EULER EQUATION

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

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

\[
\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_i} \left( \frac{(E+p) u_i} {\partial x_i} \right) = 0
\]

Label the three Cartesian components:

\((x_1, x_2, x_3) = (x, y, z)\) and

\((u_1, u_2, u_3) = (u, v, w)\)

POISSON'S EQUATION

\[\Delta g = f\]

\[\Delta = \text{LAPLACE OPERATOR}\]

\[f \neq g \text{ REAL OR COMPLEX-VALUED FUNCTIONS}\]

\[\nabla^2 g = f\]

In three-dimensional Cartesian coordinates:

\[
\left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) g(x,y,z) = f(x,y,z)
\]

When \(f = 0\) we retrieve LAPLACE'S EQUATION.

quicksort \((A_i, j, k)\):

\(i \leq k\)

\(g = \text{partition}(A_i, j, k)\)

quicksort \((A_i, p-1)\)

quicksort \((A_i, p+1, k)\)
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.

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Scientific Fields

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

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Contents

- **IP Invited Plenary Presentations**
  - Keynotes on earthquake dynamics, numerical weather prediction, and fusion plasma modelling, and a public lecture on massive-scale data analytics.

- **ID Interdisciplinary Dialogue**
  - A “colourful” discussion of quantum chromodynamics and modern-day scientific computing.

- **PNL Panel Discussion**
  - An interactive panel on Big Data and Fast Computation with perspectives from industry and academia.

- **AP ACM PASC18 Papers**
  - Eight original research papers presented in plenary or parallel sessions, and published in the ACM Digital Library.

- **MS Minisymposia**
  - Close to 200 presentations in 48 topically-focused minisymposia.

- **Poster Sessions**
  - Sixty posters presented at a flash session and evening reception.

- **CSCS Update**
  - Update from the home of Europe’s most powerful supercomputer.
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)
Erik Lindahl (Stockholm University, Sweden)
Sabine Roller (University of Siegen, Germany)
Jack Wells (Oak Ridge National Laboratory, USA)

Papers Program Chairs
Sabine Roller (University of Siegen, Germany)
Jack Wells (Oak Ridge National Laboratory, USA)

Proceedings Chair
Timothy Robinson (ETH Zurich / CSCS, Switzerland)

Chemistry & Materials
Domain Co-Chair: Edoardo Di Napoli (Forschungszentrum Jülich, Germany)
Domain Co-Chair: Aurora Clark (Washington State University, USA)
Wibe de Jong (Lawrence Berkeley National Laboratory, USA)
Matteo Giantomassi (Université Catholique de Louvain, Belgium)
Mathieu Luise (ETH Zurich, Switzerland)
Markus Meuwly (University of Basel, Switzerland)
Kristin Persson (Lawrence Berkeley National Laboratory, USA)
Giovanni Pizzi (EPFL, Switzerland)

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)

Computer Science & Applied Mathematics
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 Churnara (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)

Engineering
Domain Co-Chair: Richard Sandberg (The University of Melbourne, Australia)
Domain Co-Chair: Jackie Chen (Sandia National Laboratories, USA)
George Biros (The University of Texas at Arlington, USA)
Steve Plimpton (Sandia National Laboratories, USA)
Philipp Schlatter (KTH Royal Institute of Technology, Sweden)
Maarten van Reeuwijk (Imperial College London, UK)

Life Sciences
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
Domain Co-Chair: George Lake (University of Zurich, Switzerland)
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

10:20 – 11:10
Unveiling Earthquake Dynamics Through Extreme-Scale Multi-Physics Simulations
Alice-Agnès Gabriel (Ludwig Maximilian University of Munich, Germany)
Chair: Dimitri Komatitsch (CNRS, France)

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

AP ACM PASC18 Papers

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)

14:00 – 14:30
Training Generative Adversarial Models over Distributed Computing Systems, Hai Rui (ETH Zürich, Switzerland)

ID Interdisciplinary Dialogue

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

7:00 – 9:00
Self-justified Equilibria: existence and computation, Felix Kühler (University of Zurich, Switzerland)

ID01 The Colourful Theory, and Visible and Invisible Matter in the Universe: An Interdisciplinary Dialogue between Constantin Alexandrou and Petros Koumoutsakos

13:00 – 13:30
First-Principles Transport on Exascale Supercomputers: The Large Scale Electron Transport with Phonon Coupling, Peter Dominik Dueben (Argonne National Laboratory, USA)

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

14:30 – 15:00
Holistic Performance Engineering for Sparse Iterative Solvers, Jonas Thies (German Aerospace Center, Germany)

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

13:30 – 14:00
Distributed Training of Deep Neural Net Models for High Energy Physics
Kevin Doyle (University of Cambridge, UK)

14:00 – 14:30
Training Generative Adversarial Models over Distributed Computing Systems, Hai Rui (ETH Zürich, Switzerland)

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

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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)
MS09  Adaptive Parallel Strategies for the Exploration of Challenging Search Spaces with Applications in Particle Simulations and Optimization, Part II
Samarkand Room
Organizers: Andreas Vitalis, Marco Bacci, Amedeo Califano (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, Serena Z. Rinker (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. Stebi (Max Planck Institute of Biophysics, Germany)

MS10  Bridging the Software Productivity Gap for Climate and Weather Models
Rio Room
Organizers: 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 (Tinghua University, China)
16:00 – 16:30 Performance Portability for Next Generation HPC Architectures in ESM via the Kokkos Programming Model, Luca Bertagna (Sandia National Laboratories, USA)
16:30 – 17:00 Experience Applying the P5yclone 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, Carles E. Domsa (MeteoSwiss, Switzerland)

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

MS12  Engineering Software in times of Agile Development, Continuous Integration and Cloud Computing
Sydney Room
Organizers: Guido Juckeland (Heinrich-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 Software Development is Agile - Best Practices and Lessons Learned, Guido Juckeland (Heinrich-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
Organizers: Sofia Vallecorsa (CERN, Switzerland), Jean-Roch Vimont (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 Simulating Highly Granular Calorimeters, Tobias Golling (University of Geneva, Switzerland)

MS14  How Fintech and Big Data Change and Challenge the Insurance Sector
Nairobi Room
Organizers: Jean-Michel Benkert, Michelle Altpeter (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 (Bralzyna, 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
Organizers: 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, Alexandru 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
Organizers: Sharkeer Clin (University of Missouri - St. Louis, USA), Daniel Jacobson (Oak Ridge National Laboratory, USA)
15:30 – 16:00 ugSCIP-Jack, MPII: A Massively Parallel Steiner Tree Solver, Daniel Riefkeld (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, Sharkeer Clin (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
Organizers: Philipp Schattler (KTH Royal Institute of Technology, Sweden), Ramesh Balakrishnan (Argonne National Laboratory, USA)
15:30 – 16:00 Adaptive Mesh Refinement Based on Adjacent Error Estimators for Ne5000D, Philipp Schattler (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 Gatter-Scatter Operations in Ne5000D Using PGAS, Niclas Janson (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

**MS18**

**Addressing Resilience Challenges for Computing at Extreme Scale**

- **Organizer(s):** Aurelien Cavelan, Florina Corba (University of Basel, Switzerland)
- **Montreal Room**
- **13:30 – 14:00**

#### PNL Panel Discussion

**PNLO1**

Panel Discussion on Big Data vs. Fast Computation

- **Organizer(s):** Eng Lim Goh (Hewlett Packard Enterprise, USA), Nuria Lopez (IDG, Spain)
- **Montreal Room**
- **09:00 – 10:15**

### Poster Sessions

**FP02**

**Panel Poster Session**

- **Montreal Room**
- **10:15 – 11:00**
  - **Speaker:** Maria Grazia Gulfienda (ETH Zurich / CSCS, Switzerland)

**FP03**

**Poster Session C Reception**

- **Foyer 2nd Floor**
- **19:30 – 21:30**

### IP Invited Plenary Presentation

**IP02**

**Public Lecture on Massive-Scale Analytics Applied to Real-World Problems**

- **Organizer(s):** David Bader (Georgia Institute of Technology, USA)
- **Montreal Room**
- **18:30 – 19:30**

### ACM PASC18 Papers

#### AP02

**ACM PASC18 Popers Session II**

- **Montreal Room**
- **11:30 – 12:00**
  - **Speaker:** Jack Wells (Oak Ridge National Laboratory, USA)
  - **Title:** A Parallel Solver for Graph Laplacians, Tristan Konolige (University of Colorado Boulder, USA)

- **12:00 – 12:30**
  - **Title:** Abstractions and Directives for Adopting Wavefront Algorithms to Future Architectures, Robert Sears (University of Delaware, USA)

#### AP03

**ACM PASC18 Popers Session III**

- **Singapore Room**
- **11:30 – 12:00**
  - **Speaker:** Michael A. Heroux (Sandia National Laboratories, USA)
  - **Title:** Distributed, Shared-Memory Parallel Triangle Counting, Andrew Lamdanide (Pacific Northwest National Laboratory, USA)

- **12:00 – 12:30**
  - **Title:** MRGB – Random Number Generation for the Exascale Era, Yuruke Nagasaka (Tokyo Institute of Technology, Japan)

#### AP04

**ACM PASC18 Popers Session IV**

- **Sydney Room**
- **11:30 – 12:00**
  - **Speaker:** Olaf Schenk (Università della Svizzera italiana, Switzerland)
  - **Title:** 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**
  - **Title:** Balanced Graph Partition Re refinement Using the Graph p–Laplacian, Dimosthenis Pasadakis (Università della Svizzera italiana, Switzerland)

### MS Minisymposia Session III

**MS19**

**Advances in Computational Geosciences, Part I**

- **Organizer(s):** Eru Bunzaq (Colorado School of Mines, USA), Dimtri Komatitsch (CNRS, France)
- **Montreal Room**
- **13:30 – 14:00**
  - **Title:** 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**
  - **Title:** Elastic Full Waveform Inversion with Active Seismic Data, René-Édouard Plessy (Royal Dutch Shell, Netherlands)

- **14:30 – 15:00**
  - **Title:** 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**
  - **Title:** 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**
- **13:30 – 14:00**
  - **Title:** 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**
  - **Title:** Experiences of Porting and Maintaining the ICON Model on Accelerators, William Sawyer (ETH Zurich / CSCS, Switzerland)

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

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

### ACM PASC18 Papers

#### AP02

**APCM PASC18 Popers Session II**

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

- **12:00 – 12:30**
  - **Title:** Abstractions and Directives for Adopting Wavefront Algorithms to Future Architectures, Robert Sears (University of Delaware, USA)

#### AP03

**APCM PASC18 Popers Session III**

- **Singapore Room**
- **11:30 – 12:00**
  - **Title:** Distributed, Shared-Memory Parallel Triangle Counting, Andrew Lamdanide (Pacific Northwest National Laboratory, USA)

- **12:00 – 12:30**
  - **Title:** MRGB – Random Number Generation for the Exascale Era, Yuruke Nagasaka (Tokyo Institute of Technology, Japan)

#### AP04

**APCM PASC18 Popers Session IV**

- **Sydney Room**
- **11:30 – 12:00**
  - **Title:** 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**
  - **Title:** Balanced Graph Partition Re refinement Using the Graph p–Laplacian, Dimosthenis Pasadakis (Università della Svizzera italiana, Switzerland)

### MS Minisymposia Session III

**MS21**

**Computational Solutions to Large–Scale Data Management and Analysis Challenges in Personalized Health**

- **Organizer(s):** Leila Tamara Alexander, Torsten Schwede (Swiss Institute of Bioinformatics, Switzerland)
- **13:30 – 14:00**
  - **Title:** Semantic Interoperability Challenges for Sharing and Reusing Large Amounts of Heterogeneous Data, Marie-Christine Jaulent (INSEPAM, France)

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

- **14:30 – 15:00**
  - **Title:** HPC-Supported Therapy Development in Oncology, Oliver Michelin (University of Lausanne, Switzerland)

- **15:00 – 15:30**
  - **Title:** 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**
- **13:30 – 14:00**
  - **Title:** The Evolution of Software Practice in GROMACS: To Suit Both the Laptop and the Exascale, Neil Chue Hong (University of Edinburgh, UK)

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

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

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

### MS23

**High Performance Graph Algorithms**

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

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

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

- **15:00 – 15:30**
  - **Title:** RACE: Recursive Algebraic Coloring Engine, Christl 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 Markitis (KTH Royal Institute of Technology, Sweden)
14:00 – 14:30  Viasator – Understanding Near-Earth Space in Six Dimensions, Minna Painio (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)

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 Casasoli (INGV, Italy)
17:30 – 18:00  Full-Waveform Inversion of the Solid Earth from Crust to Core, Ebru Ozdag (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 Flandor (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)

MS25  Scientific Computing in times of MPI-X: Looking at Multiple “X” with regard to Performance and Portability
Nairobi Room  Organizer(s): Sunil Chandrasekaran (University of Delaware, USA)
13:30 – 14:00  Porting Physical Parameterizations from a Climate Model to Accelerators Thomas Küster (Università della Svizzera Italiana, Switzerland), William Sawyer (ETH Zurich / CSCS, Switzerland)
14:00 – 14:30  Zero Overhead Modern C++ for Mopping to Any Programming Model, Axel Huebl (Heinrich-Zentrum Dresden-Rossendorf, Germany)
14:30 – 15:00  Porting Quantum ESPRESSO to GPUs - Lessons Learnt and Remaining Challenges, Pietro Bonf (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)

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  Smifs: A Simulation Data Virtualizing File System Interface, Salvatore Di Grolario (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 Laboratoy, USA)
17:30 – 18:00  General Discussion and Community Input, Anshu Dubey (Argonne National Laboratory, USA)

MS27  Actionable Health Intelligence: From Precision Medicine to Population Health
Sydney Room  Organizer(s): Georgia Tourassi (Oak Ridge National Laboratory, USA)
18:00 – 18:30  Radiogenomics in the Era of Precision Medicine, Constantin Tziftchis (University of Cyprus, Cyprus)
18:30 – 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 Intercombe 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)

16:00 – 16:30  Structure and Dynamics of Au Nanoclusters Using ANN Based Interatomic Potentials, Satya Bulusu (BT Indire, India)
16:30 – 17:00  On Creating Databases for Machine Learned Interatomic Potentials, Gabor Csányi (University of Cambridge, UK)
17:00 – 17:30  Materials Modeling Using Neural Networks, Mathé Hellinghson (University of Göttingen, Germany)
17:30 – 18:00  Using Machine Learning Interatomic Potentials for Crystal Structure Prediction, Seyed-Alireza Gharami (Institute for Advanced Studies in Basic Sciences, Iran)

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 (BT Indire, India)
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MS34  Plasma II: Frontiers in Gyrokinetic Turbulence Simulation on New and Emerging HPC Platforms
Osaka Room  Organizer(s): Stephen 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, Maserun Numan (National Institute for Fusion Science, Japan)
17:00 – 17:30  CPU and GPU Parallelization of Spectral Particle Methods, Jakob Amores (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**

**IPO3**
From Weather Dwarfs to Kilometre-Scale Earth System Simulations
10:00 – 10:50
Montreal Room
Organizer(s): Maria Haney, Philippe Jetzer (University of Zurich, Switzerland)
Chair: Willem Deconinck (ECMWF, UK)

**IPO4**
Challenges in the First Principles Modelling of Magneto Hydro Dynamic Instabilities and their Control in Magnetic Fusion Devices
16:40 – 17:30
Montreal Room
Organizer(s): Maria Haney, Philippe Jetzer (University of Zurich, Switzerland)
Chair: Sinelid Ryan (Trinity College Dublin, Ireland)

**MS Minisymposia Session V**

**MS35**
Gravitational-Wave Data Analysis with the Current Generation of Advanced Detectors
11:15 – 11:45
Osaka Room
Organizer(s): Maria Haney, Philippe Jetzer (University of Zurich, Switzerland)
Chair: Willem Deconinck (ECMWF, UK)

**MS36**
HPC for HEP: Enabling Big Data from Large Instruments on Leadership Class HPC Infrastructures
11:45 – 12:15
Sydney Room
Organizer(s): Frank Vahrenholt (UC San Diego, USA), Kaushik De (The University of Texas at Arlington, USA)
Chair: Willem Deconinck (ECMWF, UK)

**MS37**
HPQc: Current Challenges in Uncertainty Quantification for Mechanistic Models, Part II: Theory, Methods and Tools
12:15 – 12:45
Singapore Room
Organizer(s): Ribaraba Dutta (Università della Svizzera italiana, Switzerland), Nikos Karathanasopoulos (ETH Zurich, Switzerland), Bastien Chopard (University of Geneva, Switzerland)
Chair: Willem Deconinck (ECMWF, UK)

**MS38**
Mass and Energy Transport Phenomena in Solid Stote
12:45 – 13:15
Boston Room
Organizer(s): Ivan Tavelli, Matthieu Mottet (IBM Research, Switzerland)
Chair: Willem Deconinck (ECMWF, UK)

**MS39**
Scalable Solvers for Forward and Inverse Problems in Geophysics
11:15 – 11:45
Darwin Room
Organizer(s): Christian Bouchu, Vâclav Hapla (ETH Zurich, Switzerland)
Chair: Willem Deconinck (ECMWF, UK)

**MS40**
Towards Weather and Climate Simulations at 1-km Resolution
11:15 – 11:45
Rio Room
Organizer(s): Peter Dominik Deuen (ECMWF, UK), Carlos E. Osuna (MeteoSwiss, Switzerland)
Chair: Willem Deconinck (ECMWF, UK)

**MS41**
Use of AI to Analyze Complex Biological Systems
11:45 – 12:15
Samarkand Room
Organizer(s): Daniel Jacobson (Oak Ridge National Laboratory, USA), Ben Brown (Lawrence Berkeley National Laboratory, USA), Georgios Gkoutos (University of Birmingham, UK)
Chair: Willem Deconinck (ECMWF, UK)

**MS42**
Coupling Strategies Towards Exascale for Complex Earth System Modelling
14:15 – 14:45
Rio Room
Organizer(s): Willem Deconinck (ECMWF, UK), Katherine Evans (Oak Ridge National Laboratory, USA)
Chair: Willem Deconinck (ECMWF, UK)

**MS43**
Distributed Asynchronous Parallel Computing: Progress and Challenges for Multi-Physics Applications on Heterogeneous Architectures
14:15 – 14:45
Darwin Room
Organizer(s): Hemant Kolla (Sandia National Laboratories, USA), Jacqueline Chen (Sandia National Laboratories, USA)
Chair: Willem Deconinck (ECMWF, UK)

**MS44**
Making the Expensive Affordable: Running a Chemistry Model in the UKESM Climate Model, Richard Hill (Met Office, UK)
15:15 – 16:15
Rio Room
Organizer(s): Willem Deconinck (ECMWF, UK), Katherine Evans (Oak Ridge National Laboratory, USA)
Chair: Willem Deconinck (ECMWF, UK)

**MS Minisymposia Session VI**

**MS45**
Data Quality for Gravitational-Wave Detectors, Andrew P. Lundgren
12:45 – 13:15
UKESM Energy Environment, Andrew P. Lundgren (University of Portsmouth, UK)

**MS46**
HPC Systems and the Integration Challenges of Large Instruments, Frank Vahrenholt (UC San Diego, USA)
12:45 – 13:15
Rio Room
Organizer(s): Willem Deconinck (ECMWF, UK), Andreas Mueller (ECMWF, UK)
Chair: Willem Deconinck (ECMWF, UK)

**MS47**
Scalable Solvers for Forward and Inverse Problems in Geophysics
12:45 – 13:15
Darwin Room
Organizer(s): Christian Bouchu, Vâclav Hapla (ETH Zurich, Switzerland)
Chair: Willem Deconinck (ECMWF, UK)

**MS48**
Near-Global RCM Simulations to Establish a Baseline for Global 1 km ECMWFSimulations, Sascha Husa (University of the Balearic Islands, Spain)
12:45 – 13:15
Darwin Room
Organizer(s): Hemanth Kolla (Sandia National Laboratories, USA), Jacqueline Chen (Oak Ridge National Laboratory, USA), Georgios Gkoutos (University of Birmingham, UK)
Chair: Willem Deconinck (ECMWF, UK)

**MS49**
Flexible Earth System Modelling at the End of Dennard Scaling, George Mozdzynski (ECMWF, UK)
14:45 – 15:15
Rio Room
Organizer(s): Willem Deconinck (ECMWF, UK), Katherine Evans (Oak Ridge National Laboratory, USA)
Chair: Willem Deconinck (ECMWF, UK)

**MS50**
Near-Global RCM Simulations to Establish a Baseline for Global 1 km ECMWFSimulations, Sascha Husa (University of the Balearic Islands, Spain)
12:45 – 13:15
Darwin Room
Organizer(s): Hemanth Kolla (Sandia National Laboratories, USA), Jacqueline Chen (Oak Ridge National Laboratory, USA), Georgios Gkoutos (University of Birmingham, UK)
Chair: Willem Deconinck (ECMWF, UK)
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- Sydney
- Montreal Auditorium
- Rio
- Nairobi

3rd 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

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, USA), 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 11:30 – 12:30  Montreal Room, Singapore Room, Sydney Room, Minisymposia Session II
AP03 11:30 – 12:30  Minisymposia Session III
AP04 11:30 – 12:30  Minisymposia Session IV

12:30 – 13:30  Foyer 2nd Floor  Lunch

Minisymposia Session III

15:00 – 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 Bailey (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
Niu-P. Yeed (CERN, UK)

10:50 – 11:15  Foyer 2nd Floor  Coffee Break

Minisymposia Session V

13:15 – 14:15  Foyer 2nd Floor  Lunch

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