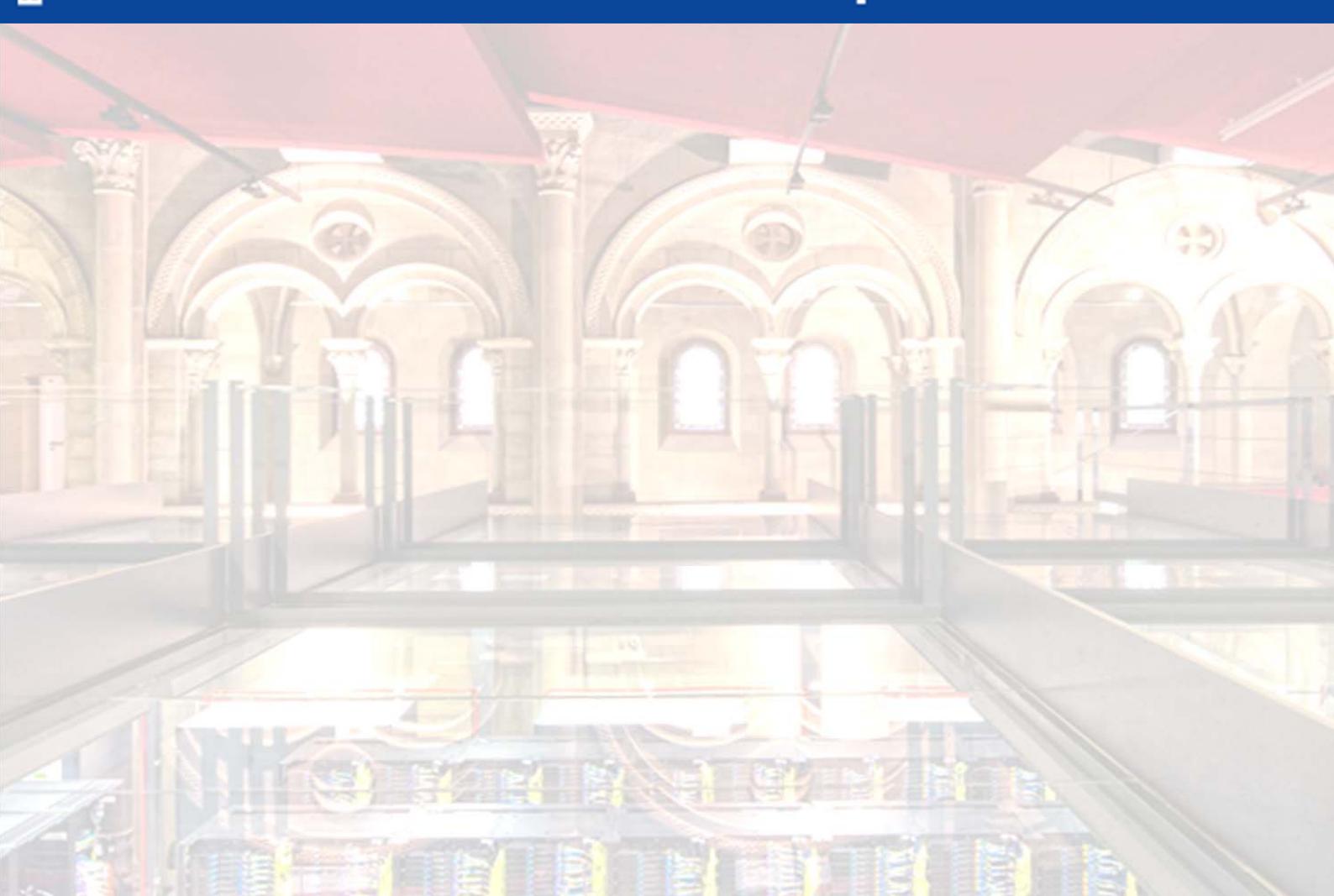


Barcelona, Spain  
**iccs**  
5-7 June **2013**



## International Conference on Computational Science



\***iCrea**

INSTITUICIÓ CATALANA DE  
RECERCA I ESTUDIS AVANÇATS



**Barcelona  
Supercomputing  
Center**

Centro Nacional de Supercomputación



EXCELENCIA  
SEVERO  
OCHOA

THE UNIVERSITY of TENNESSEE

KNOXVILLE



UNIVERSITEIT VAN AMSTERDAM



**NANYANG  
TECHNOLOGICAL  
UNIVERSITY**



**GS** Garland Science  
Taylor & Francis Group



**ho** COMPUTER  
compiler & tools

# **Conference Information**

## **Operating Hours of Registration Desk**

Wed, 05 June 9:00- 19:00

Thu, 06 June 9:00- 19:00

Fri, 07 June 9:00- 12:15

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.

## **Social Program**

- Welcome Reception

Date: Wed, 05 June 19:30-21:30

Venue: CCIB Banquette Hall, Niveau P2

- Conference Dinner & Award Ceremony

Date: Thu, 06 June 20:30-22:30

Venue: CCIB Banquette Hall, Niveau P2

*Tickets for the Conference Dinner & Award Ceremony are on sale throughout the first day of the conference at the reception and registration desk.*

## **Instruction for Speakers**

The allocation of time is as follows:

Keynote lecture: 45 minutes

Oral Presentation: 20 minutes

## **Instruction for Poster Session**

The poster presentations will take place in the 2<sup>nd</sup> floor lunch & coffee rooms 211 & 212. The size of one poster board is A0 size. Posters should be displayed on the boards using tape that

will be available from the organizers.

Presenters are asked to place their poster on the boards before their session. All posters will be hanging throughout the first two days of the conference.

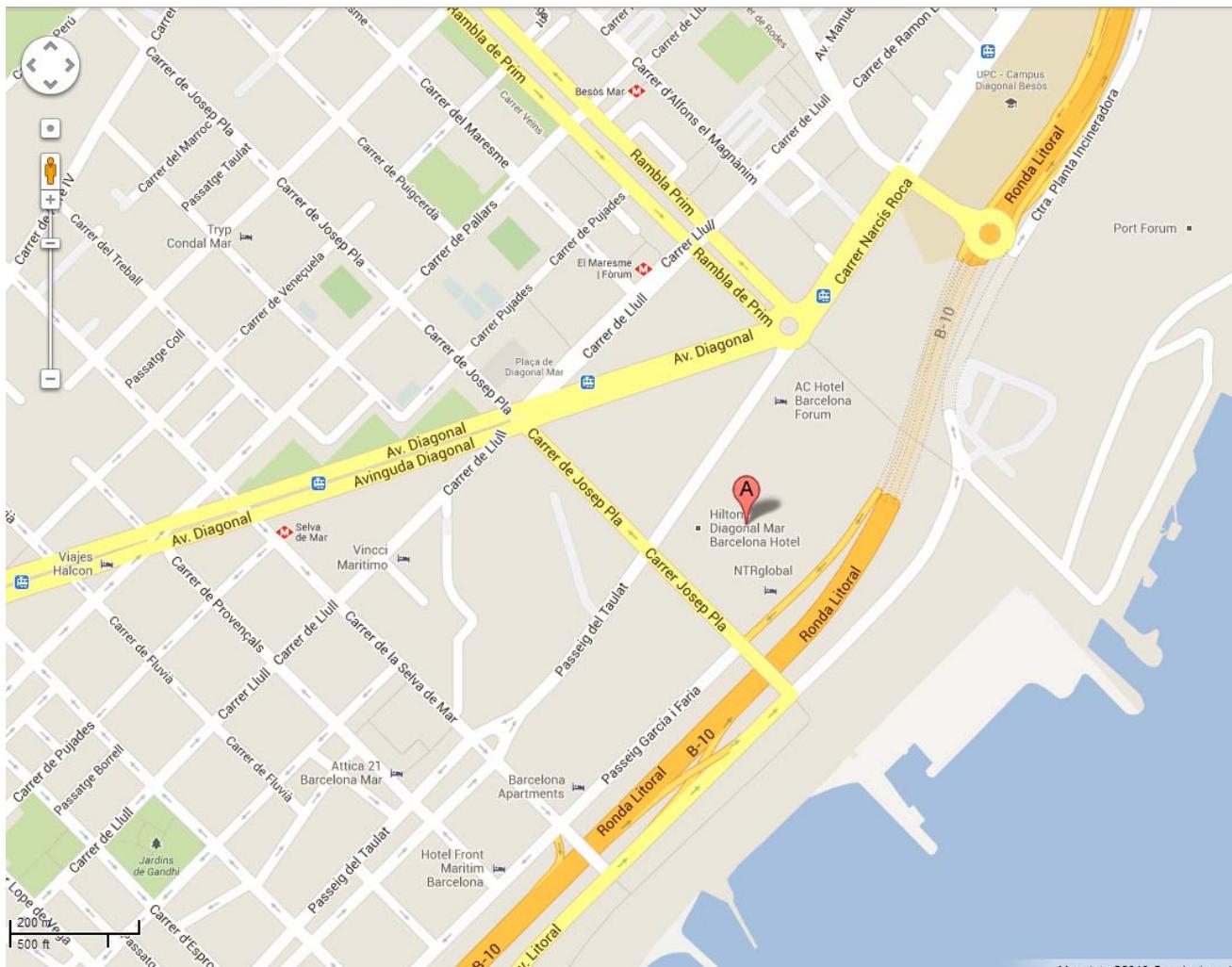
Presentation sessions:

- Wed, 05 June 13:20 – 13:50
- Thu, 06 June 13:20 – 13:50

Removal Thu, 06 June 16:30-19:30

During the presentation sessions, 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



## PRIVATE VEHICLE

If you are driving to the CCIB from the city centre, the best way to cross the city is by driving down Avenida Diagonal to the end of this avenue.

The most direct way to reach the CCIB from the airport or from outside the city is by using the Ronda Litoral (the city's coastal ringroad) and taking Salida (exit) 24.

It takes approximately 25 minutes to reach us from the airport or the city centre, depending on traffic.

## FROM & TO THE AIRPORT

El Prat airport is 13 km southeast of Barcelona and 20 km from the CCIB.

The main road artery C-31 connects the airport directly with Barcelona. To enter the city, take either of the avenues Gran Via or Avenida Diagonal – these offer the most direct road access to the city centre. Alternatively take either of the two ringroads, the Ronda de Dalt (upper) or Ronda Litoral (coastal), which circle the city.

## AIRPORT BUS

The bus shuttle service between the airport and Barcelona city centre (Plaza Cataluña) runs from 06.00 a.m. to 01.00 a.m. (airport > Barcelona) and from 05:30 to 00:15 (Barcelona > airport) every day.

Buses leave every 10-12 minutes and the trip takes around 30 minutes.

## TAXI

The trip by taxi takes approximately 20 minutes. Fares change according to the time of day (officially established fare timetable).

## PUBLIC TRANSPORT IN THE CITY

To find out the best ways of moving around the city of Barcelona by train, bus, metro and tram, please visit the following websites:

By bus and metro: Transports Municipals de Barcelona [www.tmb.cat](http://www.tmb.cat)

For local and regional trains: FGC and Rodalies de Catalunya. [www.renfe.es](http://www.renfe.es) [www.fgc.cat](http://www.fgc.cat)

**Metro** station *Urquinaona* is around 200 m from Plaza Cataluña and is on Metro line L4 (yellow): this line takes you directly to the *Maresme-Fòrum* Metro station.

You can also reach the CCIB by **bus**, using the lines 7 or 41, and by tram, alighting at the Fòrum tram stop.

Any of these means of public transport will drop you just a few steps from the CCIB.

## Floor Plan

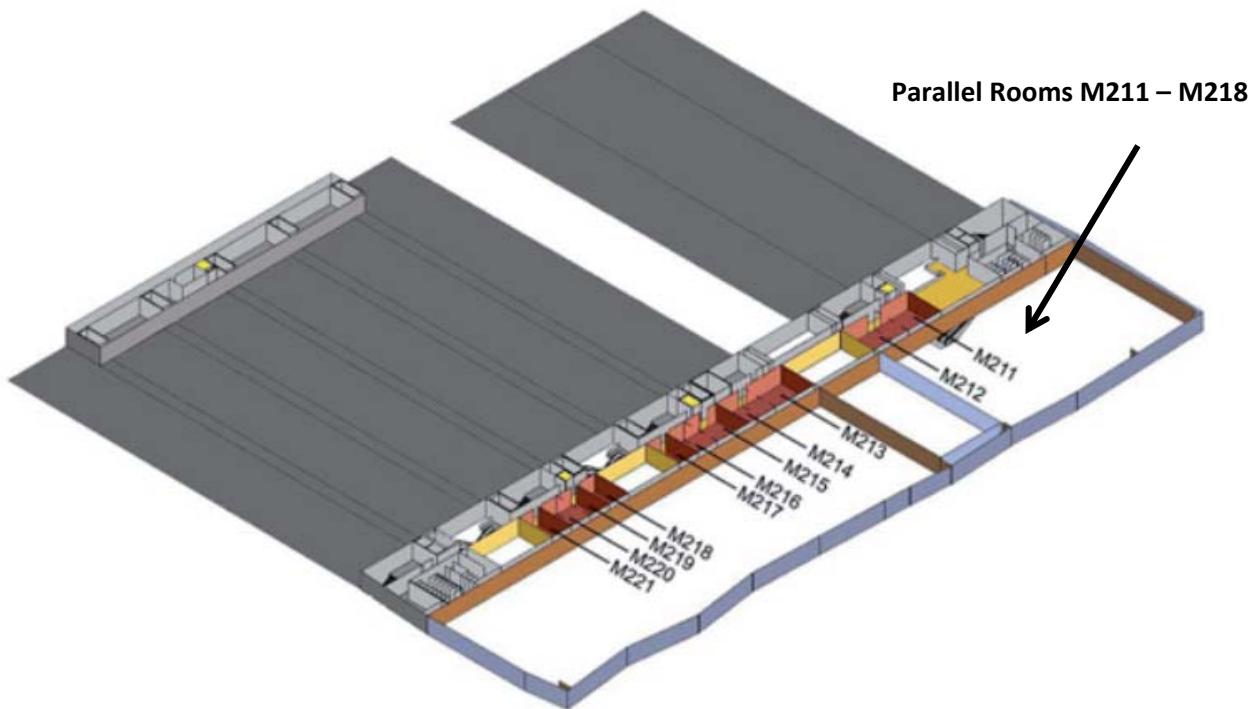
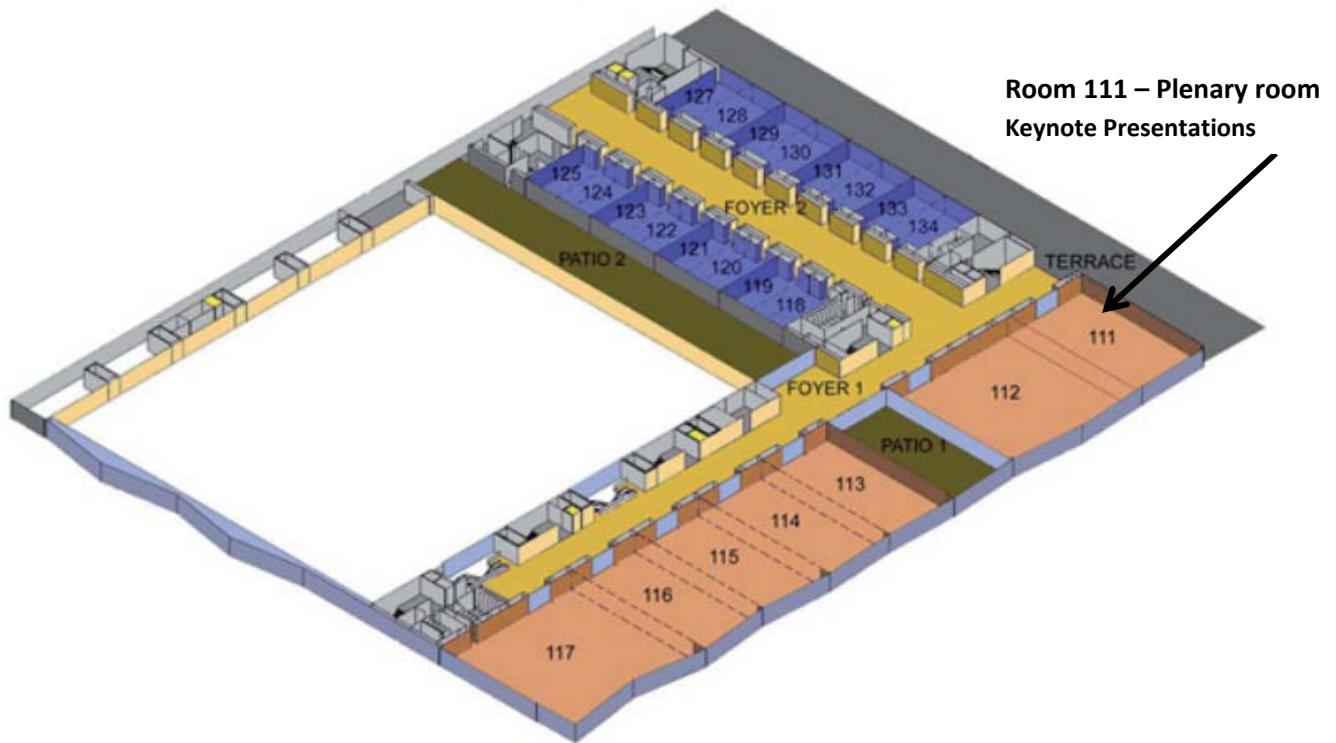
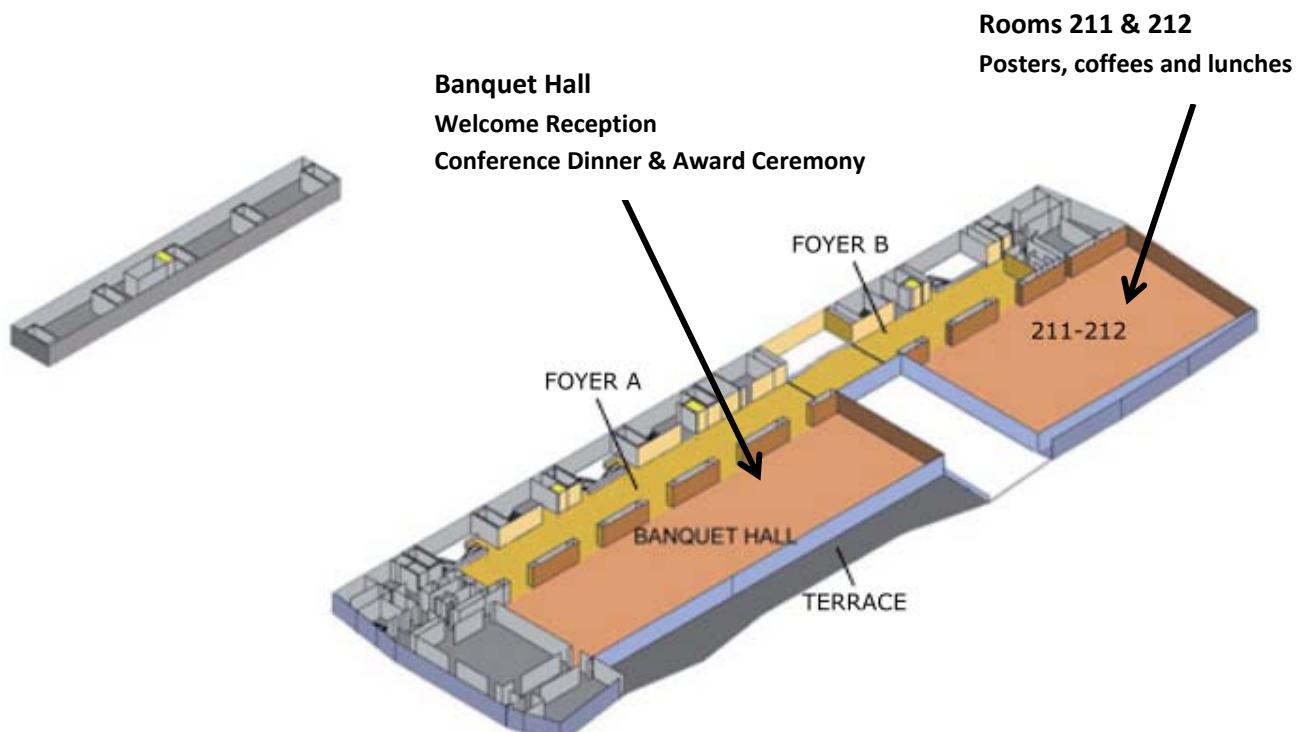


Figure 1 NIVEAU M2



**Figure 2 NIEVAU P1**



**Figure 3 NIVEAU P2**

## Program at a glance

### Day 1 – 5<sup>th</sup> of June 2013

	9:00	10:00	11:00	12:00	13:00	14:00	15:00	16:00	17:00	18:00	19:00	
	Opening Address		Keynote: Thierry van der Pyl	Keynote: David De Roure	Lunch 12:30 - 13:30	Session One 13:50 - 15:30		Session Two 15:50 - 17:30		Session Three 17:45 - 19:25		
Room 111						M01		M02		M03		
Room M211						M04		M05		M06		
Room M212						WS4a		WS4b		WS4c		
Room M213						WS32a		WS32b		WS32c		
Room M214	Registration					WS33a	Coffee				Break	
Room M215						WS48a		WS20a		WS20b		
Room M216						WS63a		WS63b		WS63c		
Room M217						WS23a		WS23b				
Room M218						WS3a		WS3b		WS18a		

### Day 2 – 6<sup>th</sup> of June 2013

	9:00	10:00	11:00	12:00	13:00	14:00	15:00	16:00	17:00	18:00	19:00		
	Session Four 10:50 - 12:30				Lunch	Poster Session Two	Session Five 15:15 - 16:55		Session Six 17:15 - 18:45				
Room 111	Keynote: Hesham Ali	Keynote: Raymond Winslow					M07		M08		M09		
Room M211							M10		M11		M12		
Room M212							WS35a		WS35b				
Room M213							WS09a		WS09b		WS09c		
Room M214	Coffee						WS52a		WS52b	Coffee	WS10a		
Room M215							WS38a		WS38b		WS38c		
Room M216							WS63d		WS63e				
Room M217							WS21a		WS21b		WS21c		
Room M218									WS36a		WS36b		

## Day 3 – 7<sup>th</sup> of June 2013

	9:00	10:00	11:00	12:00	13:00	14:00	15:00
	Session Seven 10:35 - 12:15				Session Eight 13:35 - 15:15		
Room 111	Keynote: Steve Furber		M13			M14	
Room M211			M16				
Room M212			M15			WS42a	
Room M213	Coffee		WS43a			WS43b & WS9d	
Room M214			WS10b		Lunch	WS10c	
Room M215			WS38d			WS38e	
Room M216			WS53a			WS53b	
Room M217			WS47a			WS47b	
Room M218			WS31a			WS31b	

## Plenary Program

All presentations to be held in room 111

Speakers	Session	Chair
<b>Welcome Address 1</b> Prof. Jaume Bertranpetit ICREA Director	5th of June 10:00	Vassil Alexandrov
<b>Welcome Address 2</b> Prof. Mateo Valero BSC-CNS Director	5th of June 10:00	Vassil Alexandrov
<b>Keynote 1</b> Dr Thierry van der Pyl DG CONNECT, European Commission  <i>„The European HPC strategy for growth and Jobs“</i>	5th of June 11:00	Vassil Alexandrov
<b>Keynote 2</b> Prof. David De Roure Oxford e-Research Centre, UK  <i>“Web Scale Music Analysis: a grand challenge in computational musicology”</i>	5th of June 11:00	Vassil Alexandrov
<b>Keynote 3</b> Prof. Hesham Ali University of Nebraska, Omaha, USA  <i>“High Performance Computing in Bioinformatics: A focus on next generation data analysis and integration tools”</i>	6th of June 09:00	Peter Sloot
<b>Keynote 4</b> Prof. Raimond Winslow The Johns Hopkins University, Baltimore MD, USA  <i>“The Emerging Discipline of Computational Medicine“</i>	6th of June 09:00	Peter Sloot
<b>Keynote 5</b> Prof. Vladimir Voevodin Moscow State University, Russia  <i>“Educational Landscape of the Exascale Future“</i>	6th of June 13:50	Jack Dongara
<b>PRACE</b> Marjolein Oorsprong	6th of June 14:35	Jack Dongara
<b>ho-Computers</b> Harald Odendahl	6th of June 14:55	Jack Dongara
<b>Keynote 6</b> Prof. Steve Furber University of Manchester, UK  <i>“Biologically-Inspired Massively-Parallel Computation”</i>	7th of June 09:30	Peter Sloot

## Conference sessions

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### Session 1

5<sup>th</sup> of June 2013

13:50 – 15:30

#### M01: Main Track One

13:50 - 15:30  
111

Chair: Ana Cortes

1. **Throughput constrained parallelism reduction in cyclo-static dataflow applications**  
Author(s): S. Carov, L. Cudennec, R. Sirdey  
Presenter: S. Carov, Embedded Real Time Systems Laboratory, CEA, LIST
2. **Interactive data mining by using multidimensional scaling**  
Author(s): W. DZWINEL, P. Pawliczek  
Presenter: W. DZWINEL, AGH University of Science and Technology
3. **Immunological-Based Approach for Accurate Fitting of 3D Noisy Data Points with Bezier Surfaces**  
Author(s): A. Iglesias Prieto, A. Galvez Tomida, A. Avila  
Presenter: A. Iglesias, University of Cantabria, Santander, Spain
4. **High performance computing in biomedical applications**  
Author(s): S. Bastrakov, I. Meyerov, V. Gergel, A. Gonoskov, A. Gorshkov, E. Efimenko, M. Ivanchenko, M. Kirillin, A. Malova, G. Osipov, V. Petrov, I. Surmin, A. Vildemanov  
Presenter: S. Bastrakov, State University of Nizhni Novgorod
5. **Interactive Molecular Dynamics: Scaling up to Large Systems**  
Author(s): M. Dreher, M. Piuzzi, A. Turki, M. Chavent, M. Baaden, N. Férey, S. Limet, B. Raffin, S. Robert  
Presenter: M. Dreher, INRIA - France

#### M04: Main Track Four

13:50 - 15:30  
M211

Chair: Tomas Margalref

1. **Self-Checking Spreadsheets: Recognition of Semantics**  
Author(s): M.E.M. Stewart  
Presenter: M.E.M. Stewart
2. **Elastic Memory Management of Virtualized Infrastructures for Applications with Dynamic Memory Requirements**  
Author(s): G. Moltó, M. Caballer, E. Romero, C. de Alfonso  
Presenter: G. Moltó, Universitat Politècnica de València
3. **Achieving Checkpointing Global Consistency through a Hybrid Compile Time and Runtime Protocol**  
Author(s): I. Cores, G. Rodríguez, M.J. Martín, P. González  
Presenter: I. Cores, University of A Coruña
4. **Predictive and distributed routing balancing, an application-aware approach**  
Author(s): C. Núñez Castillo, D. Lugones, D. Franco, E. Luque, M. Collier  
Presenter: C. Núñez Castillo, Universitat Autònoma de Barcelona
5. **Fault Tolerance Properties of Gossip-Based Distributed Orthogonal Iteration Methods**  
Author(s): H. Strakova, G. Niederbrucker, W.N. Gansterer  
Presenter: W.N. Gansterer, University of Vienna

**[W03a: 7th Workshop on Computational Chemistry and Its Applications](#)**13:50 - 15:30  
M218

Chair: P. Ramasami

1. **A density functional theory investigation on the properties of supramolecular catalysts for photoinitiated electron collection**  
Author(s): X. Duan, R. Pachter, K. Brewer, B. Farmer  
Presenter: R. Pachter, Air Force Research Laboratory, Materials & Manufacturing Directorate, Wright-Patterson Air Force Base, Ohio USA 45433
2. **Determination of the kinetic constants of a chemical reaction in heterogeneous phase using parameterized metaheuristics**  
Author(s): J.M. Cutillas-Lozano, D. Giménez  
Presenter: J.M. Cutillas-Lozano, Departamento de Informática y Sistemas, Universidad de Murcia, Spain
3. **TD-DFT Study of Excited-State Intramolecular Proton Transfer (ESIPT) of 2-(1,3-Benzothiazol-2-yl)-5-(N,N-Diethylamino)phenol with benzoxazole and benziidazole analogues**  
Author(s): V. Padalkar, P. Ramasami, N. Sekar  
Presenter: N. Sekar, Institute of Chemical Technology, Mumbai 400019, India
4. **Probing the structure and reactivity of Reactive Intermediates with Photoionization and Quantum Chemistry calculations**  
Author(s): J. Dyke  
Presenter: J. Dyke, University of Southampton

**[W04a: The 4th Workshop on Computational Optimization, Modelling and Simulation \(COMS2013\)](#)**13:50 - 15:30  
M212

Chairs: X.S. Yang, S. Koziel, L. Leifsson

1. **Sketch Arm, custom closets rapid prototyping system**  
Author(s): I.R.C. Iván Rodríguez Conde, S.G.M. Silvana Gómez Meire, E.B.A. Enrique Barreiro Alonso, J.R.I. Javier Rodeiro Iglesias, C.C.B. Celso Campos Bastos  
Presenter: I.R.C. Iván Rodríguez Conde, University of Vigo
2. **Multi-objective Flower Pollination Algorithm for Optimization**  
Author(s): X.S. Yang, M. Karamanoglu, X.S. He  
Presenter: X.S. Yang, Middlesex University
3. **Computational Optimization, Modelling and Simulations: Recent Trends and Challenges**  
Author(s): X.S. Yang, S. Koziel, L. Leifsson  
Presenter: X.S. Yang, Middlesex University
4. **Physics-Based Surrogates for Low-Cost Modeling of Microwave Structures**  
Author(s): S. Koziel, S. Ogurtsov, L. Leifsson  
Presenter: S. Koziel, Reykjavik University
5. **Optimizing bicriteria flow shop scheduling problem by simulated annealing algorithm**  
Author(s): D. Zelazny, J. Pempera, C. Smutnicki  
Presenter: D. Zelazny, Institute of Computer Engineering, Control and Robotics, Wroclaw University of Technology, Poland

**[W23a: 6th Workshop on "Biomedical and Bioinformatics Challenges for Computer Science" \(BBC 2013\)](#)**13:50 - 15:30  
M217*Chair: M. Cannataro*

1. **Detecting Differentially Co-expressed Genes for Drug Target Analysis**  
Author(s): T. Arodz, X. Gao  
Presenter: X. Gao, Department of Computer Science, Virginia Commonwealth University
2. **Fast comparison of microbial genomes using the Chaos Games Representation for metagenomic applications**  
Author(s): M.T. Swain  
Presenter: M.T. Swain, Aberystwyth University
3. **MetFlexo: an Automated Simulation of Realistic H1-NMR Spectra**  
Author(s): Z. Atieh, K. Suhre, H. Bensmail  
Presenter: H. Bensmail, Qatar Computing research Institute
4. **Modeling the evolution of gene regulatory networks for spatial patterning in embryo development**  
Author(s): A.V. Spirov, D.M. Holloway  
Presenter: A.V. Spirov, SUNY Stony Brook, New York
5. **Estimation of Volume Rendering Efficiency with GPU in a Parallel Distributed Environment**  
Author(s): C. Cristian Federico Perez Monte, C. Cristian Luciano, S. Silvio Rizzi, F. Fabiana Piccoli, G. German Bianchini, P. Paola Caymes Scutari  
Presenter: C. Cristian Federico Perez Monte, Grupo Gridtics - Universidad Tecnológica Nacional - Facultad Regional Mendoza

**[W32a: Agent-Based Simulations, Adaptive Algorithms and Solvers](#)**13:50 - 15:30  
M213*Chair: M. Paszynski*

1. **Nosolink: An agent-based approach to link patient flows and staff organization with the circulation of nosocomial pathogens in an intensive care unit.**  
Author(s): J. Ferrer Savall, M. Salmon, L. Temime  
Presenter: J. Ferrer Savall, Conservatoire National des Arts et Metiers
2. **Markov Chain Analysis of Agent-based Evolutionary Computing in Dynamic Optimization**  
Author(s): A. Byrski, R. Schaefer  
Presenter: R. Schaefer, AGH University of Science and Technology
3. **Evacuation Simulation supporting high level Behaviour-based Agents**  
Author(s): P.C. Tissera, A.D. Castro, A.M. Printista, E. Luque  
Presenter: E. Luque, Departamento de Arquitectura de Computadores y Sistemas Operativos - Universidad Autónoma de Barcelona
4. **Robot Task Allocation using Signal Propagation Model**  
Author(s): M. Zabinska, T. Sosnicki, W. Turek, K. Cetnarowicz  
Presenter: T. Sosnicki, AGH University of Science and Technology
5. **HPC enhanced large urban area evacuation simulations with vision based autonomously navigating multi agents**  
Author(s): M.L.L. Wijerathne, L.A. Melgar, M. Hori, T. Ichimura, S. Tanaka  
Presenter: M.L.L. Wijerathne, Earthquake Research Institute, the University of Tokyo

**W33a: Architecture, Languages, Compilation and Hardware support for Emerging ManYcore systems  
(ALCHEMY 2013)**

13:50 -  
15:30  
M214

Chair: L. CUDENNEC

1. **Extended Cyclostatic Dataflow Program Compilation and Execution for an Integrated Manycore Processor**  
Author(s): P. Aubry, P.-E. Beaucamps, F. Blanc, B. Bodin, S. Carpo, L. Cudennec, V. David, P. Dore, P. Dubrulle, B. Dupont de Dinechin, F. Galea, T. Goubier, M. Harrand, S. Jones, J.-D. Lesage, S. Louise, N. Morey Chaisemartin, T.H. Nguyen, X. Raynaud, R. Sirdey  
Presenter: R. Sirdey, CEA LIST
2. **A Dedicated Micro-Kernel to Combine Real-Time and Stream Applications on Embedded Manycores**  
Author(s): P. Dubrulle, E. Ohayon  
Presenter: P. Dubrulle, CEA
3. **PACHA : Low Cost Bare Metal Development for Shared Memory Manycore Accelerators**  
Author(s): A. Aminot, A. Guerre, J. Peeters, Y. Lhuillier  
Presenter: A. Aminot, CEA, LIST, Embedded Computing Laboratory, F-91191 Gif-sur-Yvette, France.
4. **A Distributed Run-Time Environment for the Kalray MPPA-256 Integrated Manycore Processor**  
Author(s): B. Dupont de Dinechin, P. Guironnet de Massas, G. Lager, C. Léger, B. Orgogozo, J. Reybert, T. Strudel  
Presenter: B. Dupont de Dinechin, Kalray S.A.
5. **Limits of Instruction-Level Parallelism Capture.**  
Author(s): B. Goossens, D. Parello  
Presenter: B. Goossens, Université de Perpignan, France

**W48a: Large Scale Computational Physics**

13:50 - 15:30  
M215

Chair: E.H.J. DE DONCKER

1. **Evaluation of x32-ABI in the Context of LHC Applications**  
Author(s): N. Rauschmayr, A. Streit  
Presenter: N. Rauschmayr, CERN - European Organization for Nuclear Research, Switzerland
2. **Applying high-performance computing to petascale explosive simulations**  
Author(s): J.R. Peterson, C.A. Wight, M. Berzins  
Presenter: J.R. Peterson, University of Illinois at Urbana-Champaign
3. **Hardware acceleration of an efficient and accurate proton therapy Monte Carlo**  
Author(s): T.H.O. Thomas H. Osiecki, M.T. Min-yu Tsai, A.E.G. Anne E. Gattiker, D.A.J. Damir A. Jamsek, S.R.N. Sani R. Nassif, W.E.S. W. Evan Speight, C.N.S. Cliff C. N. Sze  
Presenter: T.H.O. Thomas H. Osiecki, IBM Research, Austin, TX
4. **High Performance Solvers for Implicit Particle in Cell Simulation**  
Author(s): P. kumar, S. Markidis, G. Lapenta, K. Meerbergen, D. Roose  
Presenter: P. Kumar, KU Leuven

**W63a: Second International Young Scientists Conference 2013 "HPC technologies and computer modeling" (YSC 2013)**

13:50 -  
15:30  
M216

*Chair: Alexander Boukhanovsky*

1. **YSC-2013: Foreword**  
Author(s): A.V. Boukhanovsky  
Presenter: A.V. Boukhanovsky, University ITMO
2. **A Service-Oriented Platform for Building and Composing Computational Web Services**  
Author(s): O. Sukhoroslov  
Presenter: O. Sukhoroslov, Institute for Information Transmission Problems
3. **Visual EasyFlow scripts editor**  
Author(s): E. Alymova  
Presenter: E. Alymova, Southern Federal University
4. **Consolidation of heterogeneous HPC monitoring data: approach and architecture processing**  
Author(s): D. Ustalov  
Presenter: D. Ustalov, Institute of Mathematics and Mechanics
5. **CLAVIRE-based personal clouds for eScience**  
Author(s): T. Churov  
Presenter: T. Churov, University ITMO

## Session 2

5<sup>th</sup> June 2013

15:50 – 17:30

### M02: Main Track Two

15:50 - 17:30  
111

Chair: Ana Cortes

1. **Data analysis with intersection graphs**

Author(s): V. M. Vairinhos, V. Lobo, P. Galindo Villardón

Presenter: V. M. Vairinhos, Centro de Investigação Naval, Escola Naval, Almada 2810-001, Portugal

2. **n-step FM-Index for faster pattern matching**

Author(s): A. Chacón, J.C. Moure, A. Espinosa, P. Hernández

Presenter: A. Chacón, Computer Architecture & Operating Systems Department, Universitat Autònoma de Barcelona, Spain

3. **Model of QoS Management in a Distributed Data Sharing and Archiving System**

Author(s): D. Nikolow, R. Slota, S. Polak, D. Mitera, M. Pogoda, P. Winiarczyk, J. Kitowski

Presenter: D. Nikolow, AGH University of Science and Technology

4. **InSpace3D: A Middleware for Built Environment Data Access and Analytics**

Author(s): C. Schultz, M. Bhatt

Presenter: C. Schultz, University of Bremen

5. **Non locality, topology, formal languages: new global tools to handle large data sets**

Author(s): E. Merelli, M. Rasetti

Presenter: E. Merelli, University of Camerino, Italy

### M05: Main Track Five

15:50 - 17:30  
M211

Chair: Tomas Margalref

1. **Algorithmic Differentiation of a Complex C++ Code with Underlying Libraries**

Author(s): M. Sagebaum, N.R. Gauger, U. Naumann, J. Lotz, K. Leppkes

Presenter: M. Sagebaum, Computational Mathematics Group, Department of Mathematics and Center for Computational Engineering Science, RWTH Aachen

2. **A STUDY ON RELEVANCE OF STUDENT'S ATTITUDE, IMPLEMENTING AN INTERDISCIPLINARY APPROACH IN A POSTGRADUATE PROGRAM**

Author(s): P.K. Ragunath, R. Ravi Mohan

Presenter: P. Venkateshan, Sri Ramachandra University, India

3. **SANComSim: A Scalable, Adaptive and Non-intrusive framework to optimize performance in Computational Science applications**

Author(s): A. Núñez, R. Filgueira, M.G. Merayo

Presenter: A. Núñez, Universidad Complutense de Madrid

4. **Comparing support vector machines and artificial neural networks in the recognition of steering angle for driving of mobile robots through paths in plantations**

Author(s): D.S. Jodas, N. Marranghello, A.S. Pereira, R.C. Guido

Presenter: D.S. Jodas, Sao Paulo State University

5. **An Empirical Evaluation of the Cost and Effectiveness of Structural Testing Criteria for Concurrent Programs**

Author(s): M.A.S. Brito, S.R.S. Souza, P.S.L. Souza

Presenter: P.S.L. Souza, University of Sao Paulo

**[W03b: 7th Workshop on Computational Chemistry and Its Applications](#)**15:50 - 17:30  
M218*Chair: P. Ramasami*

1. **First Principle Attempt towards the Thermodynamic Stability of Telluroformaldehyde and its Heavier Analogues: H(n)X(2-n)A=Te (X=H, F, Cl and Br; A=C, Si and Ge; n=0, 1 and 2).**  
Author(s): P. Ramasami, N.B. Jaufeerally  
Presenter: P. Ramasami
2. **Computational Study of the Chemical Reactivity Properties of the Rhodamine B Molecule**  
Author(s): D.G.M. Daniel Glossman-Mitnik  
Presenter: D.G.M. Daniel Glossman-Mitnik, Laboratorio Virtual NANOCOSMOS - CIMAV
3. **Theoretical Investigation of the Dispersion Interaction in Argon Dimer and Trimer**  
Author(s): R. Hilal, W. Hassan, S. Elroby, S. Aziz  
Presenter: R. Hilal, King Abdulaziz University
4. **Performance Analysis of Two Quantum Reaction Dynamics Codes: Time-Dependent and Time-Independent Strategies**  
Author(s): P. Gamallo, M. González, F. Huarte-Larrañaga  
Presenter: F. Huarte-Larrañaga, Universitat de Barcelona
5. **Steric maps to evaluate the role of steric hindrance on the IPr NHC ligand**  
Author(s): A. Poater, L. Falivene, C.A. Urbina-Blanco, S. Manzini, S.P. Nolan, L. Cavallo  
Presenter: A. Poater, Universitat de Girona

**[W04b: The 4th Workshop on Computational Optimization, Modelling and Simulation \(COMS2013\)](#)**15:50 - 17:30  
M212*Chair: X.S. Yang, S. Koziel, L. Leifsson*

1. **A Small-World Network Immune from Random Failures and Resilient to Targeted Attacks**  
Author(s): H. Sawai  
Presenter: H. Sawai, Advanced ICT Research Institute, National Institute of Information and Communications Technology
2. **Genetic Algorithm for the History Matching Problem**  
Author(s): C.R.X. Xavier, E.P.S. Amorim, V.F. Vieira, R.W. dos Santos  
Presenter: C.R.X. Xavier, Federal University of São João del Rei
3. **Shape-Preserving Response Prediction for Engineering Design Optimization**  
Author(s): S. Koziel, L. Leifsson  
Presenter: S. Koziel, Reykjavik University
4. **Neighborhood Preserving Codes for Assigning Point Labels: Applications to Stochastic Search**  
Author(s): S. Baluja, M. Covell  
Presenter: S. Baluja, Google, Inc.
5. **GPU-accelerated optimization of fuel treatments for mitigating wildfire hazard**  
Author(s): B. Arca, T. Ghisu, W. Spataro, G.A. Trunfio  
Presenter: G.A. Trunfio, University of Sassari

**W20a: Third International Workshop on Advances in High-Performance Computational Earth Sciences:  
Applications and Frameworks**

15:50 -  
17:30  
M215

*Chair: Y. Cui*

1. **Surface mesh generation of large-scale digital rock images in 3D**  
Author(s): Y. Liu, H.L. Xing  
Presenter: Y. Liu, School of Earth Sciences, The University of Queensland, Australia
2. **Embarrassingly Distributed Computing for Symbiotic Weather Forecasts**  
Author(s): B. Fjukstad, J.M. Bjørndalen, O.J. Anshus  
Presenter: B. Fjukstad, University of Tromso , Faculty of Science and Technology, Department of Computer Science, Norway
3. **On scalability issues of the elastodynamics equations on multicore platforms**  
Author(s): F. Dupros, H. Do, H. aochi  
Presenter: F. Dupros, BRGM
4. **DD-OceanVar: a Domain Decomposition fully parallel Data Assimilation software for the Mediterranean Forecasting System**  
Author(s): L. D'Amore, R. Arcucci, L. Carracciolo, A. Murli  
Presenter: R. Arcucci, CMCC
5. **ParNCL and ParGAL: Data-parallel tools for postprocessing of large-scale Earth science data**  
Author(s): R. Jacob, J. Krishna, X. Xu, T. Tautges, I. Grindeanu, R. Latham, K. Peterson, P. Bochev, M. Haley, D. Brown, R. Brownrigg, D. Shea, W. Huang, D. Middleton  
Presenter: R. Jacob, Argonne National Laboratory

**W23b: 6th Workshop on "Biomedical and Bioinformatics Challenges for Computer Science" (BBC 2013)**

15:50 - 17:30  
M217

*Chair: M. Cannataro*

1. **Next steps in simulating high-risk infectious disease propagation networks**  
Author(s): A. Tirado-Ramos, C. Kelley  
Presenter: A. Tirado-Ramos, Emory University
2. **CT Image Reconstruction Based on GPUs**  
Author(s): V. Vidal, L. Flores, G. Verdú, P. Mayo, F. Rodenas  
Presenter: V. Vidal, Universitat Politècnica de València

**W32b: Agent-Based Simulations, Adaptive Algorithms and Solvers**15:50 - 17:30  
M213*Chair: M. Paszynski*

1. **Employing an adaptive projection-based interpolation to prepare discontinuous 3D material data for finite element analysis**  
Author(s): D. Goik, M. Sieniek, M. Paszynski, L. Madej  
Presenter: D. Goik, AGH University of Science and Technology, Krakow, Poland
2. **High-Accuracy Adaptive Simulations of a Petri Dish Exposed to Electromagnetic Radiation**  
Author(s): I. Gómez-Revuelto, L. García-Castillo, D. Pardo  
Presenter: D. Pardo, Department of Applied Mathematics, Statistics and Operational Research, University of the Basque Country, and IKERBASQU
3. **Hypergraph Grammars in hp-adaptive Finite Element Method**  
Author(s): G. Slusarczyk, A. Paszynska  
Presenter: M. Sieniek, AGH University of Science and Technology, Krakow, Poland
4. **Inversion of Magnetotelluric Measurements using Multigoal Oriented hp-Adaptivity**  
Author(s): J. Alvarez-Aramberri, D. Pardo, H. Barucq  
Presenter: J. Alvarez-Aramberri, Departament of Applied Mathematics, Statistics, and Operational Research, University of the Basque Country.
5. **Complex negotiations in the conclusion and realisation of the contract**  
Author(s): M. Niedzwiecki, K. Rzecki, K. Cetnarowicz  
Presenter: M. Niedzwiecki, AGH University of Science and Technology

**W63b: Second International Young Scientists Conference 2013 "HPC technologies and computer modeling" (YSC 2013)**15:50 -  
17:30  
M216*Chair: Peter Sloot*

1. **Storm surge forecast in Saint-Petersburg**  
Author(s): A. Kalyuzhnaya  
Presenter: A. Kalyuzhnaya, University ITMO
2. **Computer Simulation of Seismic Processes in Heterogenous Media and Ground Facilities using High Performance Systems**  
Author(s): V. Golubev  
Presenter: V. Golubev, Moscow Institute of Physics and Technology
3. **Using touch-table in decision support system for Saint-Petersburg flood barrier**  
Author(s): A. Zagarskikh  
Presenter: A. Zagarskikh, University ITMO
4. **Grid simulation of two-dimensional MoS<sub>2</sub> with vacancy clusters**  
Author(s): O. Kozlova  
Presenter: O. Kozlova, Belarusian State University of Informatics and Radioelectronics
5. **Physical fields parallel simulation using automated distributed systems**  
Author(s): A. Chusov  
Presenter: A. Chusov, Far Eastern Federal University

# Session 3

5<sup>th</sup> June 2013

17:45 – 19:25

## M03: Main Track Three

17:45 - 19:25

111

*Chair: Janko Strassburg*

1. **Modelling Distributed Service Systems with Resources using UML**

Author(s): M.E. Cambronero, V. Valero

Presenter: M.E. Cambronero, University of Castilla-La Mancha

2. **Data flow testing in concurrent programs with message passing and shared memory paradigms**

Author(s): P.S.L. Souza, S.R.S. Souza, M.G. Rocha, R.R. Prado, R.N. Batista

Presenter: P.S.L. Souza, University of Sao Paulo

3. **Empirical Modelling of Linear Algebra Shared-Memory Routines**

Author(s): L.-P. Garcia, J. Camara, J. Cuenca, D. Gimenez

Presenter: D. Gimenez, Universidad de Murcia

4. **Distributing Efficiently the Block-Max WAND Algorithm**

Author(s): O. Rojas, V. Gil-Costa, M. Marin

Presenter: V. Gil-Costa, Yahoo Latin America

5. **Fault-tolerant Grid-based Solvers: Combining Concepts from Sparse Grids and MapReduce**

Author(s): J.W. Larson, M. Hegland, B. Harding, S. Roberts, L. Stals, A.P. Rendell, P. Strazdins, M.M. Ali, C. Kowitz, R.

Nobes, J. Southern, N. Wilson, Y. Oishi, M. Li

Presenter: J.W. Larson, Mathematical Sciences Institute, The Australian National University

## M06: Main Track Six

17:45 - 19:25

M211

*Chair: Vassil Alexandrov*

1. **Operator-level GPU-accelerated Branch and Bound algorithms**

Author(s): I. Chakroun, N. Melab

Presenter: I. Chakroun, INRIA

2. **GPU Accelerated 3D Object Reconstruction**

Author(s): M. Denkowski

Presenter: M.D. Denkowski, Maria Curie-Sklodowska University, Institute of Computer Science, 23-210 Lublin, Poland

3. **OSL: An Algorithmic Skeleton Library with Exceptions**

Author(s): J. LEGAUX, F. LOULERGUE, S. JUBERTIE

Presenter: J. LEGAUX, Université d'Orléans, France

4. **EcoTM: Conflict-Aware Economical Unbounded Hardware Transactional Memory**

Author(s): S. Tomic, E. Akpinar, A. Cristal, O. Unsal, M. Valero

Presenter: A. Cristal, Barcelona Supercomputing Center

**[W04c: The 4th Workshop on Computational Optimization, Modelling and Simulation \(COMS2013\)](#)**17:45 - 19:25  
M212

Chair: X.S. Yang, S. Koziel, L. Leifsson

1. **Application of the maximum convex sum algorithm in determining environmental variables that affect Nigerian highland stream benthic communities**  
Author(s): M.S. Thaher, D. Umar, T. Takaoka, J. Harding  
Presenter: M.S. Thaher, University of Canterbury
2. **Solving the 2D bin packing problem by means of a hybrid evolutionary algorithm**  
Author(s): C. Blum, V. Schmid  
Presenter: C. Blum, IKERBASQUE, Basque Foundation for Science, Spain
3. **The Use of a Genetic Algorithm to Model Vasculature of a Dicotyledon Leaf**  
Author(s): D. Zimarev  
Presenter: D. Zimarev, University of Cambridge
4. **Cost-Based Multi-QoS Job Scheduling using Divisible Load Theory in Cloud Computing**  
Author(s): M. Abdullah, M. Othman  
Presenter: M. Othman, Department of Communication Technology and Network, Faculty of Computer Science and Information Technology, Universiti P
5. **Multi-level CFD-based Airfoil Shape Optimization with Automated Low-fidelity Model Selection**  
Author(s): L. Leifsson, S. Koziel  
Presenter: L. Leifsson, Reykjavik University

**[W18a: Knowledge representation and applied models and metadata in computational science \(KREAM\)](#)**17:45 - 19:25  
M218

Chair: M.A. Sicilia

1. **Automatic hypothesis checking using eScience research infrastructures, ontologies, and linked data: a case study in climate change research**  
Author(s): J. Lappalainen, M.A. Sicilia, B. Hernández  
Presenter: J. Lappalainen, University of Alcala
2. **Precision difference management using a common sub-vector to extend the extended VSM method**  
Author(s): D. Werner, C. Cruz  
Presenter: D. Werner, University of Burgundy
3. **Layered Evaluation of Multi-Criteria Collaborative Filtering for Scientific Paper Recommendation**  
Author(s): N. Manouselis, K. Verbert  
Presenter: N. Manouselis, Agro-know Technologies, Greece
4. **Data Pre-Processing Evaluation for Text Mining: Transaction/Sequence Model**  
Author(s): D. Munková, M. Munk, M. Vozár  
Presenter: M. Vozár, Constantine the Philosopher University in Nitra

**[W20b: Third International Workshop on Advances in High-Performance Computational Earth Sciences: Applications and Frameworks](#)**17:45 -  
19:25  
M215

Chair: Y. Cui

1. **Multi-GPU Implementation of a 3D Finite Difference Time Domain Earthquake Code on Heterogeneous Supercomputers**  
Author(s): J. Zhou, Y. Cui, E. Poyraz, D.J. Choi, C.C. Guest  
Presenter: Y. Cui, San Diego Supercomputer Center
2. **Large-scale Simulations of 3D Groundwater Flow using Parallel Geometric Multigrid Method**  
Author(s): K. Nakajima  
Presenter: K. Nakajima, The University of Tokyo
3. **Performance of Sediment Transport Simulations on NVIDIA's Kepler Architecture**  
Author(s): H. Su, N. Wu, M. Wen, C. Zhang, X. Cai  
Presenter: H. Su, National University of Defense Technology

**W32c: Agent-Based Simulations, Adaptive Algorithms and Solvers**17:45 - 19:25  
M213

Chair: M. Paszynski

**1. Graph Grammar Based Direct Solver for hp-adaptive Finite Element Method with Point Singularities**Author(s): P. Gurgul, A. Szymczak, A. Paszynska, M. Paszynski  
Presenter: P. Gurgul, AGH University of Science and Technology**2. Isogeometric analysis of hyperelastic materials using PetIGA**Author(s): F. Fuentes, G.A. Espinosa, J.C. Mahecha, L.M. Bernal, N. Collier, V.M. Calo  
Presenter: G.A. Espinosa, KAUST**3. Phase field modeling using PetIGA**Author(s): P.A. Vignal, N. Collier, V.M. Calo  
Presenter: P.A. Vignal, KAUST**4. Performance analysis of iterative solvers of linear equations for hp-adaptive finite element method**Author(s): P. Plaszewski, K. Banas  
Presenter: P. Plaszewski, AGH University of Science and Technology**5. Grammar-Based Multi-Frontal Solver for One Dimensional Isogeometric Analysis with Multiple Right Hand Sides**Author(s): K. Kuznik, M. Paszynski, V. Calo  
Presenter: M. Paszynski, AGH University of Science and Technology, Krakow, Poland**W63c: Second International Young Scientists Conference 2013 "HPC technologies and computer modeling" (YSC 2013)**17:45 -  
19:25  
M216

Chair: Sergey Kovalchuk

**1. Efficiency of multiagent scheduling for distributed cloud**Author(s): P. Smirnov  
Presenter: P. Smirnov, University ITMO**2. Load Balancing in GPU Implementation of Breadth-First Search**Author(s): M. Chernoskutov  
Presenter: M. Chernoskutov, Institute of Mathematics and Mechanics**3. Multiagent simulation of malicious action and security system in information systems**Author(s): M. Umnitsin  
Presenter: M. Umnitsin, Volgograd State University**4. Marrying Many-core Accelerators and InfiniBand for a New Commodity Processor**Author(s): K.S. Solnushkin  
Presenter: K.S. Solnushkin, Saint Petersburg State Polytechnic University**5. Active monitoring system for cloud computing platform**Author(s): V. Karbovsky  
Presenter: V. Karbovsky, University ITMO

# Session 4

6<sup>th</sup> June 2013

10:50 – 12:30

## M07: Main Track Seven

10:50 - 12:30  
111

Chair: Rosa Badia

1. **Dynamic distribution of workload between CPU and GPU for a parallel conjugate gradient method in an adaptive FEM**  
Author(s): J. Lang, G. Rünger  
Presenter: J. Lang, Department of Computer Science, Chemnitz University of Technology
2. **Regularity versus Load-Balancing on GPU for treefix computations**  
Author(s): D. Defour, M. Marin  
Presenter: M. Marin, University of Perpignan
3. **Optimization techniques for 3D-FWT on systems with manycore GPUs and multicore CPUs**  
Author(s): G. Gregorio Bernabé, J. Javier Cuenca, D. Domingo Giménez  
Presenter: G. Gregorio Bernabé, University of Murcia
4. **An Architecture-Aware Technique for Optimizing Sparse Matrix-Vector Multiplication on GPUs**  
Author(s): M. Maggioni, T. Berger-Wolf  
Presenter: M. Maggioni, University of Illinois at Chicago
5. **Analysis of the Task Superscalar architecture hardware design**  
Author(s): F. Yazdanpanah, D. Jimenez-Gonzalez, C. Alvarez-Martinez, Y. Etsion, R.M. Badia  
Presenter: F. Yazdanpanah, PhD Student

## M10: Main Track Ten

10:50 - 12:30  
M211

Chair: Ponnadurai Ramasami

1. **Algorithm for finding the domain intersection of a set of polytopes**  
Author(s): V.M. Tereshchenko, A.L. Fisunenko, S.V. Chevokin  
Presenter: A.L. Fisunenko, Taras Shevchenko National University of Kyiv
2. **Stability and Performance Analysis of the Castillo-Grone Mimetic Operators in Conjunction with RK3 Time Discretization in Solving Advective Equations**  
Author(s): M. Abouali, J.E. Castillo  
Presenter: J.E. Castillo, Computational Science Research Center - San Diego State University
3. **A sharp analytical bound on the spatiotemporal locality in general two-phase flow and transport phenomena**  
Author(s): R.M. Younis  
Presenter: R.M. Younis, The University of Tulsa
4. **Iterative Method for Edge Length Equalization**  
Author(s): J.P. Peçanha, J.L. Souza Filho, M.B. Vieira, M. Lobosco, S.O. Dantas  
Presenter: J.P. Peçanha, Universidade Federal de Juiz de Fora
5. **Parallel implementations of FGMRES for solving large, sparse non-symmetric linear systems**  
Author(s): B. DeVries, J. Ianello, C. Trefftz, K.A. O'Hearn, G. Wolffe  
Presenter: B. DeVries, Grand Valley State University

**W09a: 10th International Workshop on Modeling and Computing Multiscale Systems**10:50 - 12:30  
M213

Chair: Valeria Krzhizanovskaya

1. **Spatial stabilization strategies applied to multiphysics modeling of blood clotting using a modified PTT model**  
Author(s): J.E. Egger, A.M. Mallik, D.S. Szczerba, D.R. Ruefenacht, G.S. Szekely, S.H. Hirsch  
Presenter: J.E. Egger, Computer Vision Laboratory, ETH Zürich, Switzerland
2. **A framework for anti-arrhythmic drugs testing using a multi-scale computational heart employing Alya Red**  
Author(s): J. Aguado-Sierra, M. Vazquez, R. Arís, R. Sebastián  
Presenter: J. Aguado-Sierra, Barcelona Supercomputing Center
3. **An ontology-based approach to performance monitoring of MUSCLE-bound multi-scale applications**  
Author(s): W. Funika, M. Janczykowski, M. Grzegorczyk, K. Jopek  
Presenter: W. Funika, AGH University, Dept. Comp. Sci, Electronics, Telecommunication, Institute of Computer Science
4. **Multiscale Agent-based Model of Tumor Angiogenesis**  
Author(s): M.M. Olsen, H.T. Siegelmann  
Presenter: M.M. Olsen, Loyola University Maryland
5. **A multiscale approach for the coupled simulation of blood flow and thrombus formation in intracranial aneurysms**  
Author(s): S. Zimny, B. Chopard, E. Lorenz, O. Malaspinas, S. Roller, J. Bernsdorf, K. Jain  
Presenter: S. Zimny, GRS Aachen

**W21a: Eighth international Workshop on Automatic Performance Tuning (iWAPT2013)**10:50 - 12:30  
M217

Chair: D. Gimenez

1. **Code Generation and Optimization of Distributed-Memory Dense Linear Algebra Kernels**  
Author(s): B. Marker, D. Batory, R. van de Geijn  
Presenter: B. Marker, The University of Texas at Austin
2. **Self-tuning multimedia streaming system on cloud infrastructure**  
Author(s): G. Sebestyen, A. Hangan, K. Sebestyen, R. Vachter  
Presenter: G. Sebestyen, Computers Department, Technical University of Cluj-Napoca, Romania
3. **A Sparse Matrix Library with Automatic Selection of Iterative Solvers and Preconditioners**  
Author(s): T. Sakurai, T. Katagiri, H. Kuroda, K. Naono, M. Igai, S. Ohshima  
Presenter: T. Sakurai, Central Research Laboratory, Hitachi, Ltd., Yokohama, Japan
4. **Using Machine Learning in order to Improve Automatic SIMD Instruction Generation**  
Author(s): A. Trouvé, A.J. Cruz, H. Fukuyama, J. Maki, H. Clarke, K. Murakami, M. Arai, T. Nakahira, E. Yamanaka  
Presenter: A.J. Cruz, Institute of Systems, Information Technologies and Nanotechnologies

**[W35a: The Tenth Workshop on Computational Finance and Business Intelligence](#)**10:50 - 12:30  
M212*Chair: Y. Shi***1. Pricing Moving Window Parisian Option and Applications in Convertible Bonds**

Author(s): D.M. Guo, B. Song, S.Y. Wang, B.J. Zhang

Presenter: D.M. Guo, School of Economics, Central University of Finance and Economics, China.

**2. Cost-Sensitive Support Vector Machine for Semi-Supervised Learning**

Author(s): Z.Q. Qi, Y.J. Tian, Y. Shi, X.D. Yu

Presenter: Z.Q. Qi, Research Center on Fictitious Economy &amp; Data Science, Chinese Academy of Sciences, Beijing 100190, China

**3. A Simple Regularized Multiple Criteria Linear Programs for Binary Classification**

Author(s): L.F. Niu, X. Zhao, Y. Shi

Presenter: X. Zhao, Graduate University of Chinese Academy of Sciences

**4. Labor Market Forecasting by Using Data Mining**

Author(s): Y. Alsultanny

Presenter: Y. Alsultanny, Faculty of college of Graduate studies, Arabian Gulf University, Kingdom of Bahrain

**5. Local and Global Regularized Twin SVM**

Author(s): Y.N. Wang, X. Zhao, Y.J. Tian

Presenter: Y.J. Tian, Research Center on Fictitious Economy and Data Science, Chinese Academy of Sciences

**[W38a: Dynamic Data Driven Application Systems - DDDAS 2013](#)**10:50 - 12:30  
M215*Chair: C.C. Douglas***1. Dynamic Data-Driven Application Systems - DDDAS 2013**

Author(s): C.C. Douglas, A. Patra, A. Cortes

Presenter: C.C. Douglas, University of Wyoming and KAUST

**2. Using Shape Memory Alloys: a Dynamic Data Driven Approach**

Author(s): C.C. Douglas, V. Calo, D.C. Cerwinsky, L. Deng, Y. Efendiev

Presenter: C.C. Douglas, University of WYoming and KAUST

**3. Coupling Diagnostic and Prognostic Models to a Dynamic Data Driven Forest Fire Spread Prediction System**

Author(s): C. Brun, T. Margalef, A. Cortés

Presenter: C. Brun, Universitat Autònoma de Barcelona

**4. Challenges in Developing DDDAS Based Methodology for Volcanic Ash Hazard Analysis -- Effect of Numerical Weather Prediction Variability and Parameter Estimation**

Author(s): A.K. Patra, M.I. Bursik, J. Dehn, M. Jones, R. Madankan, D. Morton, M. Pavolonis, E.B. Pitman, S. Pouget, T. Singh, P. Singla, E.R. Stefanescu, P. Webley

Presenter: A.K. Patra, Department of Mechanical &amp; Aerospace Engineering, University at Buffalo, Buffalo, NY 14260

**5. A data-driven model for big forest fires behavior prediction in Europe**

Author(s): D. Rodriguez-Aseretto, D. De Rigo, M. Di Leo, A. Cortés, J. San-Miguel-Ayanz

Presenter: D. Rodriguez-Aseretto, European Commission, Joint Research Centre, Institute for Environment and Sustainability

**6. Dynamic QoS Optimization Architecture for Cloud-based DDDAS**

Author(s): T. Chen, R. Bahsoon, G. Theodoropoulos

Presenter: T. Chen, School of Computer Science, University of Birmingham, B15 2TT, United Kingdom

**W52a: Solving Problems with Uncertainties**10:50 - 12:30  
M214*Chair: V.N. Alexandrov*

1. **Quantifying Uncertainty in Phylogenetic Studies of the Slavonic Languages**  
Author(s): D. Nurbakova, S. Rusakov, V. Alexandrov  
Presenter: D. Nurbakova
2. **Relieving the Effects of Uncertainty in Forest Fire Spread Prediction by Hybrid MPI-OpenMP Parallel Strategies**  
Author(s): T. Artés, A. Cencerrado, A. Cortés, T. Margalef  
Presenter: T. Artés, UAB
3. **Monte Carlo Simulation of Ultrafast Carrier Transport: Scalability Study**  
Author(s): A. Karaivanova, E. Atanassov, T. Gurov  
Presenter: A. Karaivanova, IICT-BAS
4. **Canonical Multiattribute Utility Functions: Enumeration, Verification, and Application**  
Author(s): Y.G. Abdildin, A.E. Abbas  
Presenter: Y.G. Abdildin, University of Illinois at Urbana-Champaign
5. **A Monte Carlo Approach to Sparse Approximate Inverse Matrix Computations**  
Author(s): J. Strassburg, V.N. Alexandrov  
Presenter: J. Strassburg, The University of Reading, UK and Barcelona Supercomputing Centre, Barcelona, Spain

**W63d: Second International Young Scientists Conference 2013 "HPC technologies and computer modeling" (YSC 2013)**10:50 -  
12:30  
M216*Chair: Sergey Ivanov*

1. **Block data layout and matrix multiplication**  
Author(s): M. Yurushkin  
Presenter: M. Yurushkin, Southern Federal University
2. **Fast computation of the multivariate polynomials**  
Author(s): S. Volkov  
Presenter: S. Volkov, Institute for Information Transmission Problems
3. **Hyper-acceleration of stationary boundary value problem parallel solution by spatial decomposition with example of self-consistency Hartree-Fock problem for graphene sheet**  
Author(s): A. Svitenkov, V.G. Maslov  
Presenter: A. Svitenkov, University ITMO
4. **New approach for Stokes flow algorithm testing**  
Author(s): A. Popov  
Presenter: A. Popov, University ITMO
5. **Rendering and simulation technologies in flight simulator**  
Author(s): A. Bezgodov  
Presenter: A. Bezgodov, University ITMO

# Session 5

6<sup>th</sup> June 2013

15:15 – 16:55

## [\*\*M08: Main Track Eight\*\*](#)

15:15 - 16:55

M211

Chair: Rosa Badia

1. **Faster Betweenness Centrality Based on Data Structure Experimentation**  
Author(s): O. Green, D.A. Bader  
Presenter: O. Green, Georgia Institute of Technology
2. **A Methodology for Invasive Programming on Virtualizable Embedded MPSoC Architectures**  
Author(s): A. Biedermann, S.A. Huss  
Presenter: A.B. Biedermann, Integrated Circuits and Systems Lab, TU Darmstadt, Germany
3. **G-DBSCAN: A GPU Accelerated Algorithm for Density-based Clustering**  
Author(s): G. Andrade, G. Ramos, D. Madeira, R. Sachetto, R. Ferreira, L. Rocha  
Presenter: G. Andrade, Universidade Federal de São João del Rei
4. **Topology Aware Task stealing for On-Chip NUMA Multi-Core Processors**  
Author(s): B. Vikranth, R. Wankar, C. Raghavendra Rao  
Presenter: B. Vikranth, CVR College Of Engineering
5. **Parallelizing Alternating Direction Implicit Solver on GPUs**  
Author(s): Z. Wei, B. Jang, Y. Zhang, Y. Jia  
Presenter: B. Jang, The University of Mississippi, U.S.A.

## [\*\*M11: Main Track Eleven\*\*](#)

15:15 - 16:55

M211

Chair: David Abrahamson

1. **Hybrid-parallel algorithms for 2D Green's functions**  
Author(s): D. Gimenez, A. Alvarez-Melcon, F.D. Quesada, T. Ramirez  
Presenter: D. Gimenez, University of Murcia
2. **Pareto Front Approximation Using A Hybrid Approach**  
Author(s): S.G. Deshpande, L.T. Watson, R.A. Canfield  
Presenter: S.G. Deshpande, Virginia Polytechnic Institute and State University
3. **Applying CP(FD), CLP(FD) and CFLP(FD) to a Real-Life Employee Timetabling Problem**  
Author(s): I. Castiñeiras, F. Sáenz-Pérez  
Presenter: I. Castiñeiras, Universidad Complutense de Madrid
4. **Parallelizing the sparse matrix transposition: reducing the programmer effort using transactional memory**  
Author(s): M.A. Gonzalez-Mesa, E.D. Gutierrez, O. Plata  
Presenter: M.A. Gonzalez-Mesa, University of Malaga, Spain
5. **Sharp Interface Algorithm for Large Density Ratio Incompressible Multiphase Magnetohydrodynamic Flows**  
Author(s): R. Samulyak, T. Guo, S. Wang  
Presenter: R. Samulyak, Stony Brook Univ. and Brookhaven National Lab.

**W09b: 10th International Workshop on Modeling and Computing Multiscale Systems**15:15 - 16:55  
M213

Chair: Eric Lorenz

1. **Distributed simulation of city inundation by coupled surface and subsurface porous flow for urban flood decision support system**  
Author(s): V.V. Krzhizhanovskaya, N.B. Melnikova, A.M. Chirkin, S.V. Ivanov, A.V. Boukhanovsky, P.M.A. Sloot  
Presenter: V.V. Krzhizhanovskaya, University of Amsterdam, The Netherlands and National Research University ITMO, St. Petersburg, Russia
2. **Initialization of lattice Boltzmann models with the help of the numerical Chapman–Enskog expansion**  
Author(s): Y. Vanderhoydonc, W. Vanroose  
Presenter: Y. Vanderhoydonc, Universiteit Antwerpen
3. **Isogeometric Analysis of Coupled Thermo-Mechanical Phase-Field Models for Shape Memory Alloys Using Distributed Computing**  
Author(s): R. Dhote, H. Gomez, R. Melnik, J. Zu  
Presenter: R. Melnik, Wilfrid Laurier University, Waterloo, Canada
4. **Domain decomposition for Stokes-Darcy flows with curved interfaces**  
Author(s): I. Yotov, P. Song, C. Wang  
Presenter: I. Yotov, University of Pittsburgh
5. **Heterogeneous hardware implementation of Molecular Static method for modelling of interatomic behaviour**  
Author(s): L. Rauch  
Presenter: L. Rauch, Akademia Gorniczo-Hutnicza

**W21b: Eighth international Workshop on Automatic Performance Tuning (iWAPT2013)**15:15 - 16:55  
M217

Chair: D. Gimenez

1. **How to Determine the Topology of Hierarchical Tuning Networks for Dynamic Auto-Tuning in Large-Scale Systems**  
Author(s): A. Martinez, A. Sikora, E. César, J. Sorribes  
Presenter: A. Martinez, Universitat Autònoma de Barcelona
2. **OCOptimizer: an iterative optimization tool for OpenCL**  
Author(s): D. Andrade, J.F. Fabeiro, B.B. Fraguera  
Presenter: J.F. Fabeiro, University of A Coruña
3. **A mathematical method for online autotuning of power and energy consumption with corrected temperature effects**  
Author(s): R. Suda, C. Luo, T. Katagiri  
Presenter: R. Suda, the University of Tokyo
4. **Automatic Tuning of Compiler Optimizations and Analysis of their Impact**  
Author(s): D. Plotnikov, D. Melnik, M. Vardanyan, R. Buchatskiy, R. Zhuykov, J.H. Lee  
Presenter: D. Melnik, ISP RAS

**W35b: The Tenth Workshop on Computational Finance and Business Intelligence**15:15 - 16:55  
M212*Chair: Y. Shi*

1. **The Application of Multiple Criteria Linear Programming in Advertisement Clicking Events Prediction**  
Author(s): F. Wang, P. Zhang, Y. Shang, Y. Shi  
Presenter: F. Wang, Research Center on Fictitious Economy & Data Science, Chinese Academy of Sciences, Beijing 100093, China
2. **Sectoral Diversification and the Banks' Return and Risk: Evidence from Chinese Listed Commercial Banks**  
Author(s): Y.B. Chen, X.H. Wei, L.L. Zhang, Y. Shi  
Presenter: Y.B. Chen, University of Chinese Academy of Sciences
3. **Pillar 3 and Modelling of Stakeholders' Behaviour at the Commercial Bank Website during the Recent Financial Crisis**  
Author(s): M. Munk, A. Pilkova, J. Kapusta, P. Svec, M. Drlik  
Presenter: J. Kapusta, Constantine the Philosopher University in Nitra
4. **Two Methods of Correlation Coefficient on Compositional Data**  
Author(s): W. Long, Q. Wang  
Presenter: W. Long
5. **Securities Transaction Tax and Stock Market Behavior in an Agent-based Financial Market Model**  
Author(s): H.Q. Li, M.Y. Tang, W. Shang, S.Y. Wang  
Presenter: M.Y. Tang, Hunan Normal University

**W36a: Tools for Program Development and Analysis in Computational Science**15:15 - 16:55  
M218*Chair: K. Fuerlinger*

1. **Extending the Eclipse Parallel Tools Platform debugger with Scalable Parallel Debugging Library**  
Author(s): C. Jin, L. Ding, D. Abramson  
Presenter: D. Abramson, Monash University
2. **Implementation of Intel restricted transactional memory ISA extension in Simics**  
Author(s): G. Rechistov, A. Plotkin  
Presenter: G. Rechistov, Intel Corporation
3. **Challenges of reducing cycle-accurate simulation time for TBP applications**  
Author(s): A.C. Iordan, M. Jahre, L. Natvig  
Presenter: A.C. Iordan, Norwegian University of Science and Technology
4. **A tool for selecting the right target machine for Parallel Scientific Applications**  
Author(s): J. Panadero, A. Wong, D. Rexachs, E. Luque  
Presenter: J. Panadero, Universitat Autonoma de Barcelona
5. **Mining Software Usage with the Automatic Library Tracking Database (ALTD)**  
Author(s): B. Hadri, M. Fahey  
Presenter: M. Fahey, NICS University of Tennessee

**W38b: Dynamic Data Driven Application Systems - DDDAS 2013**15:15 - 16:55  
M215*Chair: C.C. Douglas*

1. **Scheduling Challenges in Mixed Critical Real-time Heterogeneous Computing Platforms**  
Author(s): C. Kumar N G, S.P. Vyas, R.K. Cytron, C.D. Gill, J.A. Zambreno, P.H. Jones  
Presenter: P.H. Jones, Iowa State University
2. **DDDAMS-based Dispatch Control in Power Networks**  
Author(s): N. Celik, A.E. Thanos, J.P. Saenz  
Presenter: N. Celik, University of Miami
3. **Dynamic Sensor Location Using Model Singular Vectors**  
Author(s): A. Sandu, A.G. Cioaca, V. Rao  
Presenter: A. Sandu, Virginia Tech.
4. **Retrospective Cost Methods for DDDAS**  
Author(s): A. D'Amato, A. Ali, A. Ridley, D. Bernstein  
Presenter: D. Bernstein, University of Michigan
5. **Resilient Dynamic Data Driven Application Systems (r-DDDAS)**  
Author(s): G. Dsouza, S. Hariri, Y. Al-Nashif, G. Rodriguez  
Presenter: S. Hariri, NSF Center for Cloud and Autonomic Computing, University of Arizona

**W52b: Solving Problems with Uncertainties**15:15 - 16:55  
M214*Chair: V.N. Alexandrov*

1. **A MapReduce Framework for Analysing Portfolios of Catastrophic Risk with Secondary Uncertainty**  
Author(s): B. Varghese, A. Rau-Chaplin, Z. Yao  
Presenter: B. Varghese, Dalhousie University
2. **Overcoming uncertainty on video-on-demand server design by using self-similarity and principal component analysis**  
Author(s): R. Ramirez-Velarde, L. Martinez-Elizalde, C. Barba-Jimenez  
Presenter: R. Ramirez-Velarde, Tecnologico de Monterrey

**W63e: Second International Young Scientists Conference 2013 "HPC technologies and computer modeling" (YSC 2013)**15:15 -  
16:55  
M216*Chair: Sergey Ivanov*

1. **Efficient monitoring of social networks**  
Author(s): A. Yakushev  
Presenter: A. Yakushev, University ITMO
2. **Aerodynamic and strength computing of miniature unmanned aerial vehicles with ANSYS software**  
Author(s): E. Tomilo  
Presenter: E. Tomilo, Belarusian National Technical University
3. **A heuristic optimization method for mitigating the impact of a virus attack**  
Author(s): V. Kashirin  
Presenter: V. Kashirin, University ITMO
4. **A multicomponent modeling framework for the high performance simulation of the spread of socially dangerous diseases**  
Author(s): V. Leonenko  
Presenter: V. Leonenko, Sobolev Institute of Mathematics
5. **YSC-2013 Awards**  
Author(s): P. Sloot  
Presenter: P. Sloot, University ITMO

# Session 6

6<sup>th</sup> June 2013  
17:15 – 18:55

## M09: Main Track Nine

17:15 - 18:55  
111

Chair: Ponnadurai Ramasami

1. **A Discrete Adjoint Model for OpenFOAM**  
Author(s): M. Towara, U. Naumann  
Presenter: M. Towara, Software and Tools for Computational Engineering, RWTH Aachen, Germany
2. **A parallel solver for incompressible fluid flows**  
Author(s): Y. Wang, M. Baboulin, J. Dongarra, J. Falcou, Y. Fraigneau, O.L. Maître  
Presenter: Y. Wang, University Paris-Sud, France
3. **The sparse grid combination technique for computing eigenvalues in linear gyrokinetics**  
Author(s): C. Kowitz, M. Hegland  
Presenter: C. Kowitz, Technische Universität München
4. **An Extensible Digital Library Service to Support Network Science**  
Author(s): S.M.S. Hasan, K. Bisset, E. Fox, K. Hall, J. Leidig, M. Marathe  
Presenter: J. Leidig, Grand Valley State University

## M12: Main Track Twelve

17:15 - 18:55  
M211

Chair: Michael Lees

1. **Early experience on porting and running a Lattice Boltzmann code on the Xeon-Phi co-processor**  
Author(s): S.F. Schifano, G. Crimi, F. Mantovani, M. Pivanti, R. Tripiccione  
Presenter: S.F. Schifano, University of Ferrara and INFN
2. **Streaming Breakpoint Graph Analytics for Accelerating and Parallelizing the Computation of DCJ Median of Three Genomes**  
Author(s): Z. Yin, J. Tang, S. Schaeffer, D. Bader  
Presenter: Z. Yin, School of Computational Science and Engineering, Georgia Institute of Technology, Atlanta, USA
3. **A parallel algorithm for a physiological non-linear model of the cochlea**  
Author(s): D. Sabo, S. Weiss, M. Furst  
Presenter: S. Weiss, School of Electrical Engineering, Tel Aviv University, Tel Aviv, ISRAEL
4. **Analysis of car crash simulation data with nonlinear machine learning methods**  
Author(s): B. Bohn, J. Garcke, R. Iza-Teran, A. Paprotny, B. Peherstorfer, U. Schepsmeier, C.-A. Thole  
Presenter: J. Garcke, Fraunhofer SCAI, Inst. for Numerical Simulation, University of Bonn

**[W09c: 10th International Workshop on Modeling and Computing Multiscale Systems](#)**17:15 - 18:55  
M213

Chair: Bartosz Bosak

**1. A service-oriented framework for integration of domain-specific data models in scientific workflows**

Author(s): A. Bender, A. Poschlal, S. Bozic, I. Kondov

Presenter: I. Kondov, Steinbuch Centre for Computing, Karlsruhe Institute of Technology, Germany

**2. Support for Multiscale Simulations with Molecular Dynamics**

Author(s): K.J. Rycerz, E. Ciepiela, G. Dyk, D. Groen, T. Gubala, D. Harezlak, M. Pawlik, J. Suter, S. Zasada, P. Coveney, M. Bubak

Presenter: K.J. Rycerz, Institute of Computer Science and CYFRONET AGH

**3. Distributed Multiscale Computations using the MAPPER framework**

Author(s): M. Ben Belgacem, B. Chopard, J. Borgdorff, M. Mamonski, K. Rycerz, D. Harezlak

Presenter: M. BEN BELGACEM, University of Geneva

**4. Multiscale computing with the multiscale modeling library and runtime environment**

Author(s): J. Borgdorff, M. Mamonski, B. Bosak, D. Groen, M. Ben Belgacem, K. Kurowski, A.G. Hoekstra

Presenter: J. Borgdorff, Computational Science, University of Amsterdam, Amsterdam, The Netherlands

**[W10a: Workshop on Computational and Algorithmic Finance](#)**17:15 - 18:55  
M214

Chair: A. Itkin

**1. Iterative Methods for Pricing American Options under the Bates Model**

Author(s): J. Toivanen, S. Salmi, L. von Sydow

Presenter: J. Toivanen, Stanford University

**2. Pricing discrete arithmetic Asian options under Levy processes: A meta-analysis**

Author(s): M. Staunton

Presenter: M. Staunton, London Business School

**3. Efficient solution of backward jump-diffusion PIDEs with splitting and matrix exponentials**

Author(s): A. Itkin

Presenter: A. Itkin, Numerix LLC &amp; Polytechnic Institute of NYU

**4. Monte Carlo Methods for Calibration of Equity Smile**

Author(s): A.P. Polishchuk

Presenter: A.P. Polishchuk, Bloomberg L.P.

**5. Smile Asymptotics in Stochastic Asset Price Models**

Author(s): A. Gulisashvili

Presenter: A. Gulisashvili, Ohio University

**[W21c: Eighth international Workshop on Automatic Performance Tuning \(iWAPT2013\)](#)**17:15 - 18:55  
M217

Chair: D. Gimenez

**1. Crowdsourcing auto-tuning: challenges and possible solutions**

Author(s): G. Fursin

Presenter: G. Fursin, INRIA

**2. From performance analytics to autotuning in parallel programs**

Author(s): J. Labarta

Presenter: J. Labarta, The Technical University of Catalonia

**[W36b: Tools for Program Development and Analysis in Computational Science](#)**17:15 - 18:55  
M218*Chair: K. Fuerlinger*

1. **Sensitivity analysis for mixed-language numerical models**  
Author(s): J. Utke, B.T. Reardon, R.A. Lefebvre  
Presenter: J. Utke, Argonne National Laboratory
2. **Nova: A modern platform for system dynamics, spatial, and agent-based modeling**  
Author(s): R.M. Salter  
Presenter: R.M. Salter, Oberlin College

**[W38c: Dynamic Data Driven Application Systems - DDDAS 2013](#)**17:15 - 18:55  
M215*Chair: C.C. Douglas*

1. **An Operation-time Simulation Framework for UAV Swarm Configuration and Mission Planning**  
Author(s): Y. Wei, M.B. Blake, G.R. Madey  
Presenter: G.R. Madey, University of Notre Dame
2. **An Offline/Online DDDAS Capability for Self-Aware Aerospace Vehicles**  
Author(s): D. Allaire, J. Chambers, R. Cowlagi, D. Kordonowy, M. Lecerf, L. Mainini, F. Ulker, K. Willcox  
Presenter: D. Allaire, MIT
3. **Issues Related to Parameter Estimation in Model Accuracy Assessment**  
Author(s): T.C. Henderson, N. Boonsirisumpun  
Presenter: T.C. Henderson, University of Utah
4. **Feature Matching and Adaptive Prediction Models in an Object Tracking DDDAS**  
Author(s): B. Uzkent, M.J. Hoffman, A. Vodacek, J.P. Kerekes, B. Chen  
Presenter: B. Uzkent, Rochester Institute of Technology
5. **PREDICT: Privacy and Security Enhancing Dynamic Information Collection and Monitoring**  
Author(s): L. Xiong, V. Sunderam, L. Fan, S. Goryczka, L. Pournajaf  
Presenter: L. Xiong, Emory University

# Session 7

7<sup>th</sup> June

10:35 – 12:15

## M13: Main Track Thirteen

10:35 - 12:15  
111

*Chair: David Abrahamson*

1. **Impact of Preventive Behavioral Responses to Epidemics in Rural Regions**  
Author(s): C.M. Scoglio, P.B. Schumm, W. Schumm  
Presenter: C.M. Scoglio, K-State Epicenter, Kansas State University
2. **Using an Agent-Based Simulation for predicting the effects of patients derivation policies in Emergency Departments**  
Author(s): M. Taboada, E. Cabrera, F. Epelde, M.L. Iglesias, E. Luque  
Presenter: M. Taboada, Tomas Cerda Computer Science School, University Autonoma of Barcelona
3. **Multi-agent distributed framework for swarm intelligence**  
Author(s): S. Ilie, C. Badica  
Presenter: C. Badica, University of Craiova, Romania
4. **Parallelization of shallow-water equations with the algorithmic skeleton library SkelGIS**  
Author(s): H. COULLON, S. Limet, M.H. Le  
Presenter: H. COULLON, LIFO - University of Orléans
5. **CarSh: A Commandline Execution Support for Stream-based Acceleration Environment**  
Author(s): S. Yamagiwa, S. Zhang  
Presenter: S. Yamagiwa, University of Tsukuba

## M15: Main Track Fifteen

10:35 - 12:15  
M212

*Chair: Michael Lees*

1. **Adaptive Scientific Visualization System for Desktop Computers and Mobile Devices**  
Author(s): K.V. Ryabinin, S.I. Chuprina  
Presenter: K.V. Ryabinin, Perm State University
2. **Seismic Image Restoration Using Nonlinear Least Squares Shape Optimization**  
Author(s): M. Gilardet, S. Guillou, B. Jobard, D. Komatitsch  
Presenter: M. Gilardet, TOTAL, University of Pau
3. **Virtual reality simulator for phacoemulsification cataract surgery education and training**  
Author(s): C.K. Lam, K. Sundaraj, M.N. Sulaiman  
Presenter: C.K. Lam, Universiti Malaysia Perlis
4. **Improving communication patterns for distributed cluster-based individual-oriented fish school simulations**  
Author(s): R. Solar, F. Borges, R. Suppi, E. Luque  
Presenter: F. Borges, Universitat Autònoma de Barcelona
5. **Connecting models to data in multiscale multicellular tissue simulations**  
Author(s): J. Cooper, J. Osborne  
Presenter: J. Osborne, Department of Computer Science, University of Oxford, UK

**M16: Main Track Sixteen**10:35 - 12:15  
M211*Chair: Vassil Alexandrov*1. **High-Level Programming for Medical Imaging on Multi-GPU Systems using the SkelCL Library**

Author(s): M. Steuwer, S. Gorlatch

Presenter: M. Steuwer, Department of Mathematics and Computer Science, University of Muenster, Germany

2. **PL-Science: A Scientific Software Product Line**

Author(s): G.C.B. Costa, R. Braga, J.M.N. David, F. Campos, W. Arbex

Presenter: G.C.B. Costa, Federal University of Juiz de Fora

3. **The Collage Authoring Environment: from proof-of-concept prototype to pilot service**

Author(s): E. Ciepiela, D. Harezlak, M. Kasztelnik, J. Meizner, G. Dyk, P. Nowakowski, M. Bubak

Presenter: E. Ciepiela, Academic Computer Centre Cyfronet AGH University of Science and Technology, Kraków, Poland

4. **Characteristic Boundary Conditions in LBM for Fluid and Gas Dynamics**

Author(s): M. Ehrhardt, D. Heubes, A. Bartel

Presenter: M. Ehrhardt, University of Wuppertal

5. **Numerical Evaluation of Complex Logarithms in the Cox-Ingersoll-Ross Model**

Author(s): L. Teng, M. Ehrhardt, M. Günther

Presenter: L. Teng, Chair of Applied Mathematics and Numerical Analysis, University of Wuppertal

**W10b: Workshop on Computational and Algorithmic Finance**10:35 - 12:15  
M214*Chair: A. Itkin*1. **A novel stock forecasting model based on fuzzy time series and genetic algorithm**

Author(s): Q.S. Cai, D.F. Zhang, B. Wu

Presenter: Q.S. Cai, Department of Computer Science, Xiamen University

2. **ADI FD schemes for the numerical solution of the three-dimensional Heston-Cox-Ingersoll-Ross PDE**

Author(s): T. Haentjens

Presenter: T. Haentjens, University of Antwerp, Belgium

3. **Calibration in Finance: Very Fast Greeks through Algorithmic Differentiation and Implicit Function**

Author(s): M. Henrard

Presenter: M. Henrard, Quantitative Research, OpenGamma, London

4. **Efficient and Robust IMEX schemes for option pricing under jump-diffusion models**

Author(s): S. Salmi, J. Toivanen

Presenter: S. Salmi, University of Jyväskylä

5. **Variance Reduction for Asian Options under a General Model Framework**

Author(s): K.D. Dingeç, H. Sak, W. Hörmann

Presenter: K.D. Dingeç, Department of Industrial Engineering, Bogazici University

**[W31a: Workshop on Teaching Computational Science 2013 \(WTCS 2013\)](#)**10:35 - 12:15  
M218*Chair: A.B. Shiflet*

1. **Undergraduate Module on Computational Modeling: Introducing Modeling the Cane Toad Invasion**  
Author(s): A.B. Shiflet, G.W. Shiflet, W.E. Sanders  
Presenter: A.B. Shiflet, Wofford College
2. **Measuring Business Value of Learning Technology Implementation in Higher Education Setting**  
Author(s): N. ALEXANDROV  
Presenter: N. ALEXANDROV, Barcelona Supercomputing Centre
3. **An experience of e-assessment in an introductory course on computer organization**  
Author(s): E.D. Gutierrez, M.A. Trenas-Castro, F. Corbera, J. Ramos, S. Romero  
Presenter: J. Ramos, Dept. Computer Architecture, University of Malaga, Spain
4. **Fostering the creative development of computer science students in programming and interaction design**  
Author(s): D.J.F. Ferreira  
Presenter: D.J.F. Ferreira, Federal University of Goiás
5. **Introducing: Computational Science**  
Author(s): V.R. Maxville  
Presenter: V.R. Maxville, iVEC

**[W38d: Dynamic Data Driven Application Systems - DDDAS 2013](#)**10:35 - 12:15  
M215*Chair: K. Fuerlinger*

1. **An Energy-Aware Airborne Dynamic Data-Driven Application System for Persistent Sampling and Surveillance**  
Author(s): E.W. Frew, B. Argrow, A. Houston, C. Weiss, J. Elston  
Presenter: E.W. Frew, University of Colorado
2. **A Testbed for Investigating the UAV Swarm Command and Control Problem Using DDDAS**  
Author(s): R.A. Purta, M. Dobski, A. Jaworski, G. Madey  
Presenter: R.A. Purta, Notre Dame
3. **Dynamic Data-Driven Application System methods in Economics and Financial Systems Modelling**  
Author(s): V.N. Alexandrov  
Presenter: V.N. Alexandrov, ICREA Professor in Computational Science at BSC
4. **Dynamic Data-Driven Application System Framework for Large-Composite Structures which includes Advanced FSI Simulations and Structural Health Monitoring**  
Author(s): Y. Bazilevs, M.-C. Hsu, M.T. Bement, A. Korobenko  
Presenter: A. Korobenko, University of California, San Diego
5. **Dynamic Data Driven Applications System concept for Information Fusion**  
Author(s): E.P. Blasch, G. Seetharaman, K. Reinhardt  
Presenter: E.P. Blasch, U.S. Air Force

**W43a: International Workshop on Computational Flow and Transport: Modeling, Simulations and Algorithms**

10:35 -  
12:15  
M213

Chair: S. Sun

1. **Numerical Solution of the Steady Convection-Diffusion Equation with Dominant Convection**  
Author(s): L.A. Kruckier, O.A. Pichugina, B.L. Kruckier  
Presenter: L.A. Kruckier, Southern Federal University, Computer Center, Russia
2. **On the stability of the finite difference based lattice Boltzmann method**  
Author(s): M.F. El-Amin, S. Sun, A. Salama  
Presenter: M.F. El-Amin, KAUST
3. **An NPT Monte Carlo Molecular Simulation-Based Approach to Investigate Solid-Vapor Equilibrium: Application to Elemental Sulfur-H<sub>2</sub>S System**  
Author(s): A. Kadoura, A. Salama, S. Sun, A. Sherik  
Presenter: A. Kadoura, King Abdullah University of Science and Technology
4. **The Discretization Method for Convection-Diffusion Equations in Two-Dimensional Cylindrical Coordinate Systems Based on Unstructured Grids**  
Author(s): G. Yu, B. Yu, Y. Zhao, Q. Shao, J. Xie  
Presenter: G. Yu, Beijing Key Laboratory of Urban Oil and Gas Distribution Technology, China University of Petroleum
5. **Electron beam absorption algorithms for electron beam melting processes simulated by a three-dimensional thermal free surface lattice Boltzmann method in a distributed and parallel environment**  
Author(s): M. Markl, R. Ammer, U. Ljungblad, U. Rüde, C. Körner  
Presenter: M. Markl, Chair of Metals Science and Technology, University of Erlangen-Nuremberg, Germany

**W47a: Urgent Computing: Computations for Decision Support in Critical Situations**

10:35 - 12:15  
M217

Chair: A.V. Boukhanovsky

1. **Leveraging e-Infrastructures for Urgent Computing**  
Author(s): S.H. Leong, A. Frank, D. Kranzmüller  
Presenter: S.H. Leong, Leibniz Supercomputing Centre
2. **Parallel Programming Approaches for an Agent-based Simulation of Concurrent Pandemic and Seasonal Influenza Outbreaks**  
Author(s): M. Soto-Ferrari, P. Holvenstot, D. Prieto, E. de Doncker, J. Kapenga  
Presenter: E. de Doncker, Western Michigan University
3. **Multiagent approach for building distributed adaptive computing system**  
Author(s): A.I. Kalyaev  
Presenter: A.I. Kalyaev, Scientific Research Institute of Multiprocessor Computing Systems of Southern Federal University
4. **Deadline-driven Resource Management within Urgent Computing Cyberinfrastructure**  
Author(s): S.V. Kovalchuk, P.A. Smirnov, S.V. Maryin, T.N. Tchurov, V.A. Karbovskiy  
Presenter: S.V. Kovalchuk, National Research University of Information Technologies, Mechanics and Optics
5. **Workshop opening**  
Author(s): A.V. Boukhanovsky  
Presenter: A.V. Boukhanovsky, Saint-Petersburg National Research University of Information Technologies, Mechanics and Optics

*Chair: F.M. Hoffman*

1. **Contrasting Climate Ensembles: A Model-Based Visualization Approach for Analyzing Extreme Events**  
Author(s): R. Sisneros, J. Huang, G. Ostroumov, S. Ahern, B.D. Semeraro  
Presenter: R. Sisneros, National Center for Supercomputing Applications
2. **ParCAT: Parallel Climate Analysis Toolkit**  
Author(s): B.E. Smith, D.M. Ricciuto, P.E. Thornton, G. Shipman, C.A. Steed, D.N. Williams, M. Wehner  
Presenter: B.E. Smith, Oak Ridge National Laboratory
3. **A guided hybrid genetic algorithm for feature selection with expensive cost functions**  
Author(s): M.J. Jung, J. Zscheischler  
Presenter: M.J. Jung, Max Planck Institute for Biogeochemistry
4. **Estimating basal area of spruce and fir in post-fire residual stands in Central Siberia using Quickbird, feature selection, and Random Forests**  
Author(s): M. Jung, S. Tautenhahn, C. Wirth, J. Kattge  
Presenter: M. Jung, MPI-Biogeochemistry
5. **An approach for real-time levee health monitoring using signal processing methods**  
Author(s): A.L. Pyayt, A.P. Kozionov, I.I. Mokhov, B. Lang, V.V. Krzhizhanovskaya, P.M.A. Sloot  
Presenter: A.L. Pyayt, University of Amsterdam & Siemens LLC

# Session 8

7th June 2013

13:35 – 15:15

## M14: Main Track Fourteen

13:35 - 15:15  
111

*Chair: Michael Lees*

1. **Eden's Bees: Parallelizing Artificial Bee Colony in a Functional Environment**  
Author(s): F. Rubio, A. de la Encina, P. Rabanal, I. Rodríguez  
Presenter: F. Rubio, Universidad Complutense de Madrid
2. **PDES-MAS: Distributed simulation of multi-agent systems**  
Author(s): V. Suryanarayanan, G. Theodoropoulos, M. Lees  
Presenter: G. Theodoropoulos, Durham University, UK
3. **Parallelizing the Conjugate Gradient Algorithm for Multilevel Toeplitz Systems**  
Author(s): J. Chen, T. Li  
Presenter: J. Chen, Argonne National Laboratory
4. **A Scalable Parallel LSQR Algorithm for Solving Large-Scale Linear System for Tomographic Problems: A Case Study in Seismic Tomography**  
Author(s): H. Huang, J.M. Dennis, L. Wang, P. Chen  
Presenter: H. Huang, University of Wyoming
5. **Co-evolution of Antagonistic Intelligent Agents using Genetic Algorithms**  
Author(s): L. Magnabosco, J. da Rosa, M. T. de Souza, L. de Oliveira Rech, L. Cheuk Lung  
Presenter: L. Quibem Magnabosco, Federal University of Santa Catarina

## W10c: Workshop on Computational and Algorithmic Finance

13:35 - 15:15  
M214

*Chair: A. Itkin*

1. **Parallel Risk Simulations for Linear Asset Portfolios in R**  
Author(s): H. Sak, W. Hörmann, J. Leydold  
Presenter: H. Sak, Yeditepe University
2. **A New Variance Reduction Technique for Estimating the Value-at-Risk**  
Author(s): M. Pupashenko, R. Korn  
Presenter: M. Pupashenko, Department of Mathematics, University of Kaiserslautern, Erwin-Schroedinger-Strasse, Geb. 48, 67653, Kaiserslautern, Ger
3. **A Fourier Approach to the Computation of CV@R and Optimized Certainty Equivalents**  
Author(s): S.D. Samuel Drapeau, M. Kupper, A. Papapantoleon  
Presenter: S.D. Samuel Drapeau, Humboldt University Berlin
4. **Fourier cosine method and utility indifference pricing with BSDEs**  
Author(s): M.J. Ruijter  
Presenter: M.J. Ruijter, CWI
5. **A benchmark approach of counterparty credit exposure of Bermudan option under Lévy Process: the Monte Carlo-COS Method**  
Author(s): Y. Shen, J.A.M. Van Der Weide, J.H.M. Anderluh  
Presenter: Y. Shen, Delft University of Technology
6. **Estimating the short rate from the termstructures in the Vasicek model**  
Author(s): Z.Z. Zíková, B.S. Stehlíková, J.H. Halgašová  
Presenter: Z.Z. Zíková, Comenius University in Bratislava, Slovakia

7. **A non-uniform nested simulation algorithms in portfolio risk measurement**

Author(s): S. Ben Hadj

Presenter: S. Ben Hadj, Université Catholique de Louvain

**[W31b: Workshop on Teaching Computational Science 2013 \(WTCS 2013\)](#)**

13:35 - 15:15

M218

*Chair: A.B. Shiflet*

1. **Turing Machine and Automata Simulators**

Author(s): M. Hamada

Presenter: M. Hamada

**[W38e: Dynamic Data Driven Application Systems - DDDAS 2013](#)**

13:35 - 15:15

M215

*Chair: C.C. Douglas*

1. **Tracking and Mapping Coherent Structures**

Author(s): S. Ravela, I. Sleder, T. Vigil

Presenter: S. Ravela, MIT

2. **Autonomous Data Error Detection and Recovery in Streaming Applications**

Author(s): R. Klockowski, C. Varela, S. Imai, C. Rice

Presenter: C. Varela, Rensselaer Polytechnic Institute

3. **A Dynamic Data Driven Application System for Real-time Monitoring of Stochastic Damage**

Author(s): E.E. Prudencio, P.T. Bauman, D. Faghihi, J.T. Oden, K. Ravi-Chandar, S.V. Williams

Presenter: E.E. Prudencio, The University of Texas at Austin

4. **DDDAMS-based Crowd Control via UAVs and UGVs**

Author(s): Z. Wang, M. Li, A. Khaleghi, D. Xu, A. Lobos, C. Vo, J.-M. Lien, J. Liu, Y.-J. Son

Presenter: Y.-J. Son, The University of Arizona

5. **The State of DDDAS**

Author(s): C.C. Douglas, A.K. Patra, F. Darema

Presenter: F. Darema, Air Force Office of Scientific Research

**[W42a: 2nd Workshop on Computational Approaches to Social Modeling \(ChASM\)](#)**

13:35 - 15:15

M212

*Chair: Andrea Baronchelli*

1. **Task and Time Aware Community Detection in Dynamically Evolving Social Networks**

Author(s): T. Hecking, T. Göhnert, S. Zeini, H.U. Hoppe

Presenter: T. Hecking, University of Duisburg-Essen

2. **C2M: Open and Decentralized Cloud Contact Management**

Author(s): S. Göndör, J. Devendaraj

Presenter: S. Göndör, Telekom Innovation Laboratories - TU Berlin

3. **Keynote**

Author(s): R. Pastor-Satorras

Presenter: R. Pastor-Satorras

4. **Keynote**

Author(s): L. Steels

Presenter: L. Steels

5. **How groups choose when there is no best option**

Author(s): A. Perez-Escudero, G.G. de Polavieja

Presenter: A. Perez-Escudero, Instituto Cajal, Consejo Superior de Investigaciones Cientificas. 28002, Madrid, Spain

**[W47b: Urgent Computing: Computations for Decision Support in Critical Situations](#)**13:35 - 15:15  
M217*Chair: A.V. Boukhanovsky*1. **Workflow-based Collaborative Decision Support for Flood Management Systems**

Author(s): S.V. Ivanov, S.V. Kovalchuk, A.V. Boukhanovsky

Presenter: S.V. Ivanov, National Research University of Information Technologies, Mechanics and Optics

2. **Interactive workflow-based infrastructure for urgent computing**

Author(s): K.V. Knyazkov, D.A. Nasonov, T.N. Tchurov, A.V. Boukhanovsky

Presenter: K.V. Knyazkov, National Research University of Information Technologies, Mechanics and Optics

**[W53b: Fourth Workshop on Data Mining in Earth System Science \(DMESS 2013\)](#)**13:35 - 15:15  
216*Chair: F.M. Hoffman*1. **Identification and visualization of dominant patterns and anomalies in remotely sensed vegetation phenology using a parallel tool for principal components analysis**

Author(s): R.T. Mills, J. Kumar, F.M. Hoffman, W.W. Hargrove, J.P. Spruce, S.P. Norman

Presenter: R.T. Mills, Oak Ridge National Laboratory

2. **Ophidia: toward big data analytics for eScience**

Author(s): S. Fiore, A. D'Anca, C. Palazzo, I. Foster, D.N. Williams, G. Aloisio

Presenter: S. Fiore, Euro Mediterranean Center on Climate Change and University of Salento, Italy

**[W43b: International Workshop on Computational Flow and Transport: Modeling, Simulations and Algorithms](#)**13:35 -  
14:55  
M213*Chair: S. Sun*1. **Influence of cell boundary flux distribution on well pressure**

Author(s): R.D. HAZLETT, D.K. BABU

Presenter: R.D. HAZLETT, The University of Tulsa

2. **An Efficient Method of Reweighting and Reconstructing Monte Carlo Molecular Simulation Data for Extrapolation to Different Temperature and Density Conditions**

Author(s): S. Sun, A. Kadoura, A. Salama

Presenter: S. Sun, Computational Transport Phenomena Laboratory CTPL, Division of Physical Sciences and Engineering PSE, King Abdullah Univ

3. **A Parallel CFD Model for Wind Farms**

Author(s): M.A. Avila, A. Folch, G. Houzeaux, B. Eguzkitza, L. Prieto, D. Cabezon

Presenter: M.A. Avila, Barcelona SuperComputing Center

4. **Numerical analysis of finite element method for a transient two-phase transport model of polymer electrolyte fuel cell**

Author(s): Y. Sun, M. He, P. Sun

Presenter: Y. Sun, Department of Mathematical Sciences, University of Nevada, Las Vegas, USA

**[W09d: 10th International Workshop on Modeling and Computing Multiscale Systems](#)**14:55 - 15:15  
M213*This presentation is given separately because the author cannot come earlier.**Chair: Valeria Krzhizanovskaya*1. **A multiscale model for Aberrant Crypt Foci**

Author(s): G. Romanazzi, I.N. Figueiredo, C. Leal, B. Engquist

Presenter: G. Romanazzi, CMUC, University of Coimbra

# Poster Session 1

5<sup>th</sup> of June 2013

Rooms 211 & 212

13:20 - 13:50

ID	Title
1.	Utilizing robustness of Krylov subspace methods in reducing the effort of sparse matrix vector multiplication
2.	Structuring Hierarchical Multi-Star Small-World Networks for Real-World Applications
3.	Level Set Analysis of Two-Fluid Interfacial Flows
4.	Effective Slot Selection and Co-allocation Algorithms for Economic Scheduling in Distributed Computing
5.	Synchronization efficient stencil computations using dynamic task graphs
6.	New Parallel Sphere Detector algorithm providing high-throughput for optimal MIMO detection
7.	The Modified Direct Method: An Iterative Approach for Smoothing Planar Meshes
8.	3D Quantum Dot Infrared Photodetector Simulation with modern GPU Accelerators
9.	Computing Classes of Cryptographic Sequence Generators
10.	A 1D Lattice Boltzmann Model for Ocean Acidification
11.	A Decision Making Support System for Ocean-Bottom Seismometer Position Based on GIS
12.	Adaptive Preshuffling in Hadoop clusters
13.	Research on Scheduling Scheme for Hadoop clusters

14. Operating System from the Scratch: a Problem-Based Learning Approach for the Emerging Demands on OS Development
15. A Design Methodology for Distributed Adaptive Stream Mining Systems
16. A mathematical model to study the meningococcal meningitis
17. Kernel performance improvement for the FEM-based fluid analysis code on the K computer
18. Domain triangulation between convex polytopes
19. A Parallel Method for Impulsive Image Noise Removal on Hybrid CPU/GPU Systems
20. High-level support for hybrid parallel execution of C++ applications targeting Intel Xeon Phi coprocessors
21. Bio-IR: A model for bio-inspired multi-agent systems

## Poster Session 2

6<sup>th</sup> of June 2013

Rooms 211 & 212

13:20 - 13:50

ID	Title
1.	Simulating mobile dendrites in a flow
2.	Deterministic Routing with HoL-Blocking-Awareness for Direct Topologies
3.	Formal Study of a Novel Network Role-Based Routing Intelligent Algorithm
4.	Solving Multi-criteria Vehicle Routing Problem by Parallel Tabu Search on GPU
5.	Detection and Estimation of Erroneous Positioning Data

6. Swarm Control of UAVs for Cooperative Hunting with DDDAS
7. Efficient DirOB Cache Coherency for Many-Core CMPs
8. Real-Time Sound Source Localization on Graphics Processing Units
9. Numerical parallel approach to counting Hamiltonian cycles with Proth primes
10. Using huge pages and performance counters to determine the LLC architecture
11. Aeneas: a tool to enable applications to effectively use non-relational databases
12. Multiscale modeling of blood flow: Coupling finite elements with smoothed dissipative particle dynamics
13. Dynamic and Speculative Polyhedral Parallelization of Loop Nests Using Binary Code Patterns
14. Comparative performance analysis of machine learning classifiers in detection of childhood pneumonia using chest radiographs
15. Development of a practical computer network course through Netkit virtualization tool
16. An Optimization for MapReduce Frameworks in Multi-core Architectures
17. Harnessing GPU power from high-level libraries: eigenvalues of integral operators with SLEPc
18. An Approximation of Energy Efficiency in Web Systems
19. Defining and running MapReduce operations with WS-VLAM workflow management system
20. Impact of neighborhood structure on epidemic spreading by means of Cellular Automata Approach
21. MataNui - A Distributed Storage Infrastructure for Scientific Data
22. Simulated Naïve Creature Crossing a Highway

- 23. Data-intensive Spatial Indexing on the Clouds
- 24. A heuristic optimization method for mitigating the impact of a virus attack
- 25. Performance Evaluation of Levenberg-Marquardt Technique in Error Reduction for Diabetes Condition Classification
- 26. Equation-Free Computations as DDDAS Protocols in the Study of Engineered Granular Crystals