Lectures

Once you have entered the main building you will find signposts directing to floor F and the lecture hall.

All plenary lectures take place in the Audimax (HG F 30).

The rooms HG F 26.1, HG F 26.3, HG F 26.5, HG F 33.1 and HG F 33.5 are reserved for the contributed and parallel sessions.
Welcome

The Platform for Advanced Scientific Computing (PASC) Conference series promotes scientific efforts to address key issues in different domains such as Climate and Atmospheric Modelling, Solid Earth Dynamics, Life Sciences, Material Simulations, Plasma Physics, Astrophysics and Computer Science & Mathematics.

The PASC14 conference will be hosted at ETH Zurich in June 2-3, 2014. The conference aims at bringing together all scientists and research groups within these diverse scientific domains to foster interdisciplinary collaborations and to strengthen high-performance computing (HPC) knowledge exchange.

PASC14 invites conference participants to contribute to the meeting by presenting a talk or a poster. The contribution should describe original, interesting, and solid scientific content that is relevant to computational sciences and high performance computing.

About PASC

The Swiss Platform for Advanced Scientific Computing (PASC) overarching goal is to position Swiss computational sciences in the emerging exascale-era and aims to provide the Swiss scientific community with the tools to make the best use of the new generations of supercomputing machines to solve key problems for science and society. It addresses important scientific research issues in high-performance computing and computational science in different domain sciences through interdisciplinary collaborations between domain scientists, computational scientists, software developers, computing centres and hardware developers.

PASC is a joint effort of all Swiss universities, coordinated by the Università della Svizzera italiana and by the Swiss National Supercomputing Centre of the ETH Zurich and will create a long-term research-driven cooperation network in computational science between Swiss Universities.
Overview

PASC14 will have 7 plenary speakers, 1 public lecture, 63 scientific talks, and poster sessions with 80 contributors related to the 5 different PASC areas plus one dedicated to computer science & mathematics.

Additionally, the conference includes an information event dedicated to users of the Swiss National Supercomputing Centre (CSCS).

DAY 1 – JUNE 2, 2014

10:40 – 10:50 HG F 30 - Plenary Opening
Welcome to the Conference; Ralf Eichler, President
ETH Zurich

10:50 – 11:40 HG F 30 - Invited Plenary
Weather and Climate modelling at the Petascale: achievements and perspectives; Pier Luigi Vidale, University of Reading, United Kingdom

11:40 – 12:30 HG F 30 - Invited Plenary
Big data, sparse information: Bayesian inference for large-scale models, with application to inverse modeling of Antarctic ice sheet dynamics; Omar Ghattas, Center for Computational Geosciences, The University of Texas at Austin, USA

12:30 - 13:20 Lunch

13:20 - 14:10 HG F 30 - Invited Plenary
The High Level Support Team — A support unit for petaflop computing; Roman Hatzky, Max-Planck-Institut für Plasmaphysik, IPP-EURATOM-Association, Germany

14:25 - 15:45 Parallel Sessions (4 talks 15+5 min)
HG F 26.5 - Climate Session
HG F 26.1 - Solid Earth Session
HG F 26.3 - Life Sciences Session
HG F 30 - Materials Session
HG F 33.1 - Physics Session
HG F 33.5 - Computer Science & Math. Session

15:45 - 16:15 Coffee Break

16:15 - 17:15 Parallel Sessions (3 talks 15+5 min)
HG F 26.5 - Climate Session
HG F 26.1 - Solid Earth Session
HG F 26.3 - Life Sciences Session
HG F 30 - Materials Session
HG F 33.1 - Physics Session
HG F 33.5 - Computer Science & Math. Session

17:15 - 17:30 Intermission

17:30 - 18:30 HG F 30 - Public Lecture
The Arrow of Computational Science; Petros Koumoutsakos, ETH Zurich

18:30 – 20:00 Poster Session (>75 posters)
Dinner Buffet & Drinks sponsored by NVIDIA
**Poster Session**

Based on experience from previous events, **poster sessions** are one of the most important aspects of the conference. Several collaborations have resulted from the informal discussions held at these sessions.

**Posters** should be put up on the morning of **Monday, June 2** and remain posted until the end of the meeting on **Tuesday, June 3**.

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**CSCS User Meeting**

From this year on the CSCS User Meeting will be held as part of the PASC conference. Please join us for the next meeting on **June 3, from 13:10 to 14:30, in the Audimax (HG F 30) of ETH Zurich**. The agenda includes the following topics:

- 13:10 Message from the Director
- 13:30 User Lab Overview
- 13:40 Systems Overview
- 14:00 HPC Data & Visualization Services Overview
- 14:20 Training Overview

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**DAY 2 - JUNE 3, 2014**

09:00 – 09:50 HG F 30 - Invited Plenary  
**Towards the development of wavefunction-based methods for materials modeling**; Ali Alavi, Department of Chemistry, Trinity College, University of Cambridge, United Kingdom

09:50 – 10:40 HG F 30 - Invited Plenary  
**Feedback, lineages and cancer**; John Lowengrub, University of California at Irvine, USA

10:40 – 11:05 Coffee Break

11:05 – 12:25 Parallel Sessions (4 talks 15+5 min)  
HG F 26.5 - Climate Session  
HG F 26.1 - Solid Earth Session  
HG F 26.3 - Life Sciences Session  
HG F 30 - Materials Session  
HG F 33.1 - Physics Session  
HG F 33.5 - Computer Science & Math. Session

12:25 – 13:10 Lunch sponsored by CSCS

13:10 – 14:30 HG F 30 - Plenary  
**CSCS User Meeting**

14:30 – 15:20 HG F 30 - Invited Plenary  
**Engineering for Performance in High Performance Computing**; Bill Gropp, Director of the Parallel Computing Institute, University of Illinois Urbana-Champaign, USA

15:20 – 16:10 HG F 30 - Invited Plenary  
**HPC & The Inventor’s Dilemma: Abandoing 20 years of Molecular Simulation Knowledge and Moving to GPUs**; Eric Lindahl, SciLifeLab Stockholm, KTH, Sweden

16:10 – 16:20 HG F 30 - Plenary Closing  
Piero Martinoli, President Università della Svizzera italiana
PASC Organization

Scientific Committee

The PASC14 Scientific Committee is responsible for the scientific program.

Andreas Fichtner, ETH Zurich
Maria Grazia Giuffreda, CSCS
Jan Hesthaven, EPF Lausanne
Torsten Höfler, ETH Zurich
Petros Koumoutsakos, ETH Zurich
Nicola Marzari, EPF Lausanne
Siddharta Mishra, ETH Zurich
Ben Moore, University of Zurich
Michele Parrinello, Università della Svizzera italiana
Christoph Schär, ETH Zurich
Olaf Schenk, Università della Svizzera italiana

Area Chairs

CLIMATE NETWORK
Isabelle Bey, ETH Zurich
Christoph Schär, ETH Zurich

SOLID EARTH DYNAMICS NETWORK
Andreas Fichtner, ETH Zurich
Dave May, ETH Zurich

LIFE SCIENCE NETWORK
Petros Koumoutsakos, ETH Zurich
Michele Parrinello, Università della Svizzera italiana

MATERIALS SIMULATION NETWORK
Nicola Marzari, EPF Lausanne
Thomas Schulthess, ETH Zurich

PHYSICS NETWORK
Romain Teyssier, University of Zurich
Laurent Villard, EPF Lausanne

COMPUTER SCIENCE & MATHEMATICS
Siddhartha Mishra, ETH Zurich
Markus Püschel, ETH Zurich
Olaf Schenk, Università della Svizzera italiana

Organizing Committee

The PASC14 conference has been organised by:

Michele De Lorenzi, Maria Grazia Giuffreda, CSCS
Monika Bolliger, Andreas Fichtner, ETH Zurich
Daniel Peter, Università della Svizzera italiana and ETH Zurich
Olaf Schenk, Università della Svizzera italiana
Invited Talk
Day 1 – June 2, 2014

17:30 – 18:30 Audimax (HG F 30) - Invited Plenary

The Arrow of Computational Science; Petros Koumoutsakos, ETH Zurich

Petros Koumoutsakos is Full Professor of Computational Science at ETH Zurich. He studied Naval Architecture at the National Technical University of Athens and got his Master’s at University of Michigan, Ann Arbor. He received his PhD in Aeronautics and Applied Mathematics from the California Institute of Technology. In 1997 he got his appointment as Assistant professor in the Department of Mechanical and Process Engineering, at ETH Zurich. He is founding Director of the ETH Zurich Computational Laboratory (CoLab).

Abstract

The solution of many important scientific and societal problems of our century, such as health, energy and the environment hinge on the fusion of mathematics and information technology. Computational science is the new scientific field emerging from this fusion. It provides us with unprecedented capacity to understand, predict and solve problems across disciplinary boundaries. In this talk I will demonstrate research practices in Computational science using examples ranging from aircraft aerodynamics to cancer.
Invited Talk
Day 1 - June 2, 2014

10:50 – 11:40 HG F 30 - Invited Plenary
Weather and Climate modelling at the Petascale: achievements and perspectives; Pier Luigi Vidale, University of Reading, United Kingdom (Chair: Christoph Schär, ETH Zurich)

Pier Luigi Vidale is full professor at the University of Reading and a senior scientist at the National Centre for Atmospheric Science (NCAS-Climate), leading and developing research on High-Resolution Global Climate Modelling and biosphere-atmosphere interactions.

Abstract
Increasing availability of high-performance computing has allowed the climate modeling community to construct a new generation of global coupled models, capable of resolving some of the fundamental processes that govern the climate system. More explicit representation of eddies in the ocean and of weather systems in the atmosphere has demonstrated how they contribute to the general circulation and how it is increasingly possible to rely less on uncertain physical parameterisations. These developments are potentially promising for reducing inter-model disagreement in community multi-model hindcasts and projections. We have demonstrated, for instance, how the representation of the relative importance of the remote and local processes governing the global energy and hydrological cycles converges at resolutions beyond 50km. These so-called "weather-resolving" climate models are also suitable for studying how global teleconnections might influence the long-term regional changes in storm tracks, or in understanding changes in high-impact phenomena, such as Tropical and Extra-Tropical Cyclones, as well as their contributions to the general circulation.
DAY 1 - JUNE 2, 2014
14:25 - 15:45 HG F 26.5
Chair: Isabelle Bey, ETH Zurich
14:25 - 15:05 Towards GPU-accelerated Operational Weather Forecasting; Oliver Fuhrer (MeteoSwiss)
15:05 - 15:25 Using OpenACC compiler directives to achieve performance portable code on CPU and GPU architectures; Xavier Lapillonne (ETH Zurich)
15:25 - 15:45 Towards Cloud-Resolving European-Scale Climate Simulations using a fully GPU-enabled Prototype of the COSMO Regional Climate Model; David Leutwyler (ETH Zurich)

DAY 2 - JUNE 3, 2014
11:05 - 12:25 HG F 26.5
Chair: Xavier Lapillonne, ETH Zurich
11:05 - 11:25 Big data in climate modeling; Reto Knutti (ETH Zurich)
11:25 - 11:45 Distributed Memory GPU-enabled Compression of Very Large Climate Time Series Data; William Sawyer (CSCS)
11:45 - 12:05 Statistical regression analysis of extreme events in HPC context; Olga Kaiser (Università della Svizzera Italiana)

16:15 - 17:15 HG F 26.5
Chair: Christoph Schär, ETH Zurich
16:15 - 16:35 An Application Driven, Power Efficient System Design for 1-km Scale Global Cloud System Resolving Models; David Donofrio (Lawrence Berkeley National Labs, USA)
16:35 - 16:55 Performance of semi-implicit compressible and anelastic EULAG model for all-scale atmospheric flows; Zbigniew P. Piotrowski (Instytut Meteorologii i Gospodarki Wodnej, Poland)
16:55 - 17:15 Towards a multi-node OpenACC Implementation of the ICON Model; William Sawyer (CSCS)
Invited Talk
Day 1 - June 2, 2014

11:40 – 12:30 HG F 30 - Invited Plenary

Big data, sparse information: Bayesian inference for large-scale models, with application to inverse modeling of Antarctic ice sheet dynamics; Omar Ghattas, Center for Computational Geosciences, The University of Texas at Austin, USA
(Chair: Andreas Fichtner, ETH Zurich)

Omar Ghattas is the John A. and Katherine G. Jackson Chair in Computational Geosciences, Professor of Geological Sciences and of Mechanical Engineering, and Director of the Center for Computational Geosciences in the Institute for Computational Engineering and Sciences at the University of Texas at Austin.

Abstract

Predictive models of complex geoscience systems often contain numerous uncertain parameters. Rapidly expanding volumes of observational data present opportunities to reduce these uncertainties via solution of inverse problems. Bayesian inference provides a systematic framework for inferring model parameters with associated uncertainties from (possibly noisy) data and any prior information. However, solution of the Bayesian inverse problem via conventional Markov chain Monte Carlo methods remains prohibitive for expensive models and high-dimensional parameters, as result from discretization of infinite dimensional problems with uncertain fields. Despite the large size of observational datasets, typically they can provide only sparse information on model parameters. Based on this property we design MCMC methods that adapt to the structure of the posterior probability and exploit an effectively-reduced parameter dimension, thereby making Bayesian inference tractable for some large-scale, high-dimensional inverse problems. We apply the methodology to an inverse problem for Antarctic ice sheet flow: given a non-Newtonian flow model of the ice sheet and free surface velocity observations, we seek to infer the sliding coefficient field at the base of the ice.

This work is joint with Tan Bui-Thanh, Tobin Isaac, James Martin, Noemi Petra, Georg Stadler, Hari Sundar, and Hongyu Zhu.
DAY 1 - JUNE 2, 2014

14:25 - 15:45 HG F 26.1
Chair: Andreas Fichtner, ETH Zurich

14:25 - 14:45 Opportunities and challenges in large-scale adaptive-mesh simulations; Carsten Burstedde (University of Bonn, Germany)
14:45 - 15:05 Challenges in the Simulation of Earthquakes; Christian Pelties (Ludwig Maximilian University, Germany)
15:05 - 15:25 HPC Solutions for Geophysical Exploration Problems: Efficiency, Reliability and Maintenance for Real-Life Applications; Josep de la Puente (Barcelona Supercomputing Center, Spain)
15:25 - 15:45 A Semismooth Newton-CG Method for Constrained Parameter Identification in Seismic Tomography; Christian Boehm (TU München, Germany)

16:15 - 17:15 HG F 26.1
Chair: Dave May, ETH Zurich

16:15 - 16:35 Physics-based earthquake scenarios for hazard assessment in large urban areas; Ilario Mazzieri (Politecnico di Milano, Italy)
16:35 - 16:55 Parallel Adaptive Simulation of Earthquake-Tsunami Events; Michael Bader (TU München, Germany)
16:55 - 17:15 Modelling the solid Earth plate tectonics-mantle convection system and its feedbacks with the geodynamo, atmosphere and ocean; Paul J. Tackley (ETH Zurich)

DAY 2 - JUNE 3, 2014

11:05 - 12:25 HG F 26.1
Chair: Andreas Fichtner, ETH Zurich

11:05 - 11:25 Faster and more accurate interface tracking using a level set two-way wave equation approach; Henri Samuel (Institut de Recherche en Astrophysique et Planétologie, France)
11:25 - 11:45 Immersive experimentation in a wave propagation laboratory; Johan O. A. Robertsson (ETH Zurich)
11:45 - 12:05 Constraining the Rheology of the Lithosphere Through Joint Geodynamic and Gravity Inversion; Boris Kaus (University of Maiz, Germany)
12:05 - 12:25 Towards magnetic sounding of the Earth's core by an adjoint method; Kuan Li (ETH Zurich)
Invited Talk
Day 2 – June 3, 2014

09:50 – 10:40 HG F 30 - Invited Plenary
Feedback, lineages and cancer; John Lowengrub, University of California at Irvine, USA
(Chair: Petros Koumoutsakos, ETH Zurich)

John Lowengrub is a Chancellor’s Professor at the University of California at Irvine with appointments in the departments of Mathematics, Biomedical Engineering, Chemical Engineering and Materials Science. His research interests include mathematical and computational biology, applied and computational mathematics, mathematical oncology, complex fluids and materials science.

15:20 – 16:10 HG F 30 - Invited Plenary
HPC & The Inventor’s Dilemma: Abandoing 20 years of Molecular Simulation Knowledge and Moving to GPUs; Eric Lindahl, SciLifeLab Stockholm, KTH, Sweden
(Chair: Olaf Schenk, Universita della Svizzera italiana)

Eric Lindahl heads a research division as professor of biophysics at the Department of Biochemistry & Biophysics at Stockholm University, with a dual appointment as professor of theoretical biophysics at the KTH Royal Institute of Technology. Since 2011 he is a member of the Swedish Young Academy. He completed undergraduate studies in engineering physics at Lund University, after which he received a PhD in theoretical biophysics at the KTH Royal Institute of Technology in Stockholm in 2001. He has been a visiting research scholar with Hermann Berendsen & Alan Mark at Groningen University (NL), Michael Levitt & Vijay Pande at Stanford University (US) and Mark Delarue at the Pasteur Institute (FR). In 2004 he started as assistant professor and later associate professor at Stockholm University. The team’s main research theme concerns ion channels, in particular molecular simulations – and they have written the GROMACS molecular simulation package.
DAY 1 - JUNE 2, 2014

14:25 - 15:45 HG F 26.3
Chair: Petros Koumoutsakos, ETH Zurich

14:25 - 14:45 HPC-ABGEM: High-performance agent-based general ecosystems modeling; Simone Callegari (University of Zurich)

14:45 - 15:05 Bone structure analysis on multiple GPGPUs; Peter Arbenz (ETH Zurich)

15:05 - 15:25 Computational simulation of heart function with an orthotropic active strain model of electromechanics; Toni Lassila (EPFL)

15:25 - 15:45 Red blood cells and related functions of the human spleen; Igor V. Pivkin (Università della Svizzera italiana)

16:15 - 17:15 HG F 26.3
Chair: Igor Pivkin, Università della Svizzera italiana

16:15 - 16:35 LBIBCell: A Cell-Based Simulation Environment for Morphogenetic Problems; Simon Tanaka (ETH Zurich)

16:35 - 16:55 SEM++: a particle model of cellular mechanics, growth, signaling and migration; Gerardo Tauriello (ETH Zurich)

16:55 - 17:15 Exploring the unfolded ensemble of proteins; Albert Ardevol (ETH Zurich)

DAY 2 - JUNE 3, 2014

11:05 - 12:05 HG F 26.3
Chair: Petros Koumoutsakos, ETH Zurich

11:05 - 11:25 Protein-ligand unbinding kinetics and pathways through metadynamics; Pratyush Tiwary (ETH Zurich and Università della Svizzera italiana)

11:25 - 11:45 Improving I/O Performance of ClustalW-MPI Multiple Sequence Alignment Software; Soon-Heum Ko (Linkoping University, Sweden)

11:45 - 12:05 OmicABEL: Story of a successful interdisciplinary collaboration; Diego Fabregat-Traver (RWTH Aachen, Germany)
Invited Talk
Day 2 - June 3, 2014

09:00 – 09:50 HG F 30 - Invited Plenary
Towards the development of wavefunction-based methods for materials modeling; Ali Alavi, Department of Chemistry, Trinity College, University of Cambridge, United Kingdom (Chair: Nicola Marzari, EPFL)

Ali Alavi is professor of Theoretical Chemistry at the University of Cambridge. Since 2000 he is fellow of Trinity College Cambridge. In 2000 he started at the University of Cambridge and Lecturer and then Reader in Theoretical Chemistry at the Department of Chemistry.

Abstract
We review some recent progress in using Monte Carlo methods in combination with quantum chemical methods to solve to a high degree of accuracy the many-electron Schrödinger equation, both in the molecular context as well as periodic boundary conditions. At the heart of the methods is FCIQMC which simulates an exact stochastic representation of the FCI wavefunction of a physical system expressed in a finite basis. The sampled FCI wavefunction can be used to compute the 1- and 2-electron reduced density matrix, from which a great many physical properties can be extracted. In particular, these can be used to compute a perturbative basis-set correction which very accurately accounts for the basis-set error arising from the use of finite basis sets. We have recently extended this method to periodic systems and results will be shown in this regard. Finally, we will review recent progress on alleviating the time-step bottleneck of FCIQMC, opening the possibility to simulate substantially larger systems than currently possible.
DAY 1 - JUNE 2, 2014

14:25 - 15:45 HG F 30
Chair: Nicola Marzari, EPFL

14:25 - 14:45 Nuclear quantum effects in ab initio simulations using colored noise and i-PI; Michele Ceriotti (EPFL)

14:45 - 15:05 Accelerating quantum transport simulations on massively parallel computing architectures; Mauro Calderara (ETH Zurich)

15:05 - 15:25 Enabling First Principles Simulations at the MP2 and RPA Level: An Efficient and Massively Parallel Algorithm Based on the Resolution-of-Identity Gaussian and Plane Waves Approach; Mauro Del Ben (University of Zurich)

15:25 - 15:45 SIESTA-PEXSI for large scale electronic structure calculations; Georg Huhs (Barcelona Supercomputing Center, Spain)

DAY 2 - JUNE 3, 2014

11:05 - 12:25 HG F 30
Chair: Nicola Marzari, EPFL

11:05 - 11:25 A combined classical and first-principles study to the modeling of resistance drift in phase-change materials; Federico Zipoli (IBM Research - Zurich)

11:25 - 11:45 Epitaxial strain-induced point-defect formation and ordering in oxides; Ulrich Aschauer (ETH Zurich)

11:45 - 12:05 Linear Scaling Electronic Structure Theory; Ole Schütt (ETH Zurich)

12:05 - 12:25 Massively Parallel Hartree-Fock Exact Exchange Ab Initio Molecular Dynamics Simulations; Valery Weber (IBM Research - Zurich)
Invited Talk
Day 1 – June 2, 2014

13:20 - 14:10 HG F 30 - Invited Plenary
The High Level Support Team — A support unit for petaflop computing; Roman Hatzky, Max-Planck-Institut für Plasmaphysik, IPP-EURATOM-Association, Germany
(Chair: Laurent Villard, EPFL)

Roman Hatzky is core team leader of the High Level Support Team of the European Fusion Development Agreement (EFDA) project “High Performance Computer for Fusion Applications” since 2009. He works in the Computational Physics department of IPP.

Abstract
Modern petaflop computer architectures are already so demanding that an optimal exploitation can be only performed with a special support unit. The High Level Support Team (HLST) provides support to scientists from all EFDA (European Fusion Development Agreement) Associates for the development and optimization of codes to be used on the dedicated IFERC-CSC supercomputer located in Rokkasho, Japan. The supercomputer delivers computing power of about 1.52 petaflop/s and is optimally suited for the fusion scientists’ simulation programs. The HLST consists of a core team based at the IPP Garching (Max-Planck-Institut für Plasmaphysik) and of other high level support staff provided by the Associates. The HLST members are all HPC experts with a background in developing large scientific applications and particular expertise in numerical algorithms and and visualization.
### DAY 1 - JUNE 2, 2014

**14:25 - 15:45 HG F 33.1**  
Chair: Laurent Villard, EPFL

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<tr>
<th>Time</th>
<th>Session</th>
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<tbody>
<tr>
<td>14:25 - 14:45</td>
<td>Conservation relations and accurate schemes for delta-f Particle-In-Cell simulation; Ben F. McMillan (University of Warwick, United Kingdom)</td>
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<tr>
<td>14:45 - 15:05</td>
<td>Simulations of energetic particle driven instabilities in Tokamak; Alberto Bottino (Max Planck Institut für Plasmaphysik, Germany)</td>
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<td>15:05 - 15:25</td>
<td>Towards a GPU-MIC Particle-In-Cell Code For Plasma Applications; Farah Hariri (EPFL)</td>
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<tr>
<td>15:25 - 15:45</td>
<td>Structure preserving schemes; Roger Käppeli (ETH Zurich)</td>
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**16:15 - 17:15 HG F 33.1**  
Chair: Romain Teyssier, University of Zurich

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<th>Time</th>
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<tr>
<td>16:15 - 16:35</td>
<td>Radiative transfer in multi-scale, multi-physics simulations; the big challenge in astrophysics and cosmology; Lucio Mayer (University of Zurich)</td>
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<td>16:35 - 16:55</td>
<td>Efficient Space-Charge calculation on Irregular Domains using Adaptive Mesh Refinement; Tulin Kaman (ETH Zurich and Paul Scherrer Institute)</td>
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<td>16:55 - 17:15</td>
<td>PKDGRAV2: Minimal data movement and high computation in a parallel fast multipole tree code; Joachim Stadel (University of Zurich)</td>
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### DAY 2 - JUNE 3, 2014

**11:05 - 12:25 HG F 26.1**  
Chair: Laurent Villard, EPFL

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<th>Time</th>
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<tr>
<td>11:05 - 11:25</td>
<td>Adaptively balanced parallel MLMC solver for acoustic wave propagation with log-normal coefficients; Jonas Sukys (ETH Zurich)</td>
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<td>11:25 - 11:45</td>
<td>Enabling LHC for HPC; Sigve Haug (University of Bern)</td>
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<td>11:45 - 12:05</td>
<td>DFT+DMFT study of epitaxially strained perovskite LVO; Gabriele Sclauzero (ETH Zurich)</td>
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<tr>
<td>12:05 - 12:25</td>
<td>Radiation hydrodynamics with the AMR code RAMSES; Romain Teyssier (University of Zurich)</td>
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</table>
Invited Talk
Day 2 – June 3, 2014

14:30 – 15:20 HG F 30 - Invited Plenary
Engineering for Performance in High Performance Computing; Bill Gropp, Director of the Parallel Computing Institute, University of Illinois Urbana-Champaign, USA
(Chair: Torsten Höfler, ETH Zurich)

Bill Gropp is Thomas M. Siebel Chair in Computer Science since 2013. Gropp is a Fellow of ACM, IEEE, and SIAM, and a member of the National Academy of Engineering. He received the Sidney Fernbach Award from the IEEE Computer Society in 2008 and the TCSC Award for Excellence in Scalable Computing in 2010.

Abstract
Achieving good performance on any system requires balancing many competing factors. More than just minimizing communication (or floating point or memory motion), for high end systems the goal is to achieve the lowest cost solution. And while cost is typically considered in terms of time to solution, other metrics, including total energy consumed, are likely to be important in the future.

Making effective use of the next generations of extreme scale systems requires rethinking the algorithms, the programming models, and the development process. This talk will discuss these challenges and argue that performance modeling, combined with a more dynamic and adaptive style of programming, will be necessary for extreme scale systems.
DAY 1 - JUNE 2, 2014

14:25 - 15:45 HG F 33.5
Chair: Olaf Schenk, Università della Svizzera italiana

14:25 - 14:45 Performance Engineering for Stencil Updates on Modern Processors; Gerhard Wellein (University of Erlangen-Nuremberg, Germany)

14:45 - 15:05 ppOpen-HPC: Open Source Infrastructure for Development and Execution of Large-Scale Scientific Applications on Post-Peta-Scale Supercomputers with Automatic Tuning (AT); Kengo Nakajima (The University of Tokyo, Japan)

15:05 - 15:25 A roofline model of energy; Richard Vuduc (Georgia Tech, USA)

15:25 - 15:45 Reproducible Experiments in High-Performance Computing: Techniques and Stencil Compiler Benchmark Study; Helmar Burkhart (University of Basel)

16:15 - 17:15 HG F 33.5
Chair: Markus Püschel, ETH Zurich

16:15 - 16:35 Performance, power, and energy modeling and characterization of sparse matrix-vector multiplication on multicore architectures; Cristiano Malossi (IBM Research - Zurich)

16:35 - 16:55 3D-Stacked Logic-in-Memory Hardware For Sparse Matrix Operations; Franz Franchetti (Department of Electrical and Computer Engineering, Carnegie Mellon University, USA)

16:55 - 17:15 Massively Parallel and near Linear Time Graph Analytics; Yves Ineichen (IBM Research - Zurich)

DAY 2 - JUNE 3, 2014

11:05 - 12:25 HG F 33.5
Chair: Siddharta Mishra, ETH Zurich

11:05 - 11:25 Performance Prediction for Tensor Contractions; Paolo Bientinesi (RWTH Aachen, Germany)

11:25 - 11:45 Using Adaptive Sparse Grids to Solve High-Dimensional Dynamic Economic Models; Simon Scheidegger (University of Zurich)

11:45 - 12:05 High-Performance Implementation of High-Dimensional Quadrature for Bayesian Inverse Problems; Robert Gantner (ETH Zurich)

12:05 - 12:25 Entropy-stable space-time discontinuous Galerkin schemes for hyperbolic systems of conservation laws; Andreas Hölzle (ETH Zurich)
The poster session will take place on June 2, from 18:30 to 20:00.
The following posters will be presented (gallery of HG F-Floor and HG E-Floor – see location plan here below)

**PASC CO-DESIGN PROJECTS**

**PASC-01**
GeoPC: Development of hybrid multi-level smoothers using next generation hardware  
*Dave A. May (ETH Zurich)*  
Marcus Grote (University Basel), Matthew G. Knepley (University of Chicago, USA), Karl Rupp (TU Wien, Austria), Patrick Sanan (Università della Svizzera italiana), William Sawyer (CSCS), Olaf Schenk (Università della Svizzera italiana), Sascha Schnepp (ETH Zurich), Paul J. Tackley (ETH Zurich)

**PASC-02**
GeoPC: Solid earth geodynamic applications  
*Paul J. Tackley (ETH Zurich)*  
Marcus Grote (University Basel), Matthew G. Knepley (University of Chicago, USA), Dave A. May (ETH Zurich), Karl Rupp (TU Wien, Austria), Patrick Sanan (Università della Svizzera italiana), William B. Sawyer (CSCS), Olaf Schenk (Università della Svizzera italiana), Sascha Schnepp (ETH Zurich)

**PASC-03**
Towards a comprehensive earth model across the scales  
*Michael Afanasiev (ETH Zurich)*  
Andreas Fichtner (ETH Zurich), Daniel Peter (Università della Svizzera italiana and ETH Zurich)

**PASC-04**
Heterogeneous compiler platform  
*Tobias Gysi (ETH Zurich)*  
Torsten Hoefler (ETH Zurich)

**PASC-05**
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*Carlos Osuna (ETH Zurich)*  
Oliver Fuhrer (MeteoSwiss), Tobias Gysi (ETH Zurich), Mauro Bianco (CSCS)

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*Mauro Bianco (CSCS)*  
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*Andreas Glöss (University of Zurich)*  
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Florian Schiffmann (ETH Zurich)
Samuel Andermatt (ETH Zurich), Jinwoong Cha (ETH Zurich), Ole
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Bastian Schaefer (University of Basel)
Stephan Mohr (University of Basel and CEA Grenoble), Maximilian
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Antonino La Magna (CNR-IMM, Italy), Massimo Camarda (CNR-IMM,
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Claudio Alberti (EPFL), Marco Mattavelli (EPFL), Yann Thoma (HEIG-
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Daniel Zerzlon (SIB), Ioannis Xenarios (SIB)

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Lucio Mayer (University of Zurich)
Aliereza Rahmati (Max Planck Institute for Astrophysics, Garching, Ger-
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Dominik Brunner (EMPA)
Will Sawyer (CSCS), Franziska Glassmeier (ETH Zurich), Joseph
Charles (CSCS), Lea Giordano (EMPA), Anne Roches (ETH Zurich),
Isabelle Bey (ETH Zurich), Heike Vogel (KIT, Germany), Bernhard Vogel
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A novel atmospheric large eddy simulation infrastructure
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Kyle Pressel (California Institute of Technology and ETH Zurich)
Tapio Schneider (ETH Zurich)

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on GPU-enabled clusters
Juraj Kardoš (Università della Svizzera italiana)
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Korbinian Sager (ETH Zurich)
Andreas Fichtner (ETH Zurich)

EAR-03
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Drosos Kourounis (Università della Svizzera italiana)
Olaf Schenk (Università della Svizzera italiana)

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Marlies Vasmel (ETH Zurich)
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Phillippe Marti (University of Colorado Boulder, USA), Jerome Noir (ETH Zurich), Andrew Jackson (ETH Zurich)

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Christian Pelties (LMU Munich, Germany)

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Ylona van Dinther (ETH Zurich)
Taras Gerya (ETH Zurich), Luis A. Dalguer (ETH Zurich), Martin Mai (King Abdullah University of Science and Technology, Saudi Arabia)

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Alessandro Barducci (EPFL), Michele Parrinello (ETH Zurich and Università della Svizzera italiana)

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Daniel Hupp (ETH Zurich)
Peter Arbenz (ETH Zurich), Dominik Obrist (University of Bern)

LS-03
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Bjoern H. Menze (TU München, Germany), Petros Kourmoutsakos (ETH Zurich)

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Alessandro Barducci (EPFL), Martin Tollinger (University of Innsbruck, Austria) and Michele Parrinello (ETH Zurich and Università della Svizzera italiana)
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Ralph Koitz (University of Zurich)
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Jakub Imriska (ETH Zurich)

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Marcella Iannuzzi, Jürg Hutter (University of Zurich)

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Yaël Birenbaum (ETH Zurich)
Claude Ederer (ETH Zurich)

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Giovanni Pizzi (EPFL)
Andrea Cepellotti (EPFL), Boris Kozinsky (Bosch RTC, Cambridge, USA), Marco Fornari (Central Michigan University, USA), Nicola Marzari (EPFL)

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Madhura Marathe (ETH Zurich)
Ederer (ETH Zurich)

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Boris Sangiorgio (ETH Zurich)
Michael Fechner (ETH Zurich), Nicola Spaldin (ETH Zurich)

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Mohammad Hossein Bani-Hashemian (ETH Zurich)
Sascha Brück (ETH Zurich), Mathieu Luisier (ETH Zurich), Joost VandeVondele (ETH Zurich)

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Samuel Andermatt (ETH Zurich)
Florian Schiffmann (ETH Zurich), Joost VandeVondele (ETH Zurich)

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Dorothea Golze (University of Zurich)
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Natalya Fedorova (ETH Zurich)
Andrea Scaramucci (ETH Zurich), Claude Ederer (ETH Zurich), Nicola Spaldin (ETH Zurich)

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Florian Thöle (ETH Zurich)
Michael Fechner (ETH Zurich), Nicola Spaldin (ETH Zurich)

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Clelia Spreafico (ETH Zurich)
Joost VandeVondele (ETH Zurich)

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Sergii Nichenko (Paul Scherrer Institute)
Marco Streit (Paul Scherrer Institute)

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Marcella Iannuzzi (University of Zurich)
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Ngoc Linh Nguyen (EPFL)
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## PHYSICS

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Sarunya Pumma (King Mongkut’s University of Technology Thonburi, Thailand), Sylvain Chapelain (CERN), Tiranee Achalakul (King Mongkut’s University of Technology Thonburi, Thailand)

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Simplice Donfack (Università della Svizzera italiana)  
Olaf Schenk (Università della Svizzera italiana)

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Johannes Steiner (Università della Svizzera italiana)  
Rolf Krause (Università della Svizzera italiana)

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Mattia Penati (Politecnico di Milano, Italy)  
Edie Miglio (Politecnico di Milano, Italy)

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Andreas Kreienbuehl (Università della Svizzera italiana)  
Daniel Ruprecht (Università della Svizzera italiana), Robert Speck (Forschungszentrum Juelich, Germany and Università della Svizzera italiana), Rolf Krause (Università della Svizzera italiana)

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Sandra May (ETH Zurich)
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