Using FEM Coding Environment Escript**
Author(s): A. Mohajeri, H. Muhlhaus, Y. Finzi, L. Gross
Presenter: A. Mohajeri, ESSCC

W18c: High-Performance Computational Earth Sciences

Wed, 01 Jun 2011, 16:40 - 18:20 Room: Break Out 4

1. **Data exchange algorithm and software design of KAKUSHIN coupler Jcup**
Author(s): T. Arakawa, H. Yoshimura, F. Saito, K. Ogochi
Presenter: T. Arakawa, Research Organization for Information Science and Technology
2. **A Performance Evaluation Method for Climate Coupled Models**
Author(s): I. Epicoco, S. Mocavero, G. Aloisio
Presenter: I. Epicoco, Dep. Engineering for Innovation, University of Salento, Lecce, Italy
3. **145 TFlops Performance on 3990 GPUs of TSUBAME 2.0 Supercomputer for an Operational Weather Prediction**
Author(s): T. Shimokawabe, T. Aoki, J. Ishida, K. Kawano, C. Muroi
Presenter: T. Shimokawabe, Tokyo Institute of Technology
4. **Optimization and Performance Evaluation of Stereo-Matching Software on Many-core Processors**
Author(s): K. Iwata, Y. Tanaka, R. Nakamura, T. Masuda, R. Machida, I. Kojima, S. Sekiguchi
Presenter: K. Iwata, National Institute of Advanced Industrial Science and Technology, Japan

Workshop 21

Data Mining in Earth System Science (DMESS 2011)

W21a: Data Mining in Earth System Science

Thu, 02 Jun 2011, 10:35 - 12:15 Room: Break Out 4

1. **Data Mining in Earth System Science (DMESS 2011)**
Author(s): F.M. Hoffman, J.W. Larson, R.T. Mills, B.-G.J. Brooks, A.R. Ganguly, W.W. Hargrove, J. Huang, J. Kumar, R.R. Vatsavai
Presenter: F.M. Hoffman, Oak Ridge National Laboratory , Computational Earth Sciences Group, USA
2. **Classification of Seismic Windows Using Artificial Neural Networks**
Author(s): S. Diersen, E. Lee, D. Spears, P. Chen, L. Wang
Presenter: S. Diersen, University of Wyoming, U.S.A.
3. **Visualizing Life Zone Boundary Sensitivities Across Climate Models and Temporal Spans**
Author(s): R. Sisneros, J. Huang, G. Ostrouchov, F. Hoffman
Presenter: J. Huang, University of Tennessee at Knoxville
4. **Block-Entropy Analysis of Climate Data**
Author(s): J.W. Larson, P.R. Briggs, M. Tobis
Presenter: J.W. Larson, Argonne National Laboratory
5. **Parallel k-Means Clustering for Quantitative Ecoregion Delineation using Large Data Sets**
Author(s): J. Kumar, R.T. Mills, F.M. Hoffman, W.W. Hargrove
Presenter: J. Kumar, Computer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN, USA

W21b: Data Mining in Earth System Science

Thu, 02 Jun 2011, 14:30 - 16:10 Room: Break Out 4

Joint session with WS 23

1. **Cluster Analysis-Based Approaches for Geospatiotemporal Data Mining of Massive Data Sets for Identification of Forest Threats**
Author(s): R.T. Mills, F.M. Hoffman, J. Kumar, W.W. Hargrove
Presenter: R.T. Mills, Oak Ridge National Laboratory

Workshop 22

Large Scale Computational Physics

W22a: Large Scale Computational Physics

Wed, 01 Jun 2011, 16:40 - 18:20 Room: Lecture Room 6

1. **Lattice QCD Applications on QPACE**
Author(s): T. Wettig, Y. Nakamura, A. Nobile, D. Pleiter, H. Simma, T. Streuer, F. Winter
Presenter: T. Wettig, University of Regensburg
2. **Real-time and real-space density functional calculation for electron dynamics in crystalline solids**
Author(s): K. Yabana, Y. Shinohara, T. Otobe, J.-I. Iwata, G.F. Bertsch
Presenter: K. Yabana

3. **Lattice gauge theory on a multi-core processor, Cell/B.E.**
Author(s): S. Motoki, A. Nakamura
Presenter: S. Motoki, Hiroshima University
4. **Application of graphics processing unit (GPU) to software in elementary particle/high energy physics field**
Author(s): J. Kanzaki
Presenter: J. Kanzaki, KEK

W22b: Large Scale Computational Physics

Thu, 02 Jun 2011, 10:35 - 12:15 Room: Lecture Room 6

1. **GRAPE-MP: An SIMD Accelerator Board for Multi-precision Arithmetic**
Author(s): H. DAISAKA, N. Nakasato, J. Makino, F. Yuasa, T. Ishikawa
Presenter: H. DAISAKA, Hitotsubashi University
2. **The performance of GRAPE-DR for dense matrix operations**
Author(s): J. Makino, H. Daisaka, T. Fukushige, Y. Sugawara, K. Hiraki, M. Inaba
Presenter: J. Makino, National Astronomical Observatory of Japan
3. **Development of a High-speed Eigenvalue-solver for Constant Plasma Monitoring on a Cell Cluster System**
Author(s): N. Kushida, K. Fujibayashi, H. Takemiya
Presenter: N. Kushida, Japan Atomic Energy Agency

Workshop 23

Workshop on Climate Change Data Challenges – C2DC

W23a: Climate Change

Thu, 02 Jun 2011, 14:30 - 16:10 Room: Break Out 4

Joint session with WS 21

1. **Distinguishing Provenance Equivalence of Earth Science Data**
Author(s): C.A. Tilmes, Y. Yesha, M. Halem
Presenter: C.A. Tilmes, NASA Goddard Space Flight Center
2. **Community Earth System Model Data Management: Policies and Challenges**
Author(s): G. Strand
Presenter: G. Strand, NCAR
3. **The Climate-G testbed: towards large scale distributed data management for climate change**
Author(s): S. Fiore, G. Aloisio, P. Fox, M. Petitdidier, H. Schwichtenberg, S. Denvil, J.D. Blower, A. Cofino
Presenter: S. Fiore, University of Salento and CMCC
4. **Centralized and decentralized climate model data management: technology, requirements, challenges**
Author(s): S. Kindermann, T. Weigel, J. Biercamp, H. Thiemann
Presenter: T. Weigel, German Climate Computing Center, DKRZ

Workshop 27

International Workshop on Flow and Transport: Computational Challenges

W27a: Flow and Transport

Wed, 01 Jun 2011, 11:05 - 12:45 Room: Lecture Room 6

1. **Discontinuous Galerkin and Mixed-Hybrid Finite Element Approach to Two-Phase Flow in Heterogeneous Porous Media with Different Capillary Pressures**
Author(s): R. Fucik, J. Mikyska
Presenter: R. Fucik, FNSPE Czech Technical University in Prague
2. **A Family of Multipoint Flux Mixed Finite Element Methods for Elliptic Problems on General Grids**
Author(s): G. Xue, M.F. Wheeler, I. Yotov
Presenter: G. Xue, The University of Texas at Austin
3. **Application of higher-order methods in two-phase compositional simulation**
Author(s): J. Mikyška, A. Firoozabadi
Presenter: J. Mikyška, Czech Technical University in Prague
4. **Model reduction techniques for characterization of fractured subsurfaces**
Author(s): V. Ginting, M. Presho
Presenter: V. Ginting, Department of Mathematics, University of Wyoming, Laramie, Wyoming, USA

W27b: Flow and Transport

Wed, 01 Jun 2011, 14:40 - 16:20 Room: Lecture Room 6

1. **A Finite Difference Scheme for Double-Diffusive Unsteady Free Convection from a Curved Surface to a Saturated Porous Medium with a Non-Newtonian Fluid**
Author(s): M.F. El-Amin, S. Sun
Presenter: M.F. El-Amin, King Abdullah University of Science and Technology
2. **Algorithm for Time-dependent Shortest Safety Path on Transportation Networks**
Author(s): J. Wu, S. Jin, H. Ji, T. Srikanthan
Presenter: J. Wu, Tianjin Polytechnic University
3. **A discrete fracture model for two-phase flow with matrix-fracture interaction**
Author(s): J. Jaffré, M. Mnejja, J.E. Roberts
Presenter: J.E. Roberts, INRIA Paris-Rocquencourt
4. **A Comparative Study of Locally Conservative Numerical Methods for Darcy's Flows**
Author(s): X. Ye, J. Liu, L. Mu
Presenter: X. Ye, University of Arkansas at Little Rock

Workshop 28

Knowledge representation and applied models and metadata in computational science

W28a: Knowledge representation

Thu, 02 Jun 2011, 10:35 - 12:15 Room: Break Out 3

1. **Moving from dataset metadata to semantics in ecological research: a case in translating EML to OWL**
Author(s): M.A. Sicilia, E. Mena, E. García-Barriocanal, S. Sánchez-Alonso
Presenter: M.A. Sicilia, University of Alcalá
2. **Non-functional Aspects of Information Integration and Research on Web Science**
Author(s): I. Ruiz-Rube, J.M. Doderó, J. Stoitsis
Presenter: J.M. Doderó, University of Cádiz
3. **Impact of Different Pre-Processing Tasks on Effective Identification of Users' Behavioral Patterns in Web-based Educational System**
Author(s): M. Munk, M. Drlik
Presenter: M. Drlik, Constantine the Philosopher University in Nitra, Slovakia
4. **Model-driven adaptation of question answering systems for ambient intelligence by integrating restricted-domain knowledge**
Author(s): K. Vila, J.-N. Mazón, A. Ferrández
Presenter: K. Vila, Universidad de Alicante

Workshop 29

8th Workshop on Computational Finance and Business Intelligence

W29a: Computational Finance

Fri, 03 Jun 2011, 09:30 - 11:10 Room: Lecture Room 6

1. **Property Prices and Bank Lending: Some Evidence from China's Regional Financial Centres**
Author(s): X.W. Che, B. Li, K. Guo, J. Wang
Presenter: X.W. Che, School of Economics and Management, Beijing University of Aeronautics and Astronautics
2. **Modelling the mitigation impact of insurance in Operational Risk management**
Author(s): J.P. Li, S.L. Yi, J.C. Feng, Y. Shi
Presenter: J.P. Li, Institute of Policy and Management, Chinese Academy of Sciences
3. **Exploring the Value at Risk of Oil-exporting Country Portfolio: An Empirical Analysis from the FSU Region**
Author(s): X.L. Sun, L. Tang, W. He
Presenter: X.L. Sun, Institute of Policy and Management, Chinese Academy of Sciences
4. **A multi-country prosperity index by two-dimension singular spectrum analysis**
Author(s): J.W. Zhang, H.B. Xie, S.Y. Wang
Presenter: J.W. Zhang, Academy of Mathematics and Systems Science, Chinese Academy of Sciences

5. **AUC Maximizing Support Vector Machines with Feature Selection**
Author(s): Y.J. Tian, Y. Shi, W.J. Chen, X.J. Chen
Presenter: Y.J. Tian, Research Center on Fictitious Economy and Data Science, CAS, Beijing, China

W29b: Computational Finance

Fri, 03 Jun 2011, 13:15 - 14:55 Room: Lecture Room 6

1. **Credit risk evaluation model development using support vector based classifiers**
Author(s): P.D. Paulius Danenas, G.G. Gintautas Garsva, S.G. Saulius Gudas
Presenter: P.D. Paulius Danenas, Kaunas Faculty of Humanities, Vilnius University
2. **Monte Carlo scalable algorithms for Computational Finance**
Author(s): V.N. Alexandrov, C.G. Martel, J. Strassburg
Presenter: V.N. Alexandrov, ICREA research professor in computational science at BSC
3. **Simple Portfolio Strategies Utilizing Inflation Factor in Japanese Equity Market**
Author(s): K. Sato, K. Miyazaki, J. Mawaribuchi
Presenter: K. Sato, The University of Electro-Communications
4. **Second-order Mining for Active Collaborative Filtering**
Author(s): L.-F. Niu, J.-M. Wu, Y. Shi
Presenter: L.-F. Niu, Chinese Academy of Sciences
5. **Possibilistic risk aversion with many parameters**
Author(s): I. Georgescu, J. Kinnunen
Presenter: J. Kinnunen, IAMSR, Åbo Akademi University, Finland

Workshop 31

Executable Paper Challenge

W31a: Executable Paper Grand Challenge Finalists

Wed, 01 Jun 2011, 11:05 - 12:45 Room: Auditorium

Chair: Peter Sloot

1. **Executable Paper Grand Challenge Workshop**
Author(s): R. Capone, A. Gabriel
Presenter: R. Capone, Elsevier
2. **A data and code model for reproducible research and executable papers**
Author(s): K. Hinsén
Presenter: K. Hinsén, Centre de Biophysique Moléculaire, CNRS Orléans, France
3. **SHARE: a web portal for creating and sharing executable research papers**
Author(s): P.M.E. Van Gorp, S. Mazanek
Presenter: P.M.E. Van Gorp, Eindhoven University of Technology
4. **The Planetary System: Web 3.0 & Active Documents for STEM**
Author(s): M. Kohlhase, C. David, D. Ginev, A. Kohlhase, C. Lange, B. Matican, S. Mirea, V. Zholudev, C. Jucovschi, J. Corneli
Presenter: M. Kohlhase, Computer Science, Jacobs University

W31b: Executable Paper Grand Challenge Finalists

Wed, 01 Jun 2011, 14:40 - 16:20 Room: Auditorium

Chair: Peter Sloot

1. **The Collage Authoring Environment**
Author(s): P.N. Nowakowski, E.C. Ciepiela, T.B. Bartynski, M.M. Malawski, G.D. Dyk, J.K. Kocot, D.H. Harezlak, M.K. Kasztelnik, J.M. Meizner
Presenter: E.C. Ciepiela, ACC CYFRONET AGH
2. **Executable Papers for the R Community: The R2 Platform for Reproducible Research**
Author(s): F. Leisch, M. Eugster, T. Hothorn
Presenter: F. Leisch, Ludwig-Maximilians-Universität München, Germany
3. **A-R-E: The Author-Review-Execute environment**
Author(s): W. Müller, I. Rojas, A. Eberhart, P. Haase, M. Schmidt
Presenter: W. Müller, HITS gGmbH

W31c: Executable Paper Grand Challenge Finalists

Wed, 01 Jun 2011, 16:40 - 18:20 Room: Auditorium

Chair: Peter Sloot

1. **A Universal Identifier for Computational Results**
Author(s): M. Gavish, D.L. Donoho
Presenter: M. Gavish, Stanford University
2. **A Provenance-Based Infrastructure to Support the Life Cycle of Executable Papers**
Author(s): D. Koop, E. Santos, P. Mates, H.T. Vo, P. Bonnet, B. Bauer, B. Surer, M. Troyer, D.N. Williams, J.E. Tohline, J. Freire, C.T. Silva
Presenter: D. Koop, University of Utah
Paper Mâché: Creating Dynamic Reproducible Science
Author(s): T. Williams, G. Brammer, R. Crosby, S. Matthews
Presenter: T. Williams, Texas A&M University

W31d: Executable Paper Grand Challenge Papers

Thu, 02 Jun 2011, 10:35 - 12:15 Room: Auditorium

Chair: Peter Sloot

1. **IODA - an Interactive Open Document Architecture**
Author(s): B. Wiszniewski, J. Siciarek
Presenter: B. Wiszniewski, Gdansk University of Technology, Gdansk, Poland
2. **A natural language programming solution for executable papers**
Author(s): S.M. Veres, J.P. Adolfsson
Presenter: S.M. Veres, University of Southampton
3. **Supporting the Perpetuation and Reproducibility of Numerical Method Publications**
Author(s): D. Paredes, A.T.A. Gomes, F. Valentin
Presenter: D. Paredes, Coordenação de Matemática Aplicada e Computacional, Laboratório Nacional de Computação Científica - Brasil.
4. **LabWiki: An Executable Paper Platform for Experiment-based Research**
Author(s): G. Jourjon, T. Rakotoarivelo, C. Dwertmann, M. Ott
Presenter: G. Jourjon, NICTA, Australia

W31e: Executable Paper Grand Challenge Papers

Thu, 02 Jun 2011, 14:30 - 16:10 Room: Auditorium

1. **Toward Executable Scientific Publications**
Author(s): R.J. Strijkers, R. Cushing, D. Vasyunin, A.S.Z. Belloum, C. de Laat, R.J. Meijer
Presenter: R.J. Strijkers, UvA
2. **The IPOL Initiative: Publishing and Testing Algorithms on Line for Reproducible Research in Image Processing**
Author(s): N. Limare, J.-M. Morel
Presenter: N. Limare, CMLA, ENS Cachan, France
3. **Linked Open Science—Communicating, Sharing and Evaluating Data, Methods and Results for Executable Papers**
Author(s): T.J. Kauppinen, G. Mira de Espindola
Presenter: T.J. Kauppinen, Institute for Geoinformatics, University of Münster, Germany
4. **Towards a Universal Viewer for Digital Content**
Author(s): K. McHenry, M. Ondrejcek, L. Marini, R. Kooper, P. Bajcsy
Presenter: K. McHenry, National Center for Supercomputing Applications, University of Illinois at Urbana-Champaign

W31f: Executable Paper Grand Challenge Papers

Thu, 02 Jun 2011, 16:30 - 18:10 Room: Auditorium

Chair: Peter Soot

1. **Harnessing the Scientific Data Produced by the Experimental Evaluation of Search Engines and Information Access Systems**
Author(s): N. Ferro, A. Hanbury, H. Müller, G. Santucci
Presenter: N.F. Nicola Ferro, University of Padua, Italy
2. **The Prickly Pear Archive**
Author(s): S.R. Brandt, J. Tao, F. Loeffler, O. Korobkin, E. Schnetter, I. Hinder, D. Castleberry, M. Thomas
Presenter: E. Schnetter, Louisiana State University
3. **CARMEN**
Author(s): J. Austin, B. Liang, M. Weeks, L. Smith, T. Jackson, M. Fletcher, M. Jessop, C. Ingram, P. Watson
Presenter: J. Austin, University of York

Workshop 33

Large scale computational molecular science

W33a: Large Scale Computational Molecular Science

Wed, 01 Jun 2011, 11:05 - 12:45 Room: Lecture Room 2

Chair: H. Nakai

1. **High-performance ab initio density matrix renormalization group method for quantum chemical problems**
Author(s): Y.K. Kurashige, T.Y. Yanai
Presenter: Y.K. Kurashige, Institute for Molecular Science
2. **Theoretical studies on the internal configuration inversion in helical molecules**
Author(s): A. Muraoka
Presenter: A. Muraoka, Univ. of Tokyo

3. **An ab initio study of Xe–NO(X²) and Xe–NO(A²+) potential energy surfaces**

Author(s): K. Yamashita, J.C. Castro-Palacio, K. Ishii, J. Rubayo-Soneira
Presenter: K. Yamashita, The University of Tokyo

W33b: Large Scale Computational Molecular Science

Wed, 01 Jun 2011, 14:40 - 16:20 Room: Lecture Room 2

Chair: S. Sakaki

1. **Construction of orbital-specific hybrid functional by imposing the linearity condition for orbital energies in density functional theory**

Author(s): Y. Imamura, R. Kobayashi, H. Nakai
Presenter: Y. Imamura, Waseda University

2. **On exchange interactions in large systems**

Author(s): T.T. Tsuneda
Presenter: T.T. Tsuneda, RIKEN

3. **The Fragment Molecular Orbital Method and Massively Parallel Computations**

Author(s): K. Kitaura
Presenter: K. Kitaura, Kyoto University

W33c: Large Scale Computational Molecular Science

Wed, 01 Jun 2011, 16:40 - 18:20 Room: Lecture Room 2

Chair: S. Nagase

1. **Electronic excited states of macrocyclic compounds: direct SAC-CI study**

Author(s): R. Fukuda
Presenter: R. Fukuda, Institute for molecular science

2. **Linear-scaling electronic structure calculation program based on divide-and-conquer method**

Author(s): H. Nakai, M. Kobayashi
Presenter: H. Nakai, Department of Chemistry and Biochemistry, School of Advanced Science and Engineering, Waseda University, Japan

3. **Structure Prediction of Clusters, Solids and Molecules by Global Geometry Optimization**

Author(s): S. Goedecker
Presenter: S. Goedecker

W33d: Large Scale Computational Molecular Science

Thu, 02 Jun 2011, 10:35 - 12:15 Room: Lecture Room 2

Chair: K. Yamashita

1. **A combination of the Tree code and IPS method to simulate large scale systems by molecular dynamics**

Author(s): K. Takahashi, R. Sakamaki, R. Yokota, L. Barba, T. Narumi, K. Yasuoka
Presenter: K. Takahashi, Department of Mechanical Engineering, Keio University, Yokohama, Japan

2. **Hydration Effect on Functional, Self-Organizing Systems in Aqueous Solution**

Author(s): N. Matubayasi
Presenter: N. Matubayasi, Kyoto University

3. **Computer Simulation of Surface Nonlinear Spectroscopy**

Author(s): A. Morita, T. Ishiyama, K. Shiratori
Presenter: A. Morita, Tohoku University

4. **Molecular Dynamics Study of Micelles and Lipid Bilayers**
Author(s): S. Okazaki, Y. Andoh, K. Fujimoto, N. Yoshii
Presenter: S. Okazaki, Department of Applied Chemistry, Nagoya University

Workshop 34

Poster Session

W34a: Posters

Thu, 02 Jun 2011, 12:15 - 13:35 Room: Lobby

1. **Macroscopic simulation for the internal dynamics of nano processes in ball mills**
Author(s): L.T. Handoko, G.K. Sunnardianto
Presenter: L.T. Handoko, Research Center for Physics, Indonesian Institute of Sciences
2. **Problems of antimatter evolution after Big Bang. Solutions in the frame of non-local physics.**
Author(s): B.V. Alexeev
Presenter: B.V. Alexeev, Moscow Fine Chemical Technology Institute
3. **Using reinforcement learning to vary the m in GMRES(m)**
Author(s): T.-Y. Chen, L. Peairs
Presenter: L. Peairs, Pomona College
4. **Problems of dark energy and dark matter. Solutions in the frame of non-local physics.**
Author(s): B.V. Alexeev
Presenter: B.V. Alexeev, Moscow Academy of Fine Chemical Technology, Prospekt Vernadskogo,86, Moscow 119570, Russia
5. **Resource Selection Algorithms for Economic Scheduling in Distributed Systems**
Author(s): V.V. Toporkov, A.S. Toporkova, A.V. Bobchenkov, D.M. Yemelyanov
Presenter: V.V. Toporkov, Moscow Power Engineering Institute, Computer Science Department
6. **Numerical determination of turbulization start coordinates in the jet with electrical and gas dynamics (EGD) jet control in automatic systems.**
Author(s): I.A. Mashkov, V.S. Nagorny
Presenter: I.A. Mashkov, State Polytechnical University, Saint-Petersburg, Russia
7. **A New Method for Scheduling Divisible Data on a Heterogeneous Two-Levels Hierarchical System**
Author(s): A. Shokripour, M. Othman, H. Ibrahim, S. Subramaniam
Presenter: A. Shokripour
8. **New Parallel Algorithm for Simulation of Spin-Glass System on Scales of Space-Time Periods**
Author(s): A.S. Gevorkyan, H.G. Abajyan, H.S. Sukiasyan
Presenter: A.S. Gevorkyan, Institute for Informatics and Automation Problems, NAS of Armenia
9. **Parallel GMRES Incomplete Orthogonalisation Auto-Tuning**
Author(s): P.-Y. Aquilanti, S. Petiton, H. Calandra, M. Hugues
Presenter: M. Hugues, CNRS - LIFL
10. **Implicit Second Order Weak Taylor Tau-Leaping Methods for the Stochastic Simulation of Chemical Kinetics**
Author(s): T.-H. Ahn, A. Sandu
Presenter: T.-H. Ahn, Virginia Polytechnic Institute and State University

11. **Demand-driven Movement Strategy for Moving Beacons in Distributed Sensor Localization**
Author(s): A. Iqbal, M. Murshed
Presenter: M. Murshed, Monash University
12. **Parallel Computing Flow Accumulation in Large Digital Elevation Models**
Author(s): H.-T. Do, S. Limet, E. Melin
Presenter: S. Limet, LIFO--Université d'Orléans
13. **Strategies for Fault Tolerance in Multicomponent Applications**
Author(s): A.G. Shet, W.R. Elwasif, S.S. Foley, B.H. Park, D.E. Bernholdt, R. Bramley
Presenter: D.E. Bernholdt, Oak Ridge National Laboratory
14. **Towards ensuring Satisfiability of Merged Ontology**
Author(s): M. Fahad, N. Moalla, A. Bouras
Presenter: M. Fahad, LIESP lab, University of Lyon2, France
15. **Parallel estimation of the cost function for the flexible scheduling problem**
Author(s): W. Bozejko, M. Uchroński, M. Wodecki
Presenter: W. Bozejko, Wrocław University of Technology
16. **A Multilevel Cholesky Conjugate Gradients Hybrid Solver for Linear Systems with Multiple Right-hand Sides**
Author(s): J.D. Booth, A. Chatterjee, P. Raghavan, M.R. Frasca
Presenter: P. Raghavan, The Pennsylvania State University
17. **Distributed Contract Negotiation System for Virtual Organizations**
Author(s): B. Kryza, M. Stelmach, R. Słota, J. Kitowski
Presenter: B. Kryza, Academic Computer Centre CYFRONET AGH, Krakow, Poland
18. **Global advection transport model on hexagonal-pentagonal geodesic grid by multi-moment scheme**
Author(s): J.Z. Bin, C.G. Chen, F. Xiao
Presenter: C.G. Chen, LHD, Institute of Mechanics, Chinese Academy of Sciences
19. **The lower vortical structure past the Ahmed car model**
Author(s): G. Alfonsi, L. Lauria, L. Primavera
Presenter: G. Alfonsi, Università della Calabria - Italy
20. **A Multi-Scale Electromagnetic Particle Code with Adaptive Mesh Refinement and Its Parallelization**
Author(s): H. USUI, M. Nunami, T. Moritaka, T. Matsui, Y. Yagi
Presenter: H. USUI, Graduate School of System Informatics, Kobe University, JAPAN
21. **On some recent achievements of earthquake simulation**
Author(s): M. Hori, T. Ichimura
Presenter: M. Hori, University of Tokyo
22. **A Comparison of Lock-based and Lock-free Taskpool Implementations in Haskell**
Author(s): M. Lesniak
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