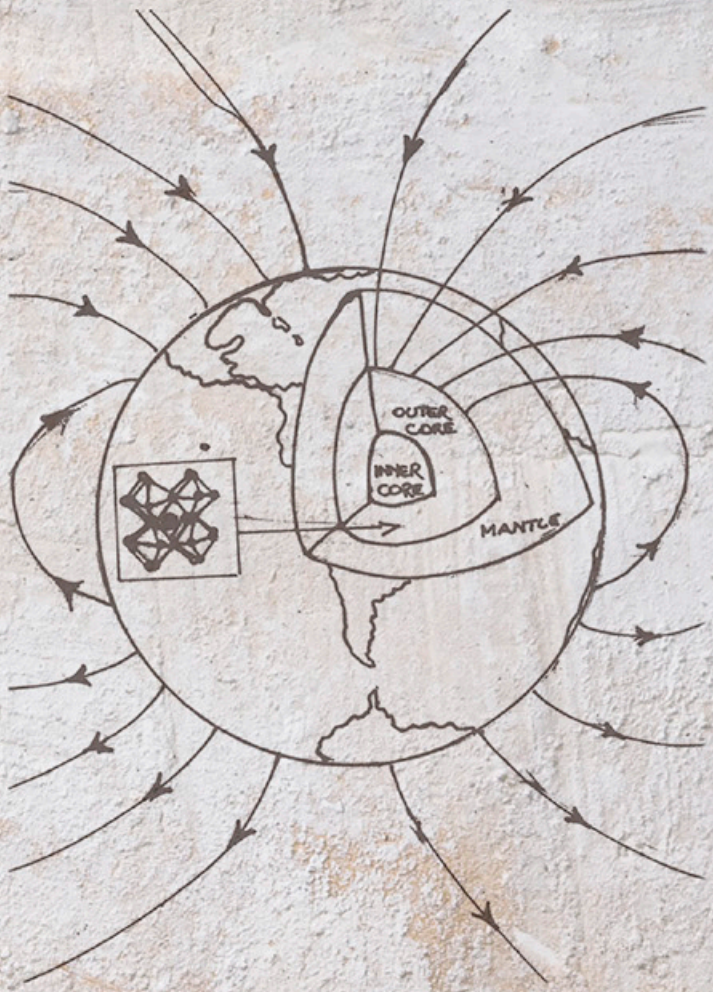

EULER EQUATION

$$\frac{\partial \rho}{\partial t} + \sum_{i=1}^{3} \frac{\partial(\rho u_i)}{\partial x_i} = 0$$

$$\frac{\partial(\rho u_j)}{\partial t} + \sum_{i=1}^{3} \frac{\partial(\rho u_i u_j)}{\partial x_i} + \frac{\partial p}{\partial x_i} = 0$$

$$\frac{\partial E}{\partial t} + \sum_{i=1}^{3} \frac{\partial((E+p)u_i)}{\partial x_i} = 0$$

i, j label the three Cartesian components:
$(x_1, x_2, x_3) = (x, y, z)$ and
$(u_1, u_2, u_3) = (u, v, w)$

PASC18

Platform for Advanced Scientific Computing Conference

Basel Switzerland

2–4 July 2018


```
quicksort(A, i, k):
    if i<k:
        p:=partition(A,i,k)
        quicksort(A, i, p-1)
        quicksort(A, p+1, k)
```

POISSON'S EQUATION

$$\Delta\varphi = f$$

Δ = LAPLACE OPERATOR

f & φ REAL OR COMPLEX-VALUED FUNCTIONS

$$\nabla^2 \varphi = f$$

IN THREE-DIMENSIONAL CARTESIAN COORDINATES:

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\varphi(x,y,z) = f(x,y,z)$$

when
$f = 0$ we retrieve LAPLACE'S EQUATION

Welcome to PASC18

We are delighted to welcome you to PASC18 at the Congress Center Basel, Switzerland. The city of Basel is situated on the river Rhine at the intersection of three countries – Switzerland, France and Germany. Home to the oldest university in Switzerland, Basel is considered the cultural capital of the country and Europe's leading research centre for life sciences, medical research, energy engineering and cultural sciences.

PASC18 is the fifth edition of the PASC Conference series, an international platform for the exchange of competences in scientific computing and computational science, with a strong focus on methods, tools, algorithms, application challenges, and novel techniques and usage of high performance computing.

The theme of PASC18 is "Fast and Big Data, Fast and Big Computation", emphasizing the close coupling of data and computation in current and future high-performance computing applications. A panel discussion bringing perspectives from various scientific domains and industry is dedicated to this theme.

The PASC Conference is first and foremost a platform for promoting interdisciplinary communication. At PASC18 we introduce a new session, the interdisciplinary dialogue, where the audience, coming from diverse research fields, can gain insight into a specific field through an interview between prominent computational scientists from different research domains. In this year's dialogue, Petros Koumoutsakos (ETH Zurich) will interview Constantia Alexandrou (University of Cyprus) about her field of research – quantum chromodynamics.

Other program highlights include keynotes from David Bader (Georgia Tech) on massive-scale analytics in real world problems, Marina Becoulet (CEA) on first-principles modelling of magnetohydrodynamics in fusion devices, Alice-Agnes Gabriel (Ludwig Maximilian University of Munich) on extreme-scale earthquake simulations, and Nils P. Wedi (ECMWF) on kilometer-scale weather and climate simulations. Minisymposium, paper and poster presentations complete the technical program, with more than 250 contributions in total from the eight scientific domains represented at the conference.

PASC18 is co-sponsored by the Association for Computing Machinery (ACM) and the PASC Structuring Project, supported by the Council of Federal Institutes of Technology (ETH Board). The PASC Conference is coordinated by the Swiss National Supercomputing Centre (CSCS).

We are grateful to our local hosts – the University of Basel and the City of Basel – and to all participants for contributing to a strong and vibrant program. We thank the following companies and organizations for their support: HPE, IBM, PSI, CRAY, DDN, MARVEL, MICROSOFT, NOVARTIS and NVIDIA.

Scientific Fields

- CLIMATE & WEATHER
- SOLID EARTH DYNAMICS
- LIFE SCIENCES
- CHEMISTRY & MATERIALS
- PHYSICS
- COMPUTER SCIENCE & APPLIED MATHEMATICS
- ENGINEERING
- EMERGING APPLICATION DOMAINS

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Conference Chairs

Florina Ciorba (University of Basel, Switzerland)
Erik Lindahl (Stockholm University, Sweden)

Scientific Committee

Minisymposia & Posters Program Chairs

Florina Ciorba (University of Basel, Switzerland)
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Chemistry & Materials
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Markus Meuwly (University of Basel, Switzerland)
Kristin Persson (Lawrence Berkeley National Laboratory, USA)
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Climate & Weather
Domain Co-Chair: **Willem Deconinck** (ECMWF, UK)
Domain Co-Chair: **Rupert Ford** (Science and Technology Facilities Council, UK)
Mario Acosta (Barcelona Supercomputing Center, Spain)
Luca Bonaventura (Politecnico di Milano, Italy)
Katherine Evans (Oak Ridge National Laboratory, USA)
Oliver Fuhrer (MeteoSwiss, Switzerland)

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Domain Co-Chair: **Michael Heroux** (Sandia National Laboratories, USA)
Domain Co-Chair: **Martin Schulz** (TU Munich, Germany)
Simone Deparis (EPFL, Switzerland)
Laura Grigori (INRIA, France)
Matthias Müller (RWTH Aachen University, Germany)
Richard Vuduc (Georgia Institute of Technology, USA)
Ulrike Yang (Lawrence Livermore National Laboratory, USA)

Emerging Application Domains
Domain Co-Chair: **Simon Scheidegger** (University of Zurich, Switzerland)
Domain Co-Chair: **Georgia Tourassi** (Oak Ridge National Laboratory, USA)
Rumi Chunara (New York University, USA)
Philipp Eisenhauer (University of Bonn, Germany)
Roger Käppeli (ETH Zurich, Switzerland)
Shannon Quinn (University of Georgia, USA)
Philipp Renner (Lancaster University, UK)
Kerstin Kleese van Dam (Brookhaven National Laboratory, USA)

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Philipp Schlatter (KTH Royal Institute of Technology, Sweden)
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Domain Co-Chair: **Dan Jacobson** (Oak Ridge National Laboratory, USA)
Domain Co-Chair: **Abigail Morrison** (Forschungszentrum Jülich, Germany)
Ben Brown (Lawrence Berkeley National Laboratory, USA)
Sharlee Climer (University of Missouri - St. Louis, USA)
Georgios Gkoutos (University of Birmingham, UK)
Susanne Kunkel (KTH Royal Institute of Technology, Sweden)
Sandipan Mohanty (Forschungszentrum Jülich, Germany)

Physics
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Domain Co-Chair: **Sinéad Ryan** (Trinity College, Ireland)
Frank Jenko (University of California, USA)
Tilo Wettig (University of Regensburg, Germany)
Frank Wuerthwein (UC San Diego, USA)

Solid Earth Dynamics
Domain Co-Chair: **Ebru Bozdag** (Colorado School of Mines, USA)
Domain Co-Chair: **Dimitri Komatitsch** (CNRS, France)
Sebastien Chevrot (CNRS, France)
David May (University of Oxford, UK)
Louise Kellogg (UC Davis, USA)
Rene-Edouard Plessix (Shell Technology Center Amsterdam, Netherlands)
James Wookey (University of Bristol, UK)

Monday 02.07

IP Invited Plenary Presentation

IP01 **Unraveling Earthquake Dynamics Through Extreme-Scale Multi-Physics Simulations**
10:20 – 11:10 | Montreal Room
Alice-Agnes Gabriel (Ludwig Maximilian University of Munich, Germany)
Chair: Dimitri Komatitsch (CNRS, France)

AP ACM PASC18 Papers

AP01 **ACM PASC18 Papers Session I**
Montreal Room | Chair: Sabine Roller (University of Siegen, Germany)

11:10 – 11:40 Extreme Computing for Extreme Adaptive Optics: The Key to Finding Life Outside our Solar System, Hatem Ltaief (King Abdullah University of Science and Technology, Saudi Arabia)

11:40 – 12:10 The CLAW DSL: Abstractions for Performance Portable Weather and Climate Models, Valentin Clement (Center for Climate System Modeling, Switzerland)

ID Interdisciplinary Dialogue

ID01 **The Colourful Theory, and Visible and Invisible Matter in the Universe: An Interdisciplinary Dialogue between Constantia Alexandrou and Petros Koumoutsakos**
18:00 – 18:45 | Montreal Room
Constantia Alexandrou (University of Cyprus, Cyprus)
Petros Koumoutsakos (ETH Zurich, Switzerland)
Chair: Erik Lindahl (Stockholm University, Sweden)

MS Minisymposia Session I

MS01 **Adaptive Parallel Strategies for the Exploration of Challenging Search Spaces with Applications in Particle Simulations and Optimization, Part I**
Samarkand Room | Organizer(s): Andreas Vitalis, Marco Bacci, Amedeo Caflisch (University of Zurich, Switzerland)

13:00 – 13:30 FAST - Goal-Oriented Adaptive Sampling of Protein Dynamics, Gregory Bowman (Washington University School of Medicine, USA)

13:30 – 14:00 Applications and Advancements of the Progress-Index Guided Sampling Method in Molecular Dynamics Simulations, Marco Bacci (University of Zurich, Switzerland)

14:00 – 14:30 iMapD: Intrinsic Map Dynamics Exploration for Uncharted Effective Free Energy Surfaces, Roberto Covino (Max Planck Institute of Biophysics, Germany)

14:30 – 15:00 Exploiting Task-Based Parallelism in Bayesian Uncertainty Quantification and Stochastic Optimization, Panagiotis Hadjidoukas (ETH Zurich, Switzerland)

MS02 **Capability Computing, Performance Portability, and Co-Design in the PASC Projects**
Sydney Room | Organizer(s): Joost VandeVondele (ETH Zurich / CSCS, Switzerland)

13:00 – 13:30 SPH-EXA: Optimizing Smooth Particle Hydrodynamics for Exascale Computing, Florina Ciorba, Ruben Cabezon (University of Basel, Switzerland)

13:30 – 14:00 Portability and Scalability of the COSMO Weather and Climate Model on Heterogeneous Architectures, Carlos E. Osuna (MeteoSwiss, Switzerland)

14:00 – 14:30 Implementing a Sparse Tensor Linear Algebra Library for Electronic Structure Calculations, Juerg Hutter (University of Zurich, Switzerland)

14:30 – 15:00 AV-FLOW: A High-Performance Library for Fluid-Structure Interaction with Complex Materials and Transitional Flow, Dominik Obrist (University of Bern, Switzerland)

MS03 **Computational Aspects of Heterogeneous Agents Macro**
Nairobi Room | Organizer(s): Felix Kubler (University of Zurich, Switzerland)

13:00 – 13:30 Exploiting MIT Shocks in Heterogeneous-Agent Economies: The Impulse Response as a Numerical Derivative, Kurt Mitman (Stockholm University, Sweden)

13:30 – 14:00 Solving Heterogeneous Agent Models with Nonconvex Optimization Problems: Linearization and Beyond, Michael Reiter (Institute for Advanced Studies, Austria)

14:00 – 14:30 Comparative Valuation Dynamics in Models with Financing Restrictions, Fabrice Tourre (Northwestern University, USA)

14:30 – 15:00 Self-Justified Equilibria: Existence and Computation, Felix Kubler (University of Zurich, Switzerland)

MS04 **Distributed Training of Deep Neural Net Models for High Energy Physics**
Osaka Room | Organizer(s): Jean-Roch Vlimant (California Institute of Technology, USA), Sofia Vallecorsa (CERN, Switzerland), Wahid Bhimji (Lawrence Berkeley National Laboratory, USA)

13:00 – 13:30 Large Scale Training for Model Optimization, Felice Pantaleo (CERN, Switzerland)

13:30 – 14:00 Training Generative Adversarial Models over Distributed Computing System, Gul Rukh Khattak (CERN, Switzerland)

14:00 – 14:30 Extreme Scale Deep Learning at NERSC, Thorsten Kurth (Lawrence Berkeley National Laboratory, USA)

14:30 – 15:00 Practical Scaling Techniques, Peter Messmer (NVIDIA Inc., Switzerland)

MS05 **Foundations and Applications of Performance Engineering**
Singapore Room | Organizer(s): Gerhard Wellein, Georg Hager (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany), Helmar Burkhart (University of Basel, Switzerland)

13:00 – 13:30 Performance Engineering - Why and How?, Georg Hager (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

13:30 – 14:00 Towards a Discipline of Performance Engineering: Lessons Learned from Stencil Kernel Benchmarks, Danilo Guerrera (University of Basel, Switzerland)

14:00 – 14:30 Holistic Performance Engineering for Sparse Iterative Solvers, Jonas Thies (German Aerospace Center, Germany)

14:30 – 15:00 Machine Learning Framework for Performance Coverage Analysis, Tanzima Z. Islam (Western Washington University, USA)

MS06 **Large Scale Electronic-Structure Calculations on Modern and Future High-Performance Supercomputers**
Boston 3 Room | Organizer(s): Stefan Goedecker (University of Basel, Switzerland), Andre Schleife (University of Illinois at Urbana-Champaign, USA), Matthieu Verstraete (Université de Liege, Belgium)

13:00 – 13:30 First-Principles Electron Transport with Phonon Coupling: Large Scale at Low Cost, Tue Gunst (Technical University of Denmark, Denmark)

13:30 – 14:00 Large-Scale First-Principles Electronic Structure Calculations in Petascale and Exascale Supercomputers: A Real-Space Density Functional Theory Code, Jun-Ichi Iwata (The University of Tokyo, Japan)

14:00 – 14:30 Potentialities of Wavelet Formalism towards a Reduction of the Complexity of Large Scale Electronic Structure Calculations, Luigi Genovese (CEA, France)

14:30 – 15:00 ABINIT on Pre-Exascale Supercomputers: Hybrid Parallelism and Numerical Stability, Marc Torrent (CEA, France)

MS07 **Machine Learning in Weather and Climate**
Rio Room | Organizer(s): Peter Dominik Dueben, Willem Deconinck (ECMWF, UK), Rupert Ford (Science and Technology Facilities Council, UK)

13:00 – 13:30 Deep Learning in Weather and Climate, Part 1: The Domain Perspective, Peter Dominik Dueben (ECMWF, UK)

13:30 – 14:00 Deep Learning in Weather and Climate, Part 2: The Computing Perspective, Christoph Angerer (NVIDIA Inc., Germany)

14:00 – 14:30 Integrating Machine Learning Algorithms and HPDA Frameworks to Run Predictive Analytics on Large-Scale Climate and Weather Datasets, Alessandro D'Anca (CMCC, Italy)

14:30 – 15:00 Using Self-Organising Maps to Understand Relationships between Clouds and Cloud Controlling Factors, Samantha V. Adams (Met Office, UK)

MS08 **On the Road to Exascale Computing: Turbulence Simulations of Complex Flows at the PetaFlops Pit Stop, Part I: Applications**
Darwin Room | Organizer(s): Ramesh Balakrishnan (Argonne National Laboratory, USA), Philipp Schlatter (KTH Royal Institute of Technology, Sweden)

13:00 – 13:30 Study of the Cyclic Flow Variability in an Internal Combustion Engine Using Spectral Elements, George Giannakopoulos (ETH Zurich, Switzerland)

13:30 – 14:00 Direct Numerical Simulation and Large Eddy Simulation of Canonical Flows for Wind Engineering Applications, Ramesh Balakrishnan (Argonne National Laboratory, USA)

14:00 – 14:30 Using a High Order Flow Solver for Generating DNS and LES Reference Databases for the Development of Turbulence Models, Ariane Frere (Cenaero, Belgium)

14:30 – 15:00	Wall Resolved and Wall Modeled Simulations of Separated Flow over Airfoils, Ramesh Balakrishnan (Argonne National Laboratory, USA)

MS Minisymposia Session II

MS09	**Adaptive Parallel Strategies for the Exploration of Challenging Search Spaces with Applications in Particle Simulations and Optimization, Part II**
Samarkand Room	Organizer(s): Andreas Vitalis, Marco Bacci, Amedeo Caflisch (University of Zurich, Switzerland)
15:30 – 16:00	Task-Based Parallelization of Replica Exchange Transition Interface Sampling in OpenPathSampling, David W. H. Swenson (University of Amsterdam, Netherlands)
16:00 – 16:30	Replica-Exchange Enveloping Distribution Sampling (RE-EDS) to Calculate Multiple Free-Energy Differences in a Single Simulation, Sereina Z. Riniker (ETH Zurich, Switzerland)
16:30 – 17:00	On the Interpretation of Non-Equilibrium MD Trajectories, Tanja Schilling (University of Freiburg, Germany)
17:00 – 17:30	Dynamic Histogram Analysis to Determine Free Energies and Rates from Biased Simulations, Lukas S. Stelzl (Max Planck Institute of Biophysics, Germany)

MS10	**Bridging the Software Productivity Gap for Climate and Weather Models**
Rio Room	Organizer(s): Xavier Lapillonne (MeteoSwiss, Switzerland), Valentin Clement (Center for Climate Systems Modeling, Switzerland)
15:30 – 16:00	Experience on Porting Atmosphere Kernels on Many-Core Processors and Accelerators, Lin Gan (Tsinghua University, China)
16:00 – 16:30	Performance Portability for Next Generation HPC Architectures in E3SM via the Kokkos Programming Model, Luca Bertagna (Sandia National Laboratories, USA)
16:30 – 17:00	Experience Applying the PSyclone Configurable Domain Specific Compiler to the Met Office LFRic Model, Rupert Ford (Science and Technology Facilities Council, UK)
17:00 – 17:30	Novel Programming Models for Large Geophysical Fluid Dynamics Models, Carlos E. Osuna (MeteoSwiss, Switzerland)

MS11	**Computing the Effect of Risk**
Montreal Room	Organizer(s): Michel Juillard (Banque de France, France)
15:30 – 16:00	Approximating Equilibria with Ex-Post Heterogeneity and Aggregate Risk, Elisabeth Proehl (University of Geneva, Switzerland)
16:00 – 16:30	The Extended Perturbation Method, Martin M. Andreasen (Aarhus University, Denmark)
16:30 – 17:00	Back in Time. Fast. Improved Time Iterations, Pablo Winant (Bank of England, UK)
17:00 – 17:30	Taking Risk into Account with Higher-Order Approximations, Michel Juillard (Banque de France, France)

MS12	**Engineering Scientific Software in times of Agile Development, Continuous Integration and Cloud Computing**
Sydney Room	Organizer(s): Guido Juckeland (Helmholtz-Zentrum Dresden-Rossendorf, Germany)
15:30 – 16:00	HPC-as-a-Service to Domain Scientists, Sunita Chandrasekaran (University of Delaware, USA)
16:00 – 16:30	The Reality of Scientific Software Development is Agile - Best Practices and Lessons Learned, Guido Juckeland (Helmholtz-Zentrum Dresden-Rossendorf, Germany)
16:30 – 17:00	Using Jetstream and High Performance Remote Research Desktops to Lower the Barrier of Entry for HPC Resources, Robert Henschel (Indiana University, USA)
17:00 – 17:30	Spack: A Package Manager for Scientific Software, Todd Gamblin (Lawrence Livermore National Laboratory, USA), Massimiliano Culpo (EPFL, Switzerland)

MS13	**Generative Models and Density Estimator for High Energy Physics**
Osaka Room	Organizer(s): Sofia Vallecorsa (CERN, Switzerland), Jean-Roch Vlimant (California Institute of Technology, USA), Michela Paganini (Yale University, USA)
15:30 – 16:00	The Success of Deep Generative Models, Jakub Tomczak (University of Amsterdam, Netherlands)
16:00 – 16:30	Generative Models for Application-Specific Fast Simulation of LHC Collision Events, Maurizio Pierini (CERN, Switzerland)
16:30 – 17:00	Using Generative Models for Fast Clusters Simulations in the TPC Detector for the ALICE Experiment, Kamil Deja (Warsaw University of Technology, Poland)
17:00 – 17:30	Generative Models for Simulating Highly Granular Calorimeters, Tobias Golling (University of Geneva, Switzerland)

MS14	**How Fintech and Big Data Change and Challenge the Insurance Sector**
Nairobi Room	Organizer(s): Jean-Michel Benkert, Michelle Allgöwer (Baloise Group, Switzerland)
15:30 – 16:00	Open Innovation at Baloise, Jean-Michel Benkert (Baloise Group, Switzerland)
16:00 – 16:30	Artificial Intelligence for Automated Investment Management, Gunter Fischer (Brainalyzed, Germany)
16:30 – 17:00	The Challenges of Big Data for a Traditional Insurance Company, Christoph Geering (Baloise Group, Switzerland)
17:00 – 17:30	Panel Discussion on How Fintech and Big Data Change and Challenge the Insurance Sector, Jean-Michel Benkert (Baloise Group, Switzerland)

MS15	**Machine Learning and Quantum Chemistry**
Boston 3 Room	Organizer(s): Roland Lindh (Uppsala University, Sweden)
15:30 – 16:00	Quantum Machine Learning in Chemical Compound Space, Anders S. Christensen (University of Basel, Switzerland)
16:00 – 16:30	Neural Networks Learning Quantum Chemistry, Olexandr Isayev (University of North Carolina, USA)
16:30 – 17:00	Neural Network Representations of Non-Equilibrium Potential Energy Surfaces Sampled in Virtual Reality, David Glowacki (University of Bristol, UK)
17:00 – 17:30	Predicting the Stability of Solids with Density Functional Theory and Machine Learning, Miguel A. L. Marques (Martin Luther University Halle-Wittenberg, Germany)

MS16	**NP-Hard Computations: Massively Parallelizing Mixed-Integer Linear Programs**
Singapore Room	Organizer(s): Sharlee Climer (University of Missouri - St. Louis, USA), Daniel Jacobson (Oak Ridge National Laboratory, USA)
15:30 – 16:00	ug[SCIP-Jack, MPI]: A Massively Parallel Steiner Tree Solver, Daniel Rehfeldt (Zuse Institute Berlin, Germany)
16:00 – 16:30	Parallel Cut-and-Solve: A Method for Solving Mixed-Integer Programs Utilizing Distributed Computational Power, Michael Chan (University of Missouri - St. Louis, USA)
16:30 – 17:00	Looking Back to Look Forward in Solving Mixed-Integer Linear Programs, Sarah Powers (Oak Ridge National Laboratory, USA)
17:00 – 17:30	Round Table Discussion: Embracing the Complexity Presented by Combinatorial Problems, Sharlee Climer (University of Missouri - St. Louis, USA)

MS17	**On the Road to Exascale Computing: Turbulence Simulations of Complex Flows at the Petaflops Pit Stop, Part II: Methods**
Darwin Room	Organizer(s): Philipp Schlatter (KTH Royal Institute of Technology, Sweden), Ramesh Balakrishnan (Argonne National Laboratory, USA)
15:30 – 16:00	Adaptive Mesh Refinement Based on Adjoint Error Estimators for Nek5000, Philipp Schlatter (KTH Royal Institute of Technology, Sweden)
16:00 – 16:30	A Minimally Intrusive Low-Memory Approach to Resilience and Multi-Level Check-Pointing for Existing Transient Solvers, Chris D. Cantwell (Imperial College London, UK)
16:30 – 17:00	Efficient Gather-Scatter Operations in Nek5000 Using PGAS, Niclas Jansson (KTH Royal Institute of Technology, Sweden)
17:00 – 17:30	Developing Methods for Exascale CFD Simulations at High Orders, David Moxey (University of Exeter, UK)

Tuesday 03.07

HPE Sponsored Keynote

Prediction: Use Science or History?
08:00 – 08:45 Eng Lim Goh (Hewlett Packard Enterprise, USA)
Montreal Room Chair: Florina Ciorba (University of Basel, Switzerland)

PNL Panel Discussion

PNL01 **Panel Discussion on Big Data vs. Fast Computation — Is HPC Facing a Game Change?**
09:00 – 10:15
Montreal Room Panelists: Eng Lim Goh (Hewlett Packard Enterprise, USA), Nuria Lopez (ICIQ, Spain) Matthias Scheffler (Fritz Haber Institute, Germany), Torsten Schwede (University of Basel, Switzerland)
Moderators: Florina Ciorba (University of Basel, Switzerland) Erik Lindahl (Stockholm University, Sweden)

Poster Sessions

10:15 – 11:00 **Flash Poster Session**
Montreal Room Chair: Maria Grazia Giuffreda (ETH Zurich / CSCS, Switzerland)

19:30 – 21:30 **Poster Session & Reception**
Foyer 2nd Floor

IP Invited Plenary Presentation

IP02 **Public Lecture on Massive-Scale Analytics Applied to Real-World Problems**
18:30 – 19:30
Montreal Room David Bader (Georgia Institute of Technology, USA)
Chair: Bastien Chopard (University of Geneva, Switzerland)

AP ACM PASC18 Papers

AP02 **ACM PASC18 Papers Session II**
Montreal Room Chair: Jack Wells (Oak Ridge National Laboratory, USA)

11:30 – 12:00 A Parallel Solver for Graph Laplacians, Tristan Konolige (University of Colorado Boulder, USA)

12:00 – 12:30 Abstractions and Directives for Adapting Wavefront Algorithms to Future Architectures, Robert Searles (University of Delaware, USA)

AP03 **ACM PASC18 Papers Session III**
Singapore Room Chair: Michael A. Heroux (Sandia National Laboratories, USA)

11:30 – 12:00 Distributed, Shared-Memory Parallel Triangle Counting, Andrew Lumsdaine (Pacific Northwest National Laboratory, USA)

12:00 – 12:30 MRG8 – Random Number Generation for the Exascale Era, Yusuke Nagasaka (Tokyo Institute of Technology, Japan)

AP04 **ACM PASC18 Papers Session IV**
Sydney Room Chair: Olaf Schenk (Università della Svizzera italiana, Switzerland)

11:30 – 12:00 A Massively Parallel Algorithm for the Approximate Calculation of Inverse p-th Roots of Large Sparse Matrices, Michael Lass (Paderborn University, Germany)

12:00 – 12:30 Balanced Graph Partition Refinement Using the Graph p-Laplacian, Dimosthenis Pasadakis (Università della Svizzera italiana, Switzerland)

MS Minisymposia Session III

MS18 **Addressing Resilience Challenges for Computing at Extreme Scale**
Montreal Room Organizer(s): Aurelien Cavelan, Florina Ciorba (University of Basel, Switzerland)

13:30 – 14:00 Characterizing Faults, Errors and Failures in Extreme-Scale Computing Systems, Christian Engelmann (Oak Ridge National Laboratory, USA)

14:00 – 14:30 Easy and Efficient Multilevel Checkpointing for Extreme Scale Systems, Leonardo Bautista (Barcelona Supercomputing Center, Spain)

14:30 – 15:00 Recent Results and Open Problems for Resilience at Scale, Yves Robert (École normale supérieure de Lyon, France)

15:00 – 15:30 Panel Discussion on Upcoming Challenges at Exascale, Aurelien Cavelan (University of Basel, Switzerland)

MS19 **Advances in Computational Geosciences, Part I**
Darwin Room Organizer(s): Ebru Bozdag (Colorado School of Mines, USA), Dimitri Komatitsch (CNRS, France)

13:30 – 14:00 High-Resolution 3D Viscoelastic Full Waveform Imaging of a Real Seismic Dataset: The Volve Oil Field Studied up to 12 Hz, Dimitri Komatitsch (CNRS, France)

14:00 – 14:30 Elastic Full Waveform Inversion with Active Seismic Data, Rene-Edouard Plessix (Royal Dutch Shell, Netherlands)

14:30 – 15:00 Accelerating Low-Order Unstructured Finite Element Earthquake Simulation by Time-Parallel Computation on Recent HPC Architectures, Kohei Fujita (University of Tokyo, Japan)

15:00 – 15:30 Computational Models of Magnetic Field Generation in the Earth, Andy Jackson (ETH Zurich, Switzerland)

MS20 **Challenges in Porting and Maintaining Atmospheric Codes on Emerging Hardware Architectures**
Rio Room Organizer(s): Richard Loft (National Center for Atmospheric Research, USA), Oliver Fuhrer (MeteoSwiss, Switzerland)

13:30 – 14:00 Porting and Maintaining a GPU-Enabled and Performance-Portable Version of the Model for Prediction Across Scales (MPAS), Richard Loft (National Center for Atmospheric Research, USA)

14:00 – 14:30 Experiences of Porting and Maintaining the ICON Model on Accelerators, William Sawyer (ETH Zurich / CSCS, Switzerland)

14:30 – 15:00 NOAA Model Development Activities Targeting Exascale, Mark Govett (NOAA, USA)

15:00 – 15:30 Experience and Challenges with Maintaining a GPU-Capable Version of COSMO in a Production Environment at MeteoSwiss and ETH, Xavier Lapillonne (MeteoSwiss, Switzerland)

MS21 **Computational Solutions to Large-Scale Data Management and Analysis Challenges in Personalized Health**
Samarkand Room Organizer(s): Leila Tamara Alexander, Torsten Schwede (Swiss Institute of Bioinformatics, Switzerland)

13:30 – 14:00 Semantic Interoperability Challenges for Sharing and Reusing Large Amounts of Heterogeneous Data, Marie-Christine Jaulent (INSERM, France)

14:00 – 14:30 Challenges of Volume Rendering in a Virtual Reality Environment, Philippe Cattin (University of Basel, Switzerland)

14:30 – 15:00 HPC-Supported Therapy Development in Oncology, Olivier Michielin (University of Lausanne, Switzerland)

15:00 – 15:30 Achieving Workflow Interoperability for Personalized Health Research in Switzerland, Thierry Sengstag (Swiss Institute of Bioinformatics, Switzerland)

MS22 **Fostering Software Engineering Best Practice within Research Teams**
Singapore Room Organizer(s): Mark Abraham (KTH Royal Institute of Technology, Sweden), Anshu Dubey (Argonne National Laboratory, USA)

13:30 – 14:00 The Evolution of Software Practice in GROMACS: To Suit Both the Laptop and the Exascale, Mark Abraham (KTH Royal Institute of Technology, Sweden)

14:00 – 14:30 Software Process for FLASH, a Code Serving Multiple Scientific Communities, Anshu Dubey (Argonne National Laboratory, USA)

14:30 – 15:00 Challenges in Evolving Software for Cryo-Electron Microscopy: From CPUs to GPUs and Back Again, Erik Lindahl (Stockholm University, Sweden)

15:00 – 15:30 More than Top-Down or Bottom-Up: Fostering Software Engineering Best Practice in Diverse Groups, Neil Chue Hong (University of Edinburgh, UK)

MS23 **High Performance Graph Algorithms**
Sydney Room Organizer(s): Olaf Schenk (Università della Svizzera italiana, Switzerland), Gerhard Wellein, Georg Hager (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

13:30 – 14:00 Tracking Communities in Streaming Graphs, David Bader (Georgia Institute of Technology, USA)

14:00 – 14:30 Parallel Mesh Partitioning with Balanced K-Means, Moritz von Looz (University of Cologne, Germany)

14:30 – 15:00 Improvement of Graph Partitions Using the Graph p-Laplacian, Drosos Kourounis (Università della Svizzera italiana, Switzerland)

15:00 – 15:30 RACE: Recursive Algebraic Coloring Engine, Christie Louis Alappat (Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)

MS24	**Plasma I: Exciting Opportunities for Plasma Simulation in the Pre-Exascale Era**
Osaka Room	Organizer(s): Frank Jenko (Max Planck Institute for Plasma Physics, Germany)
13:30 – 14:00	Design and Development of Particle-in-Cell Methods for Emerging Tensor Architectures, Stefano Markidis (KTH Royal Institute of Technology, Sweden)
14:00 – 14:30	Vlasiator – Understanding Near-Earth Space in Six Dimensions, Minna Palmroth (University of Helsinki, Finland)
14:30 – 15:00	Variable Precision: Making Every Bit Count, Jeffrey A. F. Hittinger (Lawrence Livermore National Laboratory, USA)
15:00 – 15:30	Towards a Virtual Fusion Facility on Exascale Supercomputers, Frank Jenko (Max Planck Institute for Plasma Physics, Germany)

MS25	**Scientific Computing in times of MPI+X: Looking at Multiple "X" with regard to Performance and Portability**
Nairobi Room	Organizer(s): Sunita Chandrasekaran (University of Delaware, USA)
13:30 – 14:00	Porting Physical Parameterizations from a Climate Model to Accelerators Thomas Köster (Università della Svizzera italiana, Switzerland), William Sawyer (ETH Zurich / CSCS, Switzerland)
14:00 – 14:30	Zero Overhead Modern C++ for Mapping to Any Programming Model, Axel Huebl (Helmholtz-Zentrum Dresden-Rossendorf, Germany)
14:30 – 15:00	Porting Quantum ESPRESSO to GPUs - Lessons Learnt and Remaining Challenges, Pietro Bonfà (CINECA, Italy)
15:00 – 15:30	OpenMP 4.5 Acceleration for Turbulence Simulations on GPUs, Dhawal Buaria (Max Planck Institute for Dynamics and Self Organization, Germany)

MS26	**Tensor Algebra Computation: Implementations and Applications**
Boston 3 Room	Organizer(s): Alfio Lazzaro, Juerg Hutter (University of Zurich, Switzerland), Edgar Solomonik (University of Illinois Urbana-Champaign, USA)
13:30 – 14:00	Parallel Tensor Computations in Python or C++ Using Cyclops, Edgar Solomonik (University of Illinois Urbana-Champaign, USA)
14:00 – 14:30	Tensor Transposition and Contraction on GPUs, Ponnuswamy Sadayappan (Ohio State University, USA)
14:30 – 15:00	Extending the DBCSR Library to Sparse Tensor Linear Algebra for Electronic Structure Methods beyond Density Functional Theory, Alfio Lazzaro (University of Zurich, Switzerland)
15:00 – 15:30	The Tensor Algebra Compiler, Saman Amarasinghe (Massachusetts Institute of Technology, USA)

MS Minisymposia Session IV

MS27	**Actionable Health Intelligence: From Precision Medicine to Population Health**
Sydney Room	Organizer(s): Georgia Tourassi (Oak Ridge National Laboratory, USA)
16:00 – 16:30	Radiogenomics in the Era of Precision Medicine, Constantinos Pattichis (University of Cyprus, Cyprus)
16:30 – 17:00	Deep Multi-Omics to Predict Clinical Cancer Phenotypes, Georgia Tourassi (Oak Ridge National Laboratory, USA)
17:00 – 17:30	Explainable-AI: From Human Systems Biology to the 3D Interactome and Precision Medicine, Daniel Jacobson (Oak Ridge National Laboratory, USA)
17:30 – 18:00	Drug Response Prediction in Cancer Cell Lines and Patient-Derived Xenografts, Fangfang Xia (Argonne National Laboratory, USA)

MS28	**Advances in Automation and Efficiency for the Exascale Era – Experiences from the Biomolecular Sciences**
Samarkand Room	Organizer(s): Rossen Apostolov (KTH Royal Institute of Technology, Sweden)
16:00 – 16:30	Building Blocks for Adaptive Workflows, Shantenu Jha (Rutgers University, USA)
16:30 – 17:00	Facing Compute Platform Portability Challenges with Scientific Workflows - Experiences from Common Workflow Language, Stian Soiland-Reyes (University of Manchester, UK)
17:00 – 17:30	Workflow Automation and Efficiency for Macromolecular Simulations and Screening, Adam Hospital Gasch (Institute for Research in Biomedicine, Spain)
17:30 – 18:00	Round-Table Discussion: Simulations at Exascale - Myth or Reality?, Rossen Apostolov (KTH Royal Institute of Technology, Sweden)

MS29	**Advances in Computational Geosciences, Part II**
Darwin Room	Organizer(s): Ebru Bozdag (Colorado School of Mines, USA), Dimitri Komatitsch (CNRS, France)
16:00 – 16:30	Simulating the Solid Earth and Planets over Billions of Years: From Magma Oceans to Plate Tectonics to Exoplanets, Paul J. Tackley (ETH Zurich, Switzerland)
16:30 – 17:00	Dynamic Viability of Earthquake Rupture Cascades on Complex Fault Systems, Alice-Agnes Gabriel (Ludwig Maximilian University of Munich, Germany)
17:00 – 17:30	Imaging of the Italian Lithosphere Based on Adjoint Tomography, Emanuele Casarotti (INGV, Italy)
17:30 – 18:00	Full-Waveform Inversion of the Solid Earth from Crust to Core, Ebru Bozdag (Colorado School of Mines, USA)

MS30	**Efficient Parallel Methods in High-Dimensional Approximation and Beyond**
Nairobi Room	Organizer(s): Helmut Harbrecht, Peter Zaspel (University of Basel, Switzerland)
16:00 – 16:30	Portable Distributed Sparse Grid Density Estimation for Big Data Clustering, David Pfander (University of Stuttgart, Germany)
16:30 – 17:00	Scalable Solvers for Meshless Methods on Many-Core Clusters, Peter Zaspel (University of Basel, Switzerland)
17:00 – 17:30	Inducing Input and Hyperparameter Optimization for Large Scale Sparse Gaussian Process Regression, Jannik Schürg (University of Bonn, Germany)
17:30 – 18:00	A Highly Scalable, Fault-Tolerant Implementation of the Sparse Grid Combination Technique, Michael Obersteiner (TU Munich, Germany)

MS31	**How Can We Escape the Data Avalanche in Climate Science?**
Rio Room	Organizer(s): Joachim Biercamp (German Climate Computing Centre, Germany), Oliver Fuhrer (MeteoSwiss, Switzerland), Christoph Schär (ETH Zurich, Switzerland)
16:00 – 16:30	Beating the Data Bottleneck - Write Less and Use Tiered Storage with Smart Middleware!, Bryan Lawrence (NCAS-CMS, UK)
16:30 – 17:00	Lossy Data Compression for Climate Simulation Data: Reducing Data Volume while Preserving Information, Allison H. Baker (National Center for Atmospheric Research, USA)
17:00 – 17:30	In-Situ to the Rescue?, Jan Frederik Engels (German Climate Computing Centre, Germany)
17:30 – 18:00	SimFS: A Simulation Data Virtualizing File System Interface, Salvatore Di Girolamo (ETH Zurich, Switzerland)

MS32	**Increasing Credibility of Simulation and Analytic Software for Science**
Singapore Room	Organizer(s): Anshu Dubey (Argonne National Laboratory, USA), Michael A. Heroux (Sandia National Laboratories, USA), Mark Abraham (KTH Royal Institute of Technology, Sweden)
16:00 – 16:30	Software Engineering for Simulation Neuroscience, Felix Schuermann (EPFL, Switzerland)
16:30 – 17:00	Reproducibility in Scientific Software, Michael A. Heroux (Sandia National Laboratories, USA)
17:00 – 17:30	Outreach for Better Scientific Software, David E. Bernholdt (Oak Ridge National Laboratory, USA)
17:30 – 18:00	General Discussion and Community Input, Anshu Dubey (Argonne National Laboratory, USA)

MS33	**Machine Learning Schemes with High Extrapolation Accuracy for Materials Discovery**
Boston 3 Room	Organizer(s): Stefan Goedecker (University of Basel, Switzerland)
16:00 – 16:30	Structure and Dynamics of Au Nanoclusters Using ANN Based Interatomic Potentials, Satya Bulusu (IIT Indore, India)
16:30 – 17:00	On Creating Databases for Machine Learned Interatomic Potentials, Gabor Csanyi (University of Cambridge, UK)
17:00 – 17:30	Materials Modeling Using Neural Networks, Matti Hellström (University of Göttingen, Germany)
17:30 – 18:00	Using Machine Learning Interatomic Potentials for Crystal Structure Prediction, Seyed-Alireza Ghasemi (Institute for Advanced Studies in Basic Sciences, Iran)

MS34	**Plasma II: Frontiers in Gyrokinetic Turbulence Simulation on New and Emerging HPC Platforms**
Osaka Room	Organizer(s): Stephan Brunner, Laurent Villard (EPFL, Switzerland)
16:00 – 16:30	How to Prepare the Gyrokinetic Code GYSELA for Future Exascale Machines, Virginie Grandgirard (CEA, France)
16:30 – 17:00	Advances and Optimizations of Gyrokinetic Turbulence Code GKV towards Exascale Computing, Masanori Nunami (National Institute for Fusion Science, Japan)
17:00 – 17:30	CPU and GPU Parallelization of Spectral Particle Methods, Jakob Ameres (TU Munich, Germany)
17:30 – 18:00	Porting a Legacy Global Lagrangian PIC Code on Many-Core and GPU-Accelerated Architectures, Noé Ohana (EPFL, Switzerland)

Wednesday 04.07

IP Invited Plenary Presentations

IP03 **From Weather Dwarfs to Kilometre-Scale Earth System Simulations**
10:00 – 10:50 | Montreal Room
Nils P. Wedi (ECMWF, UK)
Chair: Willem Deconinck (ECMWF, UK)

IP04 **Challenges in the First Principles Modelling of Magneto Hydro Dynamic Instabilities and their Control in Magnetic Fusion Devices**
16:40 – 17:30 | Montreal Room
Marina Becoulet (CEA, France)
Chair: Sinéad Ryan (Trinity College Dublin, Ireland)

MS Minisymposia Session V

MS35 **Gravitational-Wave Data Analysis with the Current Generation of Advanced Detectors**
Osaka Room
Organizer(s): Maria Haney, Philippe Jetzer (University of Zurich, Switzerland)

11:15 – 11:45 The LIGO/Virgo Search for Gravitational Waves, Alexander Nitz (Max Planck Institute for Gravitational Physics, Germany)

11:45 – 12:15 Methods and Challenges in the Characterization of Gravitational-Wave Sources, Salvatore Vitale (Massachusetts Institute of Technology, USA)

12:15 – 12:45 Numerical Relativity and its Applications for the Modelling of Gravitational Waves, Sascha Husa (University of the Balearic Islands, Spain)

12:45 – 13:15 Data Quality for Gravitational-Wave Detectors, Andrew P. Lundgren (University of Portsmouth, UK)

MS36 **HPC for HEP: Enabling Big Data from Large Instruments on Leadership Class HPC Infrastructures**
Sydney Room
Organizer(s): Frank Wuerthwein (UC San Diego, USA), Kaushik De (The University of Texas at Arlington, USA)

11:15 – 11:45 Running ATLAS Simulations on HPCs, Kaushik De (University of Texas at Arlington, USA)

11:45 – 12:15 Big Data on HPC via HEPCloud, Dirk Hufnagel (Fermilab, USA)

12:15 – 12:45 Perspective - Lessons from Titan, Looking to the Future, Jack Wells (Oak Ridge National Laboratory, USA)

12:45 – 13:15 HPC Systems and the Integration Challenges of Large Instruments, Frank Wuerthwein (UC San Diego, USA)

MS37 **HPUQ: Current Challenges in Uncertainty Quantification for Mechanistic Models, Part II: Theory, Methods and Tools**
Singapore Room
Organizer(s): Ritabrata Dutta (Università della Svizzera italiana, Switzerland), Nikos Karathanasopoulos (ETH Zurich, Switzerland), Bastien Chopard (University of Geneva, Switzerland)

11:15 – 11:45 ABCpy: Benchmarking ABC Algorithms from HPC Perspective, Ritabrata Dutta (Università della Svizzera italiana, Switzerland)

11:45 – 12:15 The Hierarchical Bayesian Framework Applied to Molecular Dynamics, Georgios Arampatzis (ETH Zurich, Switzerland)

12:15 – 12:45 PyMLMC + SPUX: Uncertainty Quantification Using Multi-Level and Particle Filtering Techniques, Jonas Sukys (Swiss Federal Institute of Aquatic Science and Technology, Switzerland)

12:45 – 13:15 Low-Rank Tensor Approximations for Sensitivity Analysis of Complex Models with High-Dimensional Input, Katerina Konakli (COWI, Denmark)

MS38 **Mass and Energy Transport Phenomena in Solid State**
Boston 3 Room
Organizer(s): Ivano Tavernelli, Matthieu Mottet (IBM Research, Switzerland)

11:15 – 11:45 The Materials Genome in Action, Seyed Mohamad Moosavi (EPFL, Switzerland)

11:45 – 12:15 High-Throughput Screening for New Solid-State Electrolyte Candidates, Leonid Kahle (EPFL, Switzerland)

12:15 – 12:45 Doping Solid-State Electrolytes: Classical Modelling and Insights, Matthieu Mottet (IBM Research, Switzerland)

12:45 – 13:15 Accurate Thermal Conductivities from Optimally Short Molecular Dynamics Simulations, Loris Ercole (SISSA, Italy)

MS39 **Scalable Solvers for Forward and Inverse Problems in Geophysics**
Darwin Room
Organizer(s): Christian Boehm, Václav Hapla (ETH Zurich, Switzerland)

11:15 – 11:45 Extreme Scale Seismic Wave Propagation Simulation for Mars, Vaclav Hapla (ETH Zurich, Switzerland)

11:45 – 12:15 Seismic Wave Propagation on Complex Topographies Applied in the Alpine Area Using the ExaHyPE Hyperbolic PDE Engine, Leonhard Rannabauer (TU Munich, Germany)

12:15 – 12:45 StagBL: A Scalable, Portable, High-Performance Discretization and Solver Layer for Geodynamic Simulations, Patrick Sanan (ETH Zurich, Switzerland)

12:45 – 13:15 HPC Solution Methods for Simulation of Hydro-Mechanical Processes in Geo-Environment, Radim Blaheta (Institute of Geonics CAS, Czech Republic)

MS40 **Towards Weather and Climate Simulations at 1-km Resolution**
Rio Room
Organizer(s): Peter Dominik Dueben (ECMWF, UK), Carlos E. Osuna (MeteoSwiss, Switzerland)

11:15 – 11:45 At the Edge of Resolution: Earth System Modelling at ECMWF, Nils P. Wedi (ECMWF, UK)

11:45 – 12:15 Using Global Cloud-Resolving Models for Weather Predictions and for Studies of Clouds in the Climate System, Shian-Jiann Lin (NOAA, USA)

12:15 – 12:45 Near-Global RCM Simulations to Establish a Baseline for Global 1 km GCM Simulations, Oliver Fuhrer (MeteoSwiss, Switzerland)

12:45 – 13:15 ESCAPE: Energy-Efficient Scalable Algorithms for Weather Prediction on Exascale Supercomputers, Andreas Mueller (ECMWF, UK)

MS41 **Use of AI to Analyze Complex Biological Systems**
Samarkand Room
Organizer(s): Daniel Jacobson (Oak Ridge National Laboratory, USA), Ben Brown (Lawrence Berkeley National Laboratory, USA), Georgios Gkoutos (University of Birmingham, UK)

11:15 – 11:45 Explainable AI and the Discovery of Complex Genetic Architectures: Plants, Insects and Humans: Systems Biology and the 3D Interactome, Daniel Jacobson (Oak Ridge National Laboratory, USA)

11:45 – 12:15 Scalable Deep Learning for Extracting Cancer Phenotypes from Unstructured Clinical Text, Georgia Tourassi (Oak Ridge National Laboratory, USA)

12:15 – 12:45 DeepPVP: Phenotype-Based Prioritization of Causative Variants Using Deep Learning, Georgios Gkoutos (University of Birmingham, UK)

12:45 – 13:15 Interpretable Density Estimation in Genomics Data, Ben Brown (Lawrence Berkeley National Laboratory, USA)

MS Minisymposia Session VI

MS42 **Coupling Strategies Towards Exascale for Complex Earth System Modelling**
Rio Room
Organizer(s): Willem Deconinck (ECMWF, UK), Katherine Evans (Oak Ridge National Laboratory, USA)

14:15 – 14:45 Flexible Earth System Modelling on Multiple Grids, Willem Deconinck (ECMWF, UK)

14:45 – 15:15 Comodels: A New Approach for Coupling Models for the [Tera,Exa] Scale, George Mozdzynski (ECMWF, UK)

15:15 – 15:45 Modeling Systems at the End of Dennard Scaling, Venkatramani Balaji (Princeton University, USA)

15:45 – 16:15 Making the Expensive Affordable: Running a Chemistry Model in the UKESM Climate Model, Richard Hill (Met Office, UK)

MS43 **Distributed Asynchronous Parallel Computing: Progress and Challenges for Multi-Physics Applications on Heterogeneous Architectures**
Darwin Room
Organizer(s): Hemanth Kolla (Sandia National Laboratories, USA), Jacqueline Chen (Sandia National Laboratories, USA)

14:15 – 14:45 Towards Exascale Simulations of Particle-Laden Turbulence in a Radiation Environment: The PSAAP Program at Stanford, Hilario Torres (Stanford University, USA)

14:45 – 15:15 A Scalable Asynchronous Computing Approach for Solving PDEs at Extreme Scale, Aditya Konduri (Sandia National Laboratories, USA)

15:15 – 15:45 Fault Tolerance in Asynchronous Many-Task (AMT) Programming Models and Runtimes, Hemanth Kolla (Sandia National Laboratories, USA)

15:45 – 16:15	Tools and Techniques to Enable Multiphysics Applications on Heterogeneous Architectures, James C. Sutherland (University of Utah, USA)

MS44	**Emerging Trends in Statistical Mechanics Applications to Nanostructured Materials**
Boston 3 Room	Organizer(s): Irina Paci, Jeffrey Paci (University of Victoria, Canada)
14:15 – 14:45	Bridging the Electronic, Atomistic and Mesoscopic Scales Using Machine Learned Models, Subramanian Sankaranarayanan (Argonne National Laboratory, USA)
14:45 – 15:15	Metal and Metal-Oxide Clusters at Realistic Conditions: Beyond the Static, Monostructure Description, Luca M. Ghiringhelli (Fritz Haber Institute, Germany)
15:15 – 15:45	From Computational Spectroscopy to Artificial Water Splitting, Sandra Luber (University of Zurich, Switzerland)
15:45 – 16:15	(i) Massively-Parallel Simulation of Self-Assembled Diblock-Copolymer Nano-Materials; (ii) Ab-Initio Quantum Monte Carlo Simulations for Single Vacancy Graphene and Isotropically-Strained Graphene, Ludwig Schneider (University of Göttingen, Germany), Tomonori Shirakawa (SISSA, Italy)

MS45	**Evolution of Knowledge Management in Astrophysics**
Osaka Room	Organizer(s): Roland Walter (University of Geneva, Switzerland), Claudio Gheller (ETH Zurich / CSCS, Switzerland)
14:15 – 14:45	(i) Introduction; (ii) Gravitational-Wave Detector Data and Analysis Session Summary, Roland Walter (University of Geneva, Switzerland), Maria Haney (University of Zurich, Switzerland)
14:45 – 15:15	(i) Challenges in the Gaia Mission of the European Space Agency (ESA); (ii) Data Management at ESO and ALMA, Laurent Eyer (University of Geneva, Switzerland), Felix Stoehr (ESO/ALMA, Germany)
15:15 – 15:45	(i) Data Management for the Cherenkov; (ii) Neutrino Telescope Data Management and Analysis, Etienne Lyard, Teresa Montaruli (University of Geneva, Switzerland)
15:45 – 16:15	Discussion Forum, Roland Walter (University of Geneva, Switzerland)

MS46	**HPC beyond HEP: Opening Doors for New Data Intensive Sciences at Leadership Class HPCs Using BigPanDA**
Sydney Room	Organizer(s): Kaushik De (The University of Texas at Arlington, USA), Alexei Klimentov, Torre Wenaus (Brookhaven National Laboratory, USA)
14:15 – 14:45	Enabling Biology, Chemistry and Other Sciences on Titan through BigPanDA, Danila Oleynik (The University of Texas at Arlington, USA)
14:45 – 15:15	BigPanDA Experience on Titan for the ATLAS Experiment at the LHC, Alexei Klimentov (Brookhaven National Laboratory, USA)
15:15 – 15:45	BigPanDA: Blue Brain and Beyond, Shantenu Jha (Rutgers University, USA), Fabien Delalondre (EPFL, Switzerland)
15:45 – 16:15	Panel: BigPanDA Experience at Oak Ridge - Learning from the LHC, Going Far Beyond, Torre Wenaus (Brookhaven National Laboratory, USA)

MS47	**HPUQ: Current Challenges in Uncertainty Quantification for Mechanistic Models, Part II: Applications in Life Sciences and Engineering**
Singapore Room	Organizer(s): Jonas Šukys (Swiss Federal Institute of Aquatic Science and Technology, Switzerland), Panagiotis Hadjidoukas (ETH Zurich, Switzerland), Antonietta Mira (Università della Svizzera italiana, Switzerland)
14:15 – 14:45	Combining Clinical Observations, Mathematical Modeling and HPC Approximate Bayesian Computation for Developing New Diagnosis Techniques, Bastien Chopard (University of Geneva, Switzerland)
14:45 – 15:15	Reverse Engineering of Tendons: The Data Conundrum and Current Computing Challenges, Nikolaos Karathanasopoulos (ETH Zurich, Switzerland)
15:15 – 15:45	Combined Error and Uncertainty Bound Estimates with Application to CFD Problems, Timothy Barth (NASA, USA)
15:45 – 16:15	Using One Thousand GPUs to Understand the Euler Equations, Kjetil Lye (ETH Zurich, Switzerland)

MS48	**Unconventional Methods for Partial Differential Equations**
Nairobi Room	Organizer(s): Wesley P. Petersen (ETH Zurich, Switzerland)
14:15 – 14:45	High-Order Well-Balanced Finite Volume Methods for Euler Equations with Gravity, Luc Grosheintz-Laval (ETH Zurich, Switzerland)
14:45 – 15:15	Splitting Methods for ODEs, PDEs, and SDEs - with Examples, Wesley P. Petersen (ETH Zurich, Switzerland)
15:15 – 15:45	Mutual Impact of Bubbles and Waves Studied with an Efficient Finite Volume Solver, Fabian Wermelinger (ETH Zurich, Switzerland)
15:45 – 16:15	Fight Uncertainty with Randomness: Stochastic Particle Methods for Microfluidics, Lucas Amoudruz (ETH Zurich, Switzerland)

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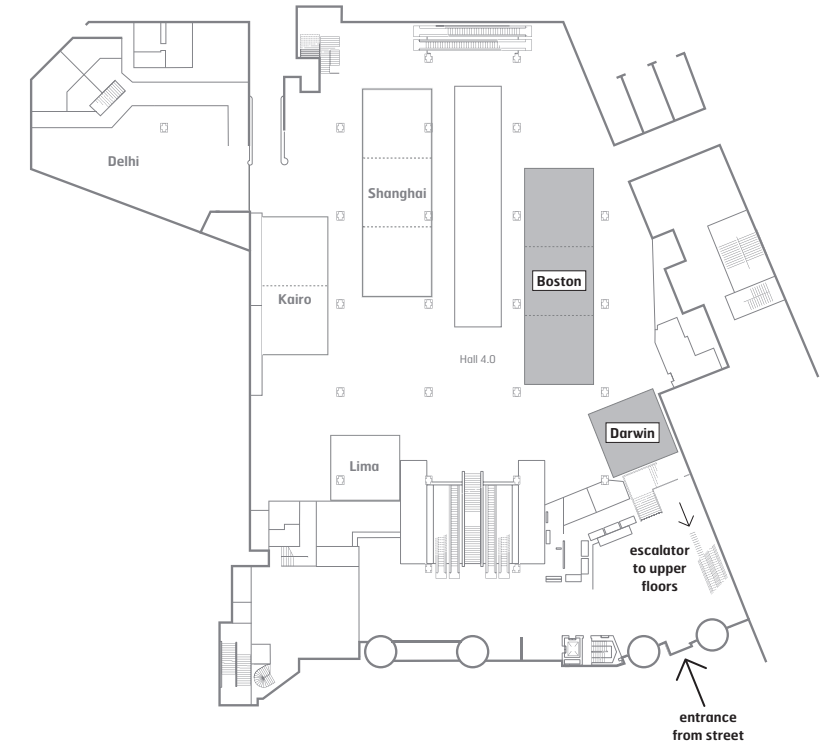
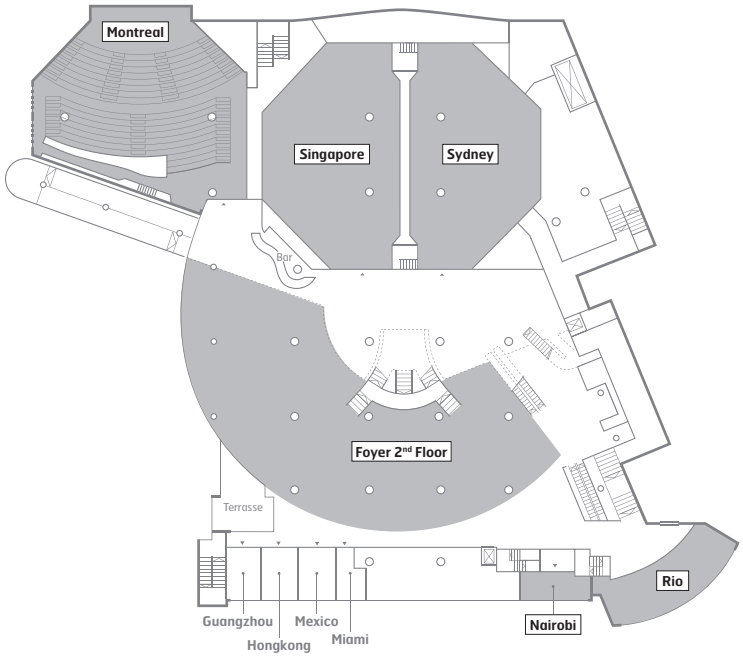


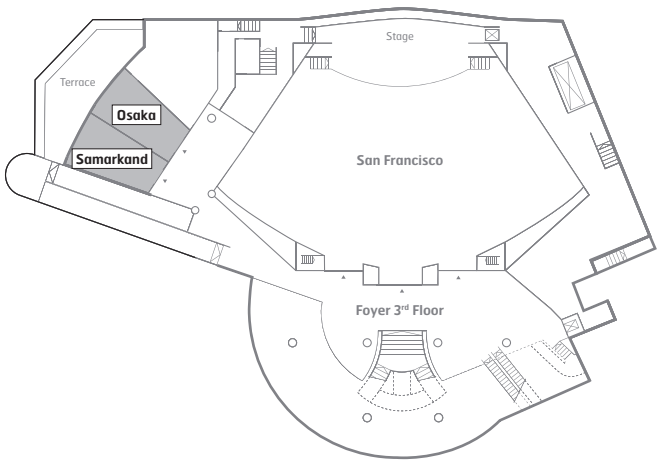
2nd Floor

Rooms
- **Foyer 2nd floor**
- **Singapore**
- **Sydney**
- **Montreal Auditorium**
- **Rio**
- **Nairobi**



3nd Floor

Rooms
- **Osaka**
- **Samarkand**



Monday 02.07

	09:00 – 10:00	Foyer 2nd Floor	**Registration**
	10:00 – 10:10	Montreal Room	**Welcome from the Local Hosts** Hans-Peter Wessels (City of Basel, Switzerland) Andrea Schenker-Wicki (University of Basel, Switzerland)
	10:10 – 10:20	Montreal Room	**Welcome from the Conference Co-Chairs** Florina Ciorba (University of Basel, Switzerland) Erik Lindahl (Stockholm University, Sweden)
IP01	10:20 – 11:10	Montreal Room	**Unraveling Earthquake Dynamics Through Extreme-Scale Multi-Physics Simulations** Alice-Agnes Gabriel (Ludwig Maximilian University of Munich, Germany)
AP01	11:10 – 12:10	Montreal Room	**ACM PASC18 Papers Session I**
	12:10 – 13:00	Foyer 2nd Floor	**Lunch**
MS	13:00 – 15:00	Samarkand Room, Sydney Room, Nairobi Room, Osaka Room, Singapore Room, Boston 3 Room, Rio Room, Darwin Room	**Minisymposia Session I**
	15:00 – 15:30	Foyer 2nd Floor	**Coffee Break**
MS	15:30 – 17:30	Samarkand Room, Rio Room, Montreal Room, Sydney Room, Osaka Room, Nairobi Room, Boston 3 Room, Singapore Room, Darwin Room	**Minisymposia Session II**
	17:30 – 18:00	Foyer 2nd Floor	**Coffee Break**
ID01	18:00 – 18:45	Montreal Room	**The Colourful Theory, and Visible and Invisible Matter in the Universe: An Interdisciplinary Dialogue between Constantia Alexandrou and Petros Koumoutsakos** Constantia Alexandrou (University of Cyprus, Cyprus) Petros Koumoutsakos (ETH Zurich, Switzerland)

Tuesday 03.07

	08:00 – 08:45	Montreal Room	**HPE Sponsored Keynote - Prediction: Use Science or History?** Eng Lim Goh (Hewlett Packard Enterprise, USA)
PNL01	09:00 – 10:15	Montreal Room	**Panel Discussion on Big Data vs. Fast Computation – Is HPC Facing a Game Change?** Panelists: Eng Lim Goh (Hewlett Packard Enterprise, US), Nuria Lopez (ICIQ, Spain), Matthias Scheffler (Fritz Haber Institute, Germany), Torsten Schwede (University of Basel, Switzerland)
	10:15 – 11:00	Montreal Room	**Flash Poster Session**
	11:00 – 11:30	Foyer 2nd Floor	**Coffee Break**
AP02 **AP03** **AP04**	11:30 – 12:30	Montreal Room, Singapore Room, Sydney Room,	**ACM PASC18 Papers Session II, III, IV**
	12:30 – 13:30	Foyer 2nd Floor	**Lunch**
MS	13:30 – 15:30	Montreal Room, Darwin Room, Rio Room, Samarkand Room, Singapore Room, Sydney Room, Osaka Room, Nairobi Room, Boston 3 Room	**Minisymposia Session III**
	15:30 – 16:00	Foyer 2nd Floor	**Coffee Break**
MS	16:00 – 18:00	Sydney Room, Samarkand Room, Darwin Room, Nairobi Room, Rio Room, Singapore Room, Boston 3 Room, Osaka Room	**Minisymposia Session IV**
	18:00 – 18:30		**Break**
IP02	18:30 – 19:30	Montreal Room	**Public Lecture on Massive-Scale Analytics Applied to Real-World Problems** David Bader (Georgia Institute of Technology, USA)
	19:30 – 21:30	Foyer 2nd Floor	**Poster Session & Reception**

Wednesday 04.07

	09:00 – 10:00	Montreal Room	**CSCS Update**
IP03	10:00 – 10:50	Montreal Room	**From Weather Dwarfs to Kilometre-Scale Earth System Simulations** Nils P. Wedi (ECMWF, UK)
	10:50 – 11:15	Foyer 2nd Floor	**Coffee Break**
MS	11:15 – 13:15	Osaka Room, Sydney Room, Singapore Room, Boston 3 Room, Darwin Room, Rio Room, Samarkand Room	**Minisymposia Session V**
	13:15 – 14:15	Foyer 2nd Floor	**Lunch**
MS	14:15 – 16:15	Rio Room, Darwin Room, Boston 3 Room, Osaka Room, Sydney Room, Singapore Room, Nairobi Room	**Minisymposia Session VI**
	16:15 – 16:40	Foyer 2nd Floor	**Coffee Break**
IP04	16:40 – 17:30	Montreal Room	**Challenges in the First Principles Modelling of Magneto Hydro Dynamic Instabilities and their Control in Magnetic Fusion Devices** Marina Becoulet (CEA, France)
	17:30 – 18:00	Montreal Room	**Closing Session**

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