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

PASC15

Platform for Advanced Scientific Computing Conference

Zürich Switzerland

01–03 June 2015

```
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

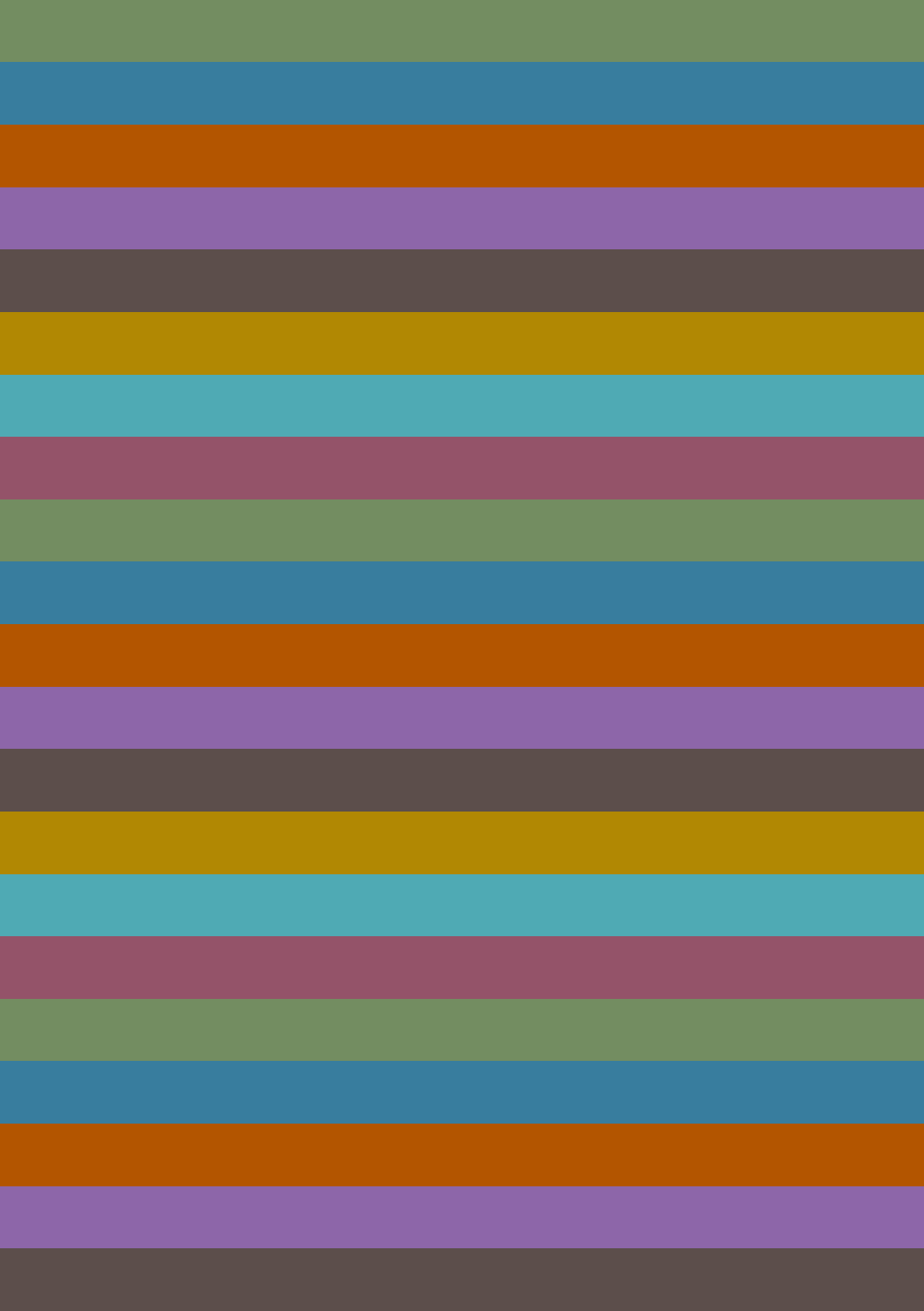
f & φ REAL OR COMPLEX-VALUED FUNCTIONS

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

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



PASC15

Platform for Advanced Scientific Computing Conference

Zürich
Switzerland

01-03 June 2015

IP
Invited Plenary Presentations

MS
Minisymposia

CTS
Contributed Talks

Wednesday, June 3, 2015

Poster Session

Monday, June 1, 2015
HG F30 – Audimax

Tuesday, June 2, 2015
HG F30 – Audimax

Wednesday, June 3, 2015
HG F30 – Audimax

IP

Invited Plenary Presentations

IP01

Simulating Cosmic Structure Formation; Volker Springel

(University of Heidelberg, Germany)

Monday,
June 1, 2015

10:15 – 11:10
Audimax
(HG F30)

Chair:
Ben Moore
(University
of Zurich,
Switzerland)

Numerical simulations on supercomputers play an ever more important role in astrophysics. They have become the tool of choice to predict the non-linear outcome of the initial conditions left behind by the Big Bang, providing crucial tests of cosmological theories. However, the problem of galaxy and star formation confronts us with a staggering multi-physics complexity and an enormous dynamic range that severely challenges existing numerical methods. In my talk, I review current strategies to address these problems, focusing on recent developments in the field such as hierarchical time integration schemes, improved particle- and mesh-based hydrodynamical solvers, and novel parallelization schemes.

Volker Springel became professor for Theoretical Astrophysics at Heidelberg University in 2010, where he now leads a research group at the Heidelberg Institute for Theoretical Studies (HITS). Springel previously was a group leader in computational cosmology at the Max-Planck-Institute for Astrophysics in Garching, after working as a postdoctoral researcher at the Harvard Center for Astrophysics in the United States. He received his PhD in 2000 from the Ludwig-Maximilian University in Munich, after studying physics at the University of Tübingen and the University of California, Berkeley.

IP02

The Great Leap; Bjorn Stevens

(Max-Planck-Institute for Meteorology, Germany)

Monday,
June 1, 2015

11:10 – 12:00
Audimax
(HG F30)

Chair:
Christoph Schär
(ETH Zurich,
Switzerland)

Increasing computational power and advances in algorithms have made it possible to resolve an ever-increasing fraction of the scales of atmospheric motion. While it remains inconceivable to resolve all the relevant scales of motion we are currently in the midst of a great leap across a range of scales that have posed some of the greatest challenges to climate science over the past sixty years. This leap is bringing wholly new insights into the structure of the climate system on both ends of the spectrum of atmospheric motions.

Bjorn Stevens's research blends modeling, theory and field work to understand the role of clouds and moist convection on the climate system. Stevens has made pioneering contributions to our understanding of how mixing and microphysical processes influence both cloud structure and its susceptibility to changes in the environment. Stevens has contributed more than 130 scholarly articles to the peer reviewed literature and received many honors, including the Clarence Leroy Meisinger Award of the American Meteorological Society for "pioneering advances in understanding and modeling of cloud-topped boundary layer." He currently co-leads the World Climate Research Programme's Grand Challenge on Clouds, Circulation and Climate Sensitivity.

IP03

Materials Discovery and Scientific Design by Computation: a Revolution Still in the Making; Giulia Galli

(University of Chicago, USA)

Tuesday,
June 2, 2015

9:00 – 10:00
Audimax
(HG F30)

Chair:
George Malcolm Stocks
(Oak Ridge National Laboratory, USA)

The need of advanced materials for sustainable energy resources and next generation information technology requires the development of integrated scientific strategies, encompassing theoretical innovations, and computational and laboratory experiments. Substantial progress has been made in the last two decades in understanding and predicting the fundamental properties of materials and molecular systems from first principles, i.e., from numerical solutions of the basic equations of quantum mechanics. However, the field of ab initio predictions is in its infancy; some formidable theoretical and computational challenges lie ahead of us, including the collection and use of data generated by simulations. We will describe recent progress and successes obtained in predicting properties of matter by quantum simulations, and discuss algorithmic challenges in connection with the use of evolving high-performance computing architectures. We will also discuss open issues related to the validation of the approximate, first principles theories used in large-scale quantum simulations.

Giulia Galli is the Liew Family Professor of Electronic Structure and Simulations in the Institute for Molecular Engineering, at the University of Chicago, Senior Scientist at Argonne National Laboratory and Senior Fellow of the Computational Institute of the University of Chicago. She holds a PhD in physics from the International School of Advanced Studies (SISSA) in Trieste, Italy. She was the head of the Quantum Simulations Group at the Lawrence Livermore National Laboratory and Professor of Chemistry and Physics at the University of California, Davis, prior to joining the University of Chicago. She is a Fellow of the American Physical Society (APS) and of the American Academy of Arts and Sciences (AAAS). She received an award of excellence from the Department of Energy (2000) and the Science and Technology Award from the Lawrence Livermore National Laboratory (2004). She served as chair of the Division of Computational Physics of the American Physical Society (2006-2007) and of the Extreme Physics and Chemistry of Carbon Directorate of the Deep Carbon Observatory (2010-2013). Her research activity is focused on quantum simulations of systems and processes relevant to condensed matter physics, physical chemistry, molecular engineering and nano-science.

IP04

Computational Challenges in Macroeconomics; Thomas Sargent

(New York University, USA)

Tuesday,
June 2, 2015

18:30 – 19:20
Audimax
(HG F30)

Chair:
Felix Kubler
(University
of Zurich,
Switzerland)

Modern macroeconomic theory has provided many qualitative insights into the functioning of financial and labor markets in our complex modern economies. But determining the quantitative importance of frequently countervailing forces requires much more than the pencil and paper methods used by economic theorists. My talk will describe some new economic ideas brought by economic theory, and how efforts to develop computational tools promise to help macroeconomists perform quantitative analyses that can inform policy choices.

Thomas J. Sargent is the W. R. Berkley Professor at New York University, a joint appointment in the Economics Department and the Stern School of Business. He has been a Senior Fellow at the Hoover Institution since 1987. He was awarded the 2011 Nobel Prize in Economics for his empirical research on cause and effect in the macroeconomy. Professor Sargent earned his BA from the University of California, Berkeley in 1964, and his PhD in economics from Harvard University in 1968. He has held Professor appointments at the University of Minnesota, University of Chicago, and Stanford University. Sargent was elected a fellow of the National Academy of Sciences in 1983.

IP05

Towards Exascale Simulation of Turbulent Combustion; Jacqueline Chen

(Sandia National Laboratories, Livermore, USA)

Wednesday, June 3, 2015

09:00 – 10:00
Audimax
(HG F30)

Chair:
Gretar Tryggvason
(University of Notre Dame, USA)

Exascale computing will enable combustion simulations in parameter regimes relevant to next-generation combustors burning alternative fuels. The first principles direct numerical simulations (DNS) are needed to provide the underlying science base required to develop vastly more accurate predictive combustion models used ultimately to design fuel efficient, clean burning vehicles, planes, and power plants for electricity generation. However, making the transition to exascale poses a number of algorithmic, software and technological challenges. As Moore's Law and Dennard scaling come to an end exascale computing will be achieved only through massive concurrency. Addressing issues of data movement, power consumption, memory capacity, interconnection bandwidth, programmability, and scaling through combustion co-design are critical to ensure that future combustion simulations can take advantage of emerging computer architectures. Co-design refers to a computer system design process where combustion science requirements influence architecture design and constraints inform the formulation and design of algorithms and software. The current state of petascale DNS of turbulent combustion will be reviewed followed by a discussion of current combustion exascale combustion co-design topics: 1) architectural modeling and simulation of the behavior of combustion applications on future extreme architectures; and 2) programming model and runtime for heterogeneous, hierarchical machines with inherent variability. While bulk synchronous programming and data parallelism have been operative at the petascale, the movement to exascale requires a shift towards asynchronous programming, where to extract maximum parallelism, both data and task parallelism accessing disjoint sets of fields is required. An example from a recent refactorization of a combustion DNS code, S3D, using an asynchronous model, Legion, with dynamic runtime analysis at scale will be presented.

Jacqueline H. Chen is a Distinguished Member of Technical Staff at the Combustion Research Facility at Sandia National Laboratories. She has contributed broadly to research in petascale direct numerical simulations (DNS) of turbulent combustion focusing on fundamental turbulence-chemistry interactions. In collaboration with computer scientists and applied mathematicians she is the founding Director of the Center for Exascale Simulation of Combustion in Turbulence (ExaCT). She received several DOE INCITE Awards in the last few years and the Asian American Engineer of the Year Award in 2009.

IP06

Algorithmic Adaptations to Extreme Scale; David Keyes

(King Abdullah University of Science and Technology, Saudi Arabia)

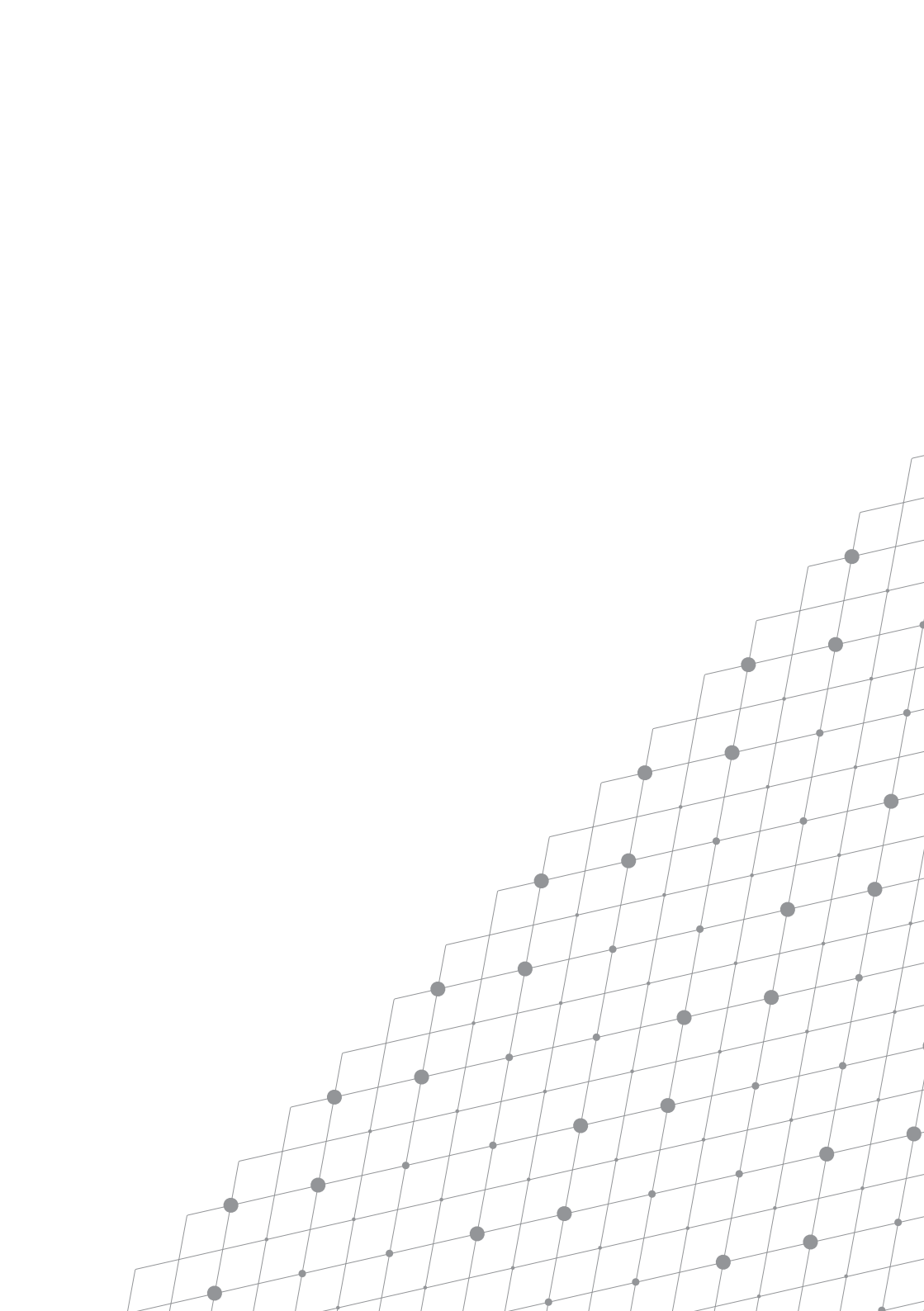
Wednesday, June 3, 2015

12:00 – 12:50
Audimax
(HG F30)

Chair:
Olaf Schenk
(Università della Svizzera italiana, Switzerland)

Algorithmic adaptations are required to use anticipated exascale hardware near its potential, since the code base has been engineered to squeeze out flops. Instead, algorithms must now squeeze out synchronizations, memory, and transfers, while extra flops on locally cacheable data represent small costs in time and energy. Today's scalable solvers, in particular, exploit frequent global synchronizations. After decades of programming model stability with bulk synchronous processing (BSP), new programming models and new algorithmic capabilities (to take advantage, e.g., of forays in data assimilation, inverse problems, and uncertainty quantification) must be co-designed with the hardware. We briefly recap the architectural constraints, highlight some work at KAUST, and outline future directions.

David Keyes is Director of the Extreme Computing Research Center at KAUST. He earned a BSE in aerospace and mechanical sciences from Princeton in 1978 and PhD in applied mathematics from Harvard in 1984. Keyes works at the interface between parallel computing and the numerical analysis of PDEs, with a focus on scalable implicit solvers. Newton-Krylov-Schwarz (NKS), Additive Schwarz Preconditioned Inexact Newton (ASPIN), and Algebraic Fast Multipole (AFM) methods are methods he helped name and popularize. Before joining KAUST as a founding dean in 2009, he led scalable solver software projects in the ASCI and SciDAC programs of the US Department of Energy, ran university collaboration programs at NASA's ICASE and the LLNL's ISCR, and taught at Columbia, Old Dominion, and Yale Universities. He is a Fellow of SIAM and AMS.



MS

Minisymposia

MS01

Advances in Numerics and Physical Modeling for Geophysical Fluid Dynamics

Organiser: *Simone Marras (Naval Postgraduate School, USA)*
Co-organiser: *Mariano Vázquez (Barcelona Supercomputing Center, Spain);*
Giovanni Tumolo (ICTP, Italy);
Alex Breuer (Technische Universität München, Germany);
Francis X. Giraldo (Naval Postgraduate School, USA)

In view of the ever increasing parallelism of supercomputing platforms and the approaching era of exascale computing, high-resolution modeling is becoming a priority for Geophysical Fluid Dynamics (GFD) numerical modelers. Today's supercomputers require highly scalable numerical methods; high-resolution permits more resolved physical processes. This mini-symposium aims to bringing together scientists from different disciplines who are contributing to the next-generation GFD model development via the definition of advanced numerical methods and more accurate physical schemes. Interest is given to scalable numerics and high-resolution physics modeling such as, but not limited to, LES.

An Accurate and Efficient Numerical Framework for Adaptive Numerical Weather Prediction; Giovanni Tumolo

(The Abdus Salam ICTP, Italy)

Monday, June 1, 2015

13:00 – 13:30
HG E1.1

We present an adaptive discretization approach for model equations typical of NWP, which combines the semi-Lagrangian technique with a TR-BDF2 semi-implicit time discretization and with a DG spatial discretization with (arbitrarily high) variable and dynamically adaptive element degree. The resulting method has full second order accuracy in time, is unconditionally stable and can effectively adapt at runtime the number of degrees of freedom employed in each element, in order to balance accuracy and computational cost. Numerical results of classical 2D benchmarks for shallow water equations on the sphere and Euler equations on a vertical slice confirm the potential of the proposed formulation.

Co-Authors: **Luca Bonaventura** (Politecnico di Milano, Italy)

Towards a 3D Dynamical Core Based on Mixed Finite Element Methods; Andrew McRae

(Imperial College London, United Kingdom) Abstract

Monday, June 1, 2015

13:30 – 14:00
HG E1.1

There are known scaling issues with the otherwise-successful combination of C-grid finite difference methods on a global latitude-longitude grid. Direct extensions of C-grid methods to quasi-uniform grids have known inadequacies. Mixed finite element methods, recently unified under the label of finite element exterior calculus, provide a way of recovering desirable numerical properties but on arbitrary meshes. After some initial work in 2D, we implemented a method for the automated generation of sophisticated 'tensor-product' finite elements. The use of finite element methods also invites the possibility of high-order approaches, though we are not actively exploring this.

Co-Authors: **Colin Cotter** (Imperial College London, United Kingdom); **David Ham** (Imperial College London, United Kingdom)

Scalable Dynamic Load Balancing of Detailed Cloud Physics with FD4; Matthias Lieber

(Technische Universität Dresden, Germany)

Monday,
June 1, 2015

14:00 – 14:30
HG E1.1

Load balancing of large-scale scientific simulations is a challenging task. My talk shows how the open source framework FD4 (Four-Dimensional Distributed Dynamic Data structures) enables scalable dynamic load balancing of detailed cloud physics in the atmospheric model COSMO-SPECS+FD4. The concept is based on separating data structures and decomposition such that the cloud physics model can be partitioned independently of the atmospheric model. To increase scalability, a hierarchical space-filling curve partitioning algorithm is used. Benchmarks on a Blue Gene/Q system show the scalability up to 256k ranks. FD4 can also be applied to other multiphase or multiphysics problems.

Using GPUs Productively for the ICON Climate Model; William Sawyer

(CSCS / ETH Zurich, Switzerland)

Monday,
June 1, 2015

14:30 – 15:00
HG E1.1

The Swiss National Supercomputing Centre (CSCS) has undertaken a full port of the Icosahedral Non-hydrostatic (ICON) climate model currently under development at the Max Planck Institute for Meteorology (MPI-M) and the German Weather Service (DWD). Central to this port is the co-design with MPI-M and DWD developers to ensure that the code changes are minimal and non-intrusive, do not impose any significant changes in CPU performance, and can be incorporated directly into the development trunk. In this talk we present some of the techniques which facilitate this co-design project and initial results indicating that the performance is directly related to the peak memory bandwidth.

Co-Authors: **Markus Wetzstein** (CSCS / ETH Zurich, Switzerland); **Leonidas Linardakis** (Max Planck Institute for Meteorology, Germany)

Development of a Vertical Slice Model Using Mixed FEM Discretizations; Hiroe Yamazaki

(Imperial College London, United Kingdom)

Monday, June 1, 2015

15:30 – 16:00
HG E1.1

A vertical slice model is developed for the Euler-Boussinesq equations with a constant temperature gradient in the y-direction (the Eady-Boussinesq model). The model is a solution of the full 3D equations with no variation normal to the slice, which is an idealized problem used to study the formation and subsequent evolution of weather fronts. Mixed FEM discretizations on an extruded mesh are performed using Firedrake, a high-level Python framework for the portable solution of PDEs on unstructured meshes. I will discuss the details of the vertical slice model implementations and the preliminary results obtained through test simulations developed to implement the modelling of fronts.

Co-Authors: **Colin Cotter** (Imperial College London, United Kingdom); **Jemma Shipton** (Imperial College London, United Kingdom); **Lawrence Mitchell** (Imperial College London, United Kingdom); **David A Ham** (Imperial College London, United Kingdom); **Andrew McRae** (Imperial College London, United Kingdom)

Nonlinear Stabilization Techniques for Finite Element Approximations of Fluid Problems; Murtazo Nazarov

(Uppsala University, Sweden)

Monday, June 1, 2015

16:00 – 16:30
HG E1.1

This talk will discuss recent developments in stabilized finite element approximations using nonlinear viscosity methods. The regularization terms are constructed by the residual of the system or entropy equations. The method is successfully applied to compressible and incompressible Navier-Stokes equations and variable density flows in two and three space dimensions. Then we discuss about maximum principle preserving continuous finite element schemes for scalar conservation laws. The new method does not require any a priori knowledge of quantities like local wave-speed, proportionality constant, or local mesh-size and it is independent of the cell type.

preCICE – a Library for Flexible Surface-Coupling on Massively Parallel Systems; Benjamin Uekermann

(Technische Universität München, Germany)

Monday,
June 1, 2015

16:30 – 17:00
HG E1.1

With increasing compute power, the simulation of multi-physics gains more and more popularity. At the same time, a flexible software development process including existing single-physics codes becomes a necessity to cope with the overall complexity. preCICE is an open-source library to surface-couple single-physics codes. Its high-level API allows to write adapters for single-physics codes in 30 lines. Afterwards various codes can be coupled in a nearly plug-and-play manner. preCICE offers methods for interpolation, means for parallel communication, and sophisticated fix-point acceleration schemes. In this talk, we present our efforts and tests on the parallel efficiency of preCICE.

Co-Authors: **Hans-Joachim Bungartz** (Technische Universität München, Germany); **Florian Lindner** (Universität Stuttgart, Germany); **Miriam Mehl** (Universität Stuttgart, Germany)

Implicit Monolithic Time Scheme and Preconditioned Variational Multiscale Stabilization (PVMS) for Low Mach Flows; Mariano Vázquez

(Barcelona Supercomputing Center, Spain)

Monday,
June 1, 2015

17:00 – 17:30
HG E1.1

In this work we present an implicit scheme for solving the Navier-Stokes equations at Low Mach regimes. The method can cope efficiently with both stiffness and numerical instabilities thanks to the following procedure. A local preconditioner is applied to the Navier-Stokes equations. Next, the preconditioned local system is discretized according to the Variational Multiscale Stabilization (VMS) method. Finally, a monolithic implicit Jacobi (i.e. fixed point) scheme is applied, which, in turn, uses an algebraic diagonal preconditioner on a GMRES iterative solver. The scheme is assessed on large-scale 3D problems, particularly on its accuracy, convergence and parallel efficiency.

Co-Authors: **Margarida Moragues** (Barcelona Supercomputing Center, Spain); **Guillaume Houzeaux** (Barcelona Supercomputing Center, Spain)

High-Performance Computing and Big Data Challenges for NWP and Climate; Peter Bauer

(ECMWF, United Kingdom)

Tuesday,
June 2, 2015

10:30 – 11:00
HG E1.1

There is growing concern that the energy cost to produce weather forecasts, to quantify their uncertainty, and to handle the associated I/O load from enhanced observing systems as well as large forecast ensembles will be unaffordable with current HPC and data management technologies. NWP centres face enormous challenges due to the rising cost of energy associated with running complex high-resolution models on more and more processors in time for delivering forecasts with substantial societal benefit.

High-Order Schemes for Schemes for Atmospheric Dynamics on Unstructured Meshes; Antonis Antoniadis

(Cranfield University, United Kingdom)

Tuesday,
June 2, 2015

11:00 – 11:30
HG E1.1

This paper presents an extension of the Weighted Essentially Non-Oscillatory (WENO) type schemes for the non-hydrostatic compressible Euler equations in conjunction with two and three-dimensional unstructured meshes. The schemes are suitable for regional and global climate models dynamical cores. Their potential lies in their simplicity; accuracy; robustness; non-oscillatory properties; versatility in handling any type of grid topology; computational and parallel efficiency. The WENO schemes (up to 5th -order) are applied to two- and three-dimensional test cases: a 2D rising thermal bubble; the 2D density current and the 3D Robert smooth bubble.

Co-Authors: **Panagiotis Tsoutsanis** (Cranfield University, United Kingdom)

2D Adaptivity for 2.5D Flow Problems; Michael Bader

(Technische Universität München, Germany)

Tuesday,
June 2, 2015

11:30 – 12:00
HG E1.1

Many geophysical fluid dynamics problems feature a noticeably smaller extension in the vertical dimension compared to the horizontal dimensions. For such scenarios, we evaluate the potential of 2.5D grids that extend dynamically adaptive triangular meshes by a uniformly refined third dimension. While we tolerate a slight increase in the total number of degrees of freedom, we aim at improved performance due to vectorisation along the vertical dimension. Examples will be presented for simulation of tsunamis and porous media flow.

Co-Authors: **Kaveh Rahnema** (Technische Universität München, Germany); **Oliver Meister** (Technische Universität München, Germany)

A Conservative and Grid Adaptive Stabilization Scheme for Spectral Elements Based on a Dynamic SGS Model for LES. Application in Numerical Weather Prediction; Simone Marras

(Naval Postgraduate School, USA)

Tuesday,
June 2, 2015

12:00 – 12:30
HG E1.1

The solution of the Euler equations by high-order spectral elements is prone to instabilities that must be damped in some way. We approach the problem of stabilization via an adaptive subgrid-scale scheme meant to treat the instabilities by modeling the sub-grid scale features of the flow. The equations are regularized via a dynamically adaptive stress proportional to the residual of the unperturbed equations. Its effect is close to none where the solution is smooth and it increases elsewhere. This is a first step toward LES for hurricanes and extreme weather forecast with the Nonhydrostatic Unified Model of the Atmosphere, NUMA, the dynamical core of the next-generation Navy model NEPTUNE.

Co-Authors: **Francis X. Giraldo** (Naval Postgraduate School, USA)

MS02

Big Data Analytics for Novel Materials Discovery

Organiser: *Luca Ghiringhelli (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)*
Co-organiser: *Matthias Scheffler (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)*

To achieve deeper and novel scientific insight, to decide what new materials should be studied next as most promising novel candidates, and to identify interesting anomalies, the big data generated in computational materials science must be shared and efficient and physically meaningful analytic tools must be developed. The field has evolved in two main directions: constructing large databases of internally consistent materials data and development of advanced, machine-learning based, analysis techniques. Speakers of this symposium will discuss the strong and weak points of the different strategies adopted to perform big-data analytics, towards the discovery of new materials.

On-The-Fly Machine Learning of QM Forces for Big Data-Augmented Molecular Dynamics; Alessandro De Vita

(King's College London, United Kingdom)

Monday, June 1, 2015

13:00 –13:30
HG F1

I will present a 'big-data'-based MD technique where QM-accurate information is either located in massive databases or generated on the fly if unavailable, and used to predict atomic forces via Bayesian inference [1]. The approach is efficient as it concentrates QM subroutine calls where/when 'chemically novel' configurations are encountered along the system's trajectory. Interestingly, QM-zone partitioning followed by execution by standard O(N3) QM engines is predicted to be a better option than using O(N) QM methods when dealing with large QM zones in machine learning-augmented QM/MM calculations running on HPC platforms. [1] Z. Li, J. R. Kermode and A. De Vita, PRL 114, 096405 (2015).

Co-Authors: **Marco Caccin** (King's College London, United Kingdom); **Zhenwei Li** (University of Basel, Switzerland); **James Kermode** (University of Warwick, United Kingdom)

Mapping the Structure of Complex Materials Using Sketch-Map; Michele Ceriotti

(EPFL, Switzerland)

Monday, June 1, 2015

13:30 – 14:00
HG F1

A crucial step in understanding the behavior of complex materials is the introduction of coarse-grained order parameters that describe meta-stable states and transitions on the free energy surface, with a simpler, more intuitive representation than using the Cartesian coordinates of all the atoms. I will present sketch-map, a non-linear dimensionality reduction algorithm loosely based on multidimensional scaling, which obtains automatically such a simplified description, mapping with exquisite detail the stability of different conformations. Applications ranging from polypeptides to small clusters will be presented, demonstrating the potential and transferability of the method.

Co-Authors: **Margarida Moragues** (Barcelona Supercomputing Center, Spain); **Guillaume Houzeaux** (Barcelona Supercomputing Center, Spain)

Soft Matter and Data Repositories, a Personal View; Kurt Kremer

(Max Planck Institute for Polymer Research, Germany)

Monday, June 1, 2015

14:00 – 14:30
HG F1

Compared to many low molecular weight materials soft matter is not that perfectly characterized. E.g. polydispersity directly affects material properties. Furthermore chemical variation, for both synthetic and biological soft matter, is huge. Thus there are two options to provide data repositories, i.e. by experiment or simulation and quantum chemistry or by combination of both. I will present some thoughts of how, mainly based on theoretical work, they might be extended to form a basis of generally applicable data repositories.

Quantum Energy Regression Using Scattering Transforms; Matthew Hirn

(École normale supérieure, France)

Monday, June 1, 2015

14:30 – 15:00
HG F1

Physical functionals are usually computed as solutions of variational problems or from solutions of partial differential equations, which may require huge computations for complex systems. Quantum chemistry calculations of molecular energies is such an example. We present a novel approach for the regression of quantum mechanical energies based on the scattering transform of an intermediate electron density representation. The scattering transform is a deep convolutional network, composed of iterated wavelet transforms, that possesses appropriate invariant and stability properties for quantum energy regression. Numerical experiments give state of the art accuracy on planar organic molecules.

Co-Authors: **Stéphane Mallat** (École normale supérieure, France); **Nicolas Poilvert** (Pennsylvania State University, USA)

Machine Learning Approaches to Simulate Nanoscale Heat Transport; Davide Donadio

(Ikerbasque, Spain)

Monday, June 1, 2015

15:30 – 16:00
HG F1

Simulating thermal transport in nanostructures at atomistic level often requires the use of large-scale models, thus making it necessary to recur to empirical potentials. However, systems with complex chemistry, such as materials for phase change memories (PCM) and advanced thermoelectrics (TE), are poorly described by standard potentials. Here we propose an alternative approach to compute phonon properties and the thermal conductivity of nanostructures, which makes use of neural network potentials fitted on a large database of density functional theory calculation. We demonstrate its application on GeTe nanostructures for PCM and on nanostructured Ge-Mn alloys for TE application.

Co-Authors: **Claudia Mangold** (ETH Zurich, Switzerland); **Emanuele Bosoni** (University of Milano Bicocca, Italy); **Davide Campi** (University of Milano Bicocca, Italy); **Joerg Behler** (Ruhr University Bochum, Germany); **Marco Bernasconi** (University of Milano Bicocca, Italy)

Challenges in Big Data: When Materials Go Beyond the Periodic Table; Martin Uhrin

(EPFL, Switzerland)

Monday, June 1, 2015

16:00 – 16:30
HG F1

The properties of any material are, on some level, a function of its internal structure making an understanding of structure key to the discovery process. We use a simple model for particles that attract at long range and repel at short to probe possible structures over a wide range of parameters and stoichiometries. In exploring their energy landscapes we populate a schemaless, MongoDB, database with over 20M entries, many more than current databases populated from experiment or electronic structure calculations. We discuss some challenges of performing local and global analysis over such a large dataset and detail some interesting finds including never before seen structures.

Co-Authors: **Chris J. Pickard** (University College London, United Kingdom)

From Sharing to Big-Data Analytics: The NoMaD Project; Claudia Draxl

(Humboldt-Universität zu Berlin, Germany)

Monday,
June 1, 2015

16:30 – 17:00
HG F1

Essentially every new commercial product depends on new or improved materials. To identify such materials, computational approaches are increasingly employed, with millions of CPU hours spent every day and an enormous amount of data created. The goal of the Novel Materials Discovery (NoMaD) Project is not boosting more high-throughput calculations. The issue of NoMaD is: What to do with the data? In this talk, I will introduce the NoMaD Repository (https://nomad-repository.eu) that was established to host, organize, and share materials data, and I will demonstrate an example how big-data analytics based on statistical-learning approaches can lead to new insight into materials properties.

Co-Authors: **Luca M. Ghiringhelli** (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany); **Jan Vybiral** (Charles University, Czech Republic); **Sergey V. Levchenko** (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany); **Matthias Scheffler** (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany)

MS03

Data Assimilation and Predictive Models in the Earth Sciences

Organiser: *Christian Boehm (ETH Zurich, Switzerland)*
Co-organiser: *Andreas Fichtner (ETH Zurich, Switzerland);*
Dave A. May (ETH Zurich, Switzerland)

Nearly all fields in the Earth sciences combine numerical models and data measurements to infer unknown parameters or to predict the future state of a dynamical system. With the widespread availability of massively parallel supercomputers researchers can continually increase both the resolution and the physical complexity within their numerical models. By combining observations and model simulations, data assimilation offers a powerful tool to iteratively solve these systems, which may be highly nonlinear with extremely large numbers of unknowns. This minisymposium aims at discussing examples from various Earth science applications, including geodynamics, geomagnetism and seismic imaging.

Preconditioning Strategies for Multi-Parameter Full Waveform Inversion; Ludovic Métivier

(CNRS, France)

Monday, June 1, 2015

13:00 – 13:30
HG F3

Full Waveform Inversion (FWI) is a high-resolution seismic imaging method, based on the minimization of the misfit between observed and synthetic data. FWI is now routinely used in seismic exploration, as a velocity-building method. However, the formalism of FWI allows for the simultaneous reconstruction not only of P- and S-wave velocities, but also for parameters such as density, attenuation and anisotropy. This current limitation is due to trade-offs between parameters, making difficult to decipher between them only from seismic data. We propose to review and analyze the issues related to multi-parameter FWI, and propose a preconditioning strategy trying to mitigate these difficulties.

Co-Authors: **Romain Brossier** (University of Grenoble Alpes, France); **Stéphane Operto Géoazur** (University of Sophia-Antipolis, France); **Jean Virieux** (University of Grenoble Alpes, France)

Data Assimilation for Source Encoding Strategies in Full-Waveform Seismic Inversion; Christian Boehm

(ETH Zurich, Switzerland)

Monday, June 1, 2015

13:30 – 14:00
HG F3

Full-Waveform seismic tomography infers the material properties of the Earth based on the observation of seismograms. Since the costs of solving this inverse problem are roughly proportional to the number of seismic events, source-encoding strategies can reduce the computational effort substantially. We exploit statistical properties of a sample average approximation to gradually incorporate more information into the problem formulation and to update the weights of the encoded sources. This alternates with a Newton-type method based on mini-batch Hessian approximations to update the material model.

Co-Authors: **Andreas Fichtner** (ETH Zurich, Switzerland); **Alessandro Lechmann** (ETH Zurich, Switzerland)

Full Waveform Inversion for the Identifiable Subspace; Drosos Kourounis

(Università della Svizzera italiana, Switzerland)

Monday, June 1, 2015

14:00 – 14:30
HG F3

Full-waveform inversion (FWI) optimizes subsurface model estimates to derive high-fidelity geological models. A mathematically sound method is described for selecting the part of the geological parameters that is best identifiable from the seismic acquisition geometry. This is combined with either interior-point or sequential quadratic programming methods for performing FWI for the subset of parameters that have been characterized as identifiable. Numerical results are presented on several examples of increased complexity.

Co-Authors: **Olaf Schenk** (Università della Svizzera italiana, Switzerland)

A Data-Comprehensive Seismic Earth Model across the Scales; Michael Afanasiev

(ETH Zurich, Switzerland)

Monday, June 1, 2015

14:30 – 15:00
HG F3

The Comprehensive Seismic Earth Model (CSEM) is a 3D multi-scale visco-elastic model of Earth's interior. Designed to combat scaling issues in seismic inversion, the CSEM incorporates models generated from a variety of forward problem solvers, on a variety of spatial scales. Approaching global-scale seismic inversion in this manner allows us to exploit the benefits of both high resolution numerical techniques, such as full waveform inversion via the spectral element method, and more classical inversion techniques, such as traveltime tomography, where each may contribute model updates within their specific regimes of validity.

Co-Authors: **Andreas Fichtner** (ETH Zurich, Switzerland); **Daniel Peter** (ETH Zurich / Università della Svizzera italiana, Switzerland); **Korbinian Sager** (ETH Zurich, Switzerland); **Saulé Zukauskaité** (ETH Zurich, Switzerland); **Laura Ermet** (ETH Zurich, Switzerland)

Data Assimilation in Geodynamical Modelling: Methods and Applications; Alik Ismail-Zadeh

(Karlsruhe Institute of Technology, Germany)

Monday, June 1, 2015

15:30 – 16:00
HG F3

Present geophysical, geochemical, and geodetic observations together with geological information provide a clue to understanding dynamics of the Earth interior in the past. Assimilation of present observations allows to constrain mantle temperature/composition and flow in the past using dynamical models. Quantitative tools are required to assimilate the data and hence to solve inverse retrospective problems in geodynamics. The basic inversion methods (adjoint and quasi-reversibility) including the methodologies uncertainties and requirements for HPC, and two case studies related to mantle/lithosphere dynamics and to a volcanic lava flow will be presented and discussed.

Towards Joint Reconstruction of Paleo Mantle-Litho-Sphere Dynamics Using Data Assimilation; Nicolas Coltice

(Université Lyon 1, France)

Monday, June 1, 2015

16:00 – 16:30
HG F3

Data assimilation becomes suitable when the observations are sufficient in number and accurate enough, and if the forward model contains sufficient complexity to necessary for predictions. When it comes to reconstructing convection in the Earth's mantle, data assimilation raises questions for both observations and models. I will review inverse methods used so far, for which seismic tomography is central, and present another angle for data assimilation: using tectonic data as the data to match. I will describe preliminaries and present a sequential data assimilation scheme, and a variational data assimilation scheme, both using tectonic information as the data to match.

Data Assimilation and Predictive Models in Geomagnetism; Alexandre Fournier

(Institut de Physique du Globe de Paris, France)

Monday,
June 1, 2015

16:30 – 17:00
HG F3

Assimilating geomagnetic data in numerical models of Earth's core dynamics is a challenging problem, since the information contained in the geomagnetic record is intrinsically restricted to the large scales of the poloidal geomagnetic field at the core-mantle boundary. After a general introduction on terrestrial magnetism and the observation of Earth's magnetic field, I will report more specifically on recent efforts carried out to investigate the feasibility of resorting to three-dimensional, buoyancy-driven, numerical dynamo models for geomagnetic data assimilation practice. For this symposium, I will discuss in particular the computational cost associated with this exercise.

Co-Authors: **Julien Aubert** (Institut de Physique du Globe de Paris, France); **Lars Nerger** (Alfred Wegener Institute, Germany); **Sabrina Sanchez** (Institut de Physique du Globe de Paris, France)

On Ensemble and Particle Filters for Large-Scale Data Assimilation; Roland Potthast

(Deutscher Wetterdienst, Germany)

Monday,
June 1, 2015

17:00 – 17:30
HG F3

Ensemble data assimilation techniques are of rapidly growing importance. Ensemble techniques allow to describe and forecast uncertainty of the analysis, but they also improve the assimilation result itself, by allowing estimates of the covariance or, more general, the prior and posterior probability distribution of atmospheric states. In our talk, we will first give a survey about recent activities of the German Meteorological Service DWD. Then, we present recent work on the further development of the ensemble data assimilation towards a particle filter for large-scale atmospheric systems, which keeps the advantages of the LETKF, but overcomes some of its limitations.

Co-Authors: **Andreas Rhodin** (Deutscher Wetterdienst, Germany); **Christoph Schraff** (Deutscher Wetterdienst, Germany); **Hendrik Reich** (Deutscher Wetterdienst, Germany)

MS04

Fluid–Structure Interaction in the Cardiovascular System

Organiser: *Dominik Obrist (University of Bern, Switzerland)*
Co-organiser: *Simone Deparis (EPFL, Switzerland)*

The mechanical interaction between blood and soft tissue is a central mechanism in the cardiovascular system (e.g. heart valve dynamics, myocardial motion). A detailed understanding of these processes is the basis for the development of diagnostic methods, therapeutic devices and prostheses. To this end, large fluid-structure problems have to be solved accurately and efficiently on high-performance computing platforms with sophisticated numerical methods and with parallelization paradigms, which comply with large structural deformations and a range of inherent time scales. This minisymposium presents the work of leading groups in this field.

Numerical Modeling of the Fluid Dynamics in the Heart; Simone Deparis

(EPFL, Switzerland)

Monday, June 1, 2015

13:00 – 13:30
HG E21

The challenge of the modeling and simulation of blood flow dynamics in the heart and in the aortic root includes at least the following components: large deformations of the computational domain, opening and closing of the valves, interaction with the cardiac muscle, and changing flow regime. In this talk we focus mainly on the flow components. We first look at the flow in an idealized left ventricle. The flow is discretized by finite elements and stabilized by the variational multiscale method. The valve is modeled by a zero-dimensional resistance model. We then present a three-dimensional model for the leaflets. We conclude by showing simulations of blood flow in the aortic root.

Co-Authors: **L. Dede** (EPFL, Switzerland); **E. Faggiano** (Università di Pavia, Italy); **M. Fedele** (Università di Pavia, Italy); **A. Gerbi** (EPFL, Switzerland); **A. Quarteroni** (EPFL, Switzerland); **A. Tagliabue** (Politecnico di Milano, Italy)

Coupling in Vivo Human Mitral Valve to the Left Ventricle; Hao Gao

(University of Glasgow, United Kingdom)

Monday, June 1, 2015

13:30 – 14:00
HG E21

I will present an integrated model of mitral valve (MV) coupled with the left ventricle (LV) by using an immersed boundary method along with a finite element description of valvular and myocardial mechanics. The model is derived from clinical images and takes into account of the important valvular features, left ventricular contraction, nonlinear soft tissue mechanics, fluid structure interaction, and the MV-LV interaction. The integrated MV and LV model can simulate the cardiac function both in diastole and systole. Further work is required to ensure that the highly complex valvular-ventricular interaction, and the fluid-structure interaction, can be reliably represented.

Co-Authors: **Boyce E. Griffith** (University of North Carolina, USA); **Colin Berry** (University of Glasgow, United Kingdom); **Xiaoyu Luo** (University of Glasgow, United Kingdom)

Fluid-Structure Interaction Simulations of Heart Valves on Parallel Computing Clusters; Iman Borazjani

(University at Buffalo SUNY, USA)

Monday,
June 1, 2015

14:00 - 14:30
HG E21

We will discuss our new developments for simulating mechanical heart valves in left-ventricle geometries. Specifically, we discuss the development of a Newton-Krylov solver with an analytical jacobian, which has improved the performance of our flow solver on curvilinear grids by several folds, with parallel efficiency of 80-90%. Furthermore, we discuss advancements in parallelized implementation of platelet activation models into numerical simulations to quantify the probability of blood clot formation in heart valves. We present the results of our recent fluid-structure interaction simulations, and discuss the flow physics. Finally, we discuss our future plans to advance FSI simulations.

Co-Authors: **Hafez Asgharzadeh** (University at Buffalo, USA); **Mohammadali Hedayat** (University at Buffalo, USA)

HPC Framework for Aortic Valve Simulation with Hybrid Discretization for Fluid and Soft Tissue; Dominik Obrist

(University of Bern, Switzerland)

Monday,
June 1, 2015

14:30 – 15:00
HG E21

The numerical simulation of aortic valves is a multi-physics problem involving large deformations of soft tissue and transient vortical flow fields. Whereas soft tissue is most appropriately discretized on unstructured meshes in Lagrangian formulation, the three-dimensional flow field is discretized on a structured Cartesian grid to obtain an efficient implementation on modern HPC platforms. The tissue dynamics on the unstructured mesh and the flow on the structured grid are coupled with the immersed boundary method. The parallelization of such a hybrid discretization approach raises interesting questions with respect to data locality and load balancing under a domain decomposition paradigm.

Co-Authors: **Barna Becsek** (University of Bern, Switzerland)

MS05

HPC in Systems Biology

Organiser: *Manuel Peitsch (Philip Morris Int. & Swiss Institute of Bioinformatics, Switzerland)*

Systems Biology is a highly multidisciplinary approach to decoding life that combines computational with experimental methods to elucidate biological mechanisms and their dynamic behavior at all levels of biological organization. Systems Biology enables new approaches in pharmacology, toxicology, diagnostics, as well as drug development. The presentations will exemplify how computational Systems Biology can enable the understanding of biological systems both at the genomic and at the structural level, how mechanistic understanding is likely to change product risk assessment and how HPC will turn Big Data into knowledge about biological systems.

From Genomes to Systems Biology; Ioannis Xenarios

(Swiss Institute of Bioinformatics, Switzerland)

Monday,
June 1, 2015

13:00 – 13:30
HG E1.2

From the part list genes, proteins and chemical compounds to the complex dynamics of biological systems, computational approaches are critical. In this presentation I'll describe the challenges linking the genotypes to the phenotypes and the ability/inability to reconstruct what we understand of the biological system. I'll take examples in the field of immunology and more 'simple' model organism to explain the methodologies used to both characterize a system and also to predict novel regulations or unexpected combination of perturbation.

Big Data in Life Sciences: Harnessing Supercomputing to Make Big Data Accessible and Actionable; Matthias Reumann

(IBM Research, Switzerland)

Monday,
June 1, 2015

13:30 – 14:00
HG E1.2

Big data in life sciences is experiencing the perfect storm: The volume is increasing exponentially with accelerating speed, the variety of data ranges from multi-omics information to lifestyle measures with the help of mobile devices backed by cloud infrastructures. State of the art analytical methods are generally limited by computational approaches. The researcher is forced to limit their investigation to selected data rather than exhaustively mining the data. We have demonstrated that supercomputing methodologies enables discovery beyond traditional methods. Add cognitive computing to supercomputing and the perfect storm can be conquered.

Building Computable Biological Network Models and their Application to Product Risk Assessment; Julia Hoeng

(Philip Morris Int., Switzerland)

Monday,
June 1, 2015

14:00 – 14:30
HG E1.2

Systems Toxicology is aimed at decoding the toxicological blueprint of active substances that interact with living systems. It integrates classic toxicology with network models and quantitative measurements of molecular and functional changes across multiple levels of biological organization. It combines high content experimental data obtained with computational and mathematical sciences to identify Pathways of Toxicity and the Key Events in Adverse Outcome Pathways. These findings are applied to perform a mechanism-by-mechanism evaluation of the impact of products on these pathways. The presentation will focus on the computational aspects of Systems Toxicology and its applications.

Co-Authors: **Manuel C. Peitsch** (Philip Morris International, Switzerland)

Towards Computing Aerosol Flow and Exposure for In-Vitro Research Purposes; Arkadiusz Kuczaj

(Philip Morris Int. & University of Twente, Switzerland/Netherlands)

Monday,
June 1, 2015

14:30 – 15:00
HG E1.2

Systems Toxicology combines high content experimental data obtained at the molecular, cellular, organ, organism, and with computational and mathematical sciences aims to identify Pathways of Toxicity. Linking conditions occurring in a respiratory tract with those in the exposure systems requires detailed understanding of flow and deposition of aerosols. The presentation will showcase the application of Computational Fluid Dynamics in simulating flow in a human lung airway model and outlines opportunities for leveraging simulated data to develop well-designed in-vitro respiratory toxicology experiments that have the potential to allow in-vitro to in-vivo exposure extrapolations.

Co-Authors: **Markus Nordlund** (Philip Morris International, Switzerland)

MS06

Mathematical Aspects of Multi-Scale Methods in Computational Chemistry

Organiser: *Benjamin Stamm (Sorbonne Université, France)*

In the last decades, multi-scale strategies have been the object of a wide and fruitful development. Such methodologies, including QM/MM methods and QM/Continuum methods, allow to model different chemical parts with different accuracies in the description of a molecular system. For strongly inhomogeneous systems, as it is the case for biological environments, such techniques are extremely important resulting in a large variety of real-world applications at an affordable computational price. The scope of this mini-symposium is to bring chemists and mathematicians working on the methodological development of such methods together and foster this inter-disciplinary research field.

A Fast Domain Decomposition Algorithm for Continuum Solvation Models; Yvon Maday

(Université Pierre et Marie Curie, France)

Monday, June 1, 2015

13:00 – 13:30
HG E3

Continuum solvation models are nowadays among the most popular tools in computational chemistry to include the effects of the chemical environment in the description of a molecular property or process. The strength of these models is their simplicity of use and cost-effectiveness. Continuum solvation models have been used together with both classical molecular mechanics (MM), quantum mechanics (QM) and hybrid (QM/MM) levels of theory to describe the solute. In this talk, I will present the basics of an efficient, parallel, linear scaling implementation of the conductor-like screening model (COSMO), based on a domain decomposition algorithm adapted to the integral formulation of the problem.

Co-Authors: **Filippo Lipparini** (Université Pierre et Marie Curie, France); **Louis Lagardère** (Université Pierre et Marie Curie, France); **Benjamin Stamm** (Université Pierre et Marie Curie, France); **Eric Cancès** (École des Ponts ParisTech, France / INRIA, France); **Jean-Philip Piquemal** (Université Pierre et Marie Curie, France); **Benedetta Mennucci** (Università di Pisa, Italy)

High Performance Polarizable Molecular Dynamics; Jean-Philip Piquemal

(Université Pierre et Marie Curie, France)

Monday, June 1, 2015

13:30 – 14:00
HG E3

In this talk, I will present new advances in the development of scalable polarizable force fields for extensive molecular dynamics simulations. The discussed techniques are grounded on solid applied mathematic techniques enabling gain ranging from to 2 to 3 orders in magnitude in time thanks to parallelism. Potential applications will be discussed.

Extension and Implementation of Ewald-Based Methods for Classical Simulations of a Density-Based Force Field; G. Andres Cisneros

(Wayne State University, USA)

Monday, June 1, 2015

14:00 – 14:30
HG E3

We have developed a novel polarizable force field, called the Gaussian Electrostatic Model (GEM). GEM is designed to reproduce each term of the QM intermolecular interaction by fitting electronic densities using Hermite Gaussians. GEM enables the evaluation of intermolecular interactions for molecular systems with errors below chemical accuracy for each component, and provides a novel procedure to obtain distributed multipoles (GEM--DM). The use of Hermite Gaussian result in the need to evaluate a large number of two center (Coulomb and overlap) integrals. I will discuss the extension of two approximate Ewald methods (PME and FFP) to evaluate these integrals and timings for H2O.

Co-Authors: **Robert E. Duke** (Wayne State University, USA); **Oleg Starovoytov** (University of Houston, USA); **Jean-Philip Piquemal** (Université Pierre et Marie Curie, France)

Accelerated Dynamics in Molecular Simulations; Tony Lelièvre

(Ecole des Ponts, France)

Monday, June 1, 2015

14:30 – 15:00
HG E3

I will present multiscale-in-time strategies to accelerate molecular dynamics simulations. Starting from a metastable stochastic process, the idea is to use the underlying jump process between metastable states in order to accelerate exit events in a statistically consistent way. For example, it is possible to parallelize in time the integration of the dynamics. These ideas have been proposed A.F. Voter in the nineties, and their mathematical foundations have been recently understood thanks to the notion of quasi-stationary distribution.

Multi-Scale Exploration of Protein Interiors; Markus Meuwly

(University of Basel, Switzerland)

Monday,
June 1, 2015

15:30 – 16:00
HG E3

Proteins exhibit dynamics on multiple length scales. This presentation will highlight computational approaches to characterize such motions ranging from fully atomistic simulations to network simulations. The focus will be on small ligand diffusion in globular proteins which is of physiological significance.

Quantum Biochemistry; Jan H. Jensen

(University of Copenhagen, Denmark)

Monday,
June 1, 2015

16:00 – 16:30
HG E3

I will give an overview of my groups latest work in applying quantum chemistry to biochemical problems such as enzyme catalysis, enzyme design, protein-ligand binding and protein structure determination by NMR.

Multi-Scale Modeling Techniques for the Exploration of Complex Systems: Polypeptides, Crystals, and Quantum Systems; Mark Tuckerman

(New York University, USA)

Monday,
June 1, 2015

16:30 – 17:00
HG E3

I will discuss our recent advances in the development of multi-scale approaches for studying complex condensed-phase systems. For polypeptide and crystal structure prediction, I will discuss heterogeneous multi-scaling techniques we have introduced for the exploration of high-dimensional free energy surfaces. A two-part strategy will be described wherein landmark features of the surface, i.e., minima and saddles, are first identified and then fed into an enhanced sampling scheme for generating free energy differences. I will then discuss our attempts to combine adaptive resolution techniques with the Feynman path integral for treating systems in which nuclear quantum effects are important.

Tensor Product Approximation and Tensor Networks for Many Particle Schrödinger Equation; Reinhold Schneider

(Technische Universität Berlin, Germany)

Monday,
June 1, 2015

17:00 – 17:30
HG E3

Hierarchical tensor formats and tensor trains introduced recently in numerical analysis have the same parametrization as tree tensor networks and matrix product states. These representations offer stable and robust approximation of high-order tensors and multi-variate functions by a low order cost. For many high dimensional problems, including many body quantum mechanics, uncertainty quantification etc., this approach has a certain potential to circumvent from the curse of dimensionality. For numerical computations, the groundstate computation can be cast into optimization problems constraint by restricting to set of d tensors of bounded multilinear ranks.

Co-Authors: **Max Pfeffer** (Technische Universität Berlin, Germany)

MS07

Modeling and Simulation in Geo-Energy and Hydro-Power

Organiser: *Rolf Krause (Università della Svizzera italiana, Switzerland)*
Co-organiser: *Thomas Driesner (ETH Zurich, Switzerland)*

Mathematical modeling and numerical simulation are of fundamental importance for the development of new and innovative technologies in the energy sector. In this minisymposium, we focus on the exchange of methods, concepts and ideas in modeling and simulation of complex application problems from the two areas geo-energy and hydro-power. This includes the efficient numerical solution of coupled nonlinear systems, or problems involving interface effects and highly complex geometries.

Modeling of Inelastic Strain Induced by CO2 Injection; Victor Vilarrasa

(EPFL, Switzerland)

Monday, June 1, 2015

13:00 – 13:30
HG E22

Inelastic strain, which is associated to the induced microseismicity observed in CO2 injection sites like Weyburn or In Salah, is likely to occur in CO2 storage sites. Furthermore, CO2 will reach the storage formation at a colder temperature than the rock, which will induce a thermal stress reduction. We model non-isothermal injection of CO2 in a deep saline formation using the fully coupled finite element code CODE_BRIGHT. We find that despite inelastic strain is likely to occur in the cooled region around the injection well, fracture propagation does not extend into the caprock in the normal faulting stress regime simulated in this study.

Co-Authors: **Lyesse Laloui** (EPFL, Switzerland)

CFD Computations of a Cavitation Vortex Rope; Jean Decaix

(HES-SO//Valais-Wallis, Switzerland)

Monday, June 1, 2015

13:30 – 14:00
HG E22

Due to the increase in renewable energies in the electricity market, hydraulic power plants have to run at off-design operating points. For Francis turbines, this leads to the formation of a vortex rope known to promote cavitation surge. If the flow discharge is higher than the nominal one, an axisymmetric cavitation vortex rope develops in the draft tube cone. Such a vortex rope leads to high-pressure fluctuations that interact with the entire power plant and limit the range of operating points. To better understand the physics of the phenomenon and to provide input to 1D models, two-phase 3D CFD calculations are performed and compared with experimental data.

Co-Authors: **Sebastien Alligné** (Power Vision Engineering Sàrl, Switzerland); **Andres Müller** (EPFL, Switzerland); **Cécile Münch** (HES-SO//Valais-Wallis, Switzerland); **François Avellan** (EPFL, Switzerland)

Challenges of Simulating Geothermal Reservoir Processes; Thomas Driesner

(ETH Zurich, Switzerland)

Monday, June 1, 2015

14:00 – 14:30
HG E22

Future geothermal power production in Switzerland requires circulating water through deep (~ 5km), fractured rock masses at temperatures exceeding 180°C. The extreme conditions massively limit direct, in situ observation and steering of reservoir processes, making numerical simulation a key research and development technology. The biggest challenges are a combination of complex but poorly know geometries (thin, irregular fracture networks in a large rock mass) and strongly coupled, non-linear processes (thermo-hydro-mechanical-chemical interactions). This contribution outlines the goals and challenges of numerical code development in the SCCER-SoE and related initiatives.

A New Volcanic Hydrothermal System in Java; the Lusi Mud Eruption and Aftermath; Stephen Miller

(University of Neuchatel, Switzerland)

Monday, June 1, 2015

14:30 – 15:00
HG E22

In 2006 a magnitude 6.3 earthquake occurred in Yogyakarta on the island of Java. This relatively shallow earthquake resulted in 20,000 deaths and widespread destruction of the city. About 48 hours later, in the town of Sidoarjo about 250 km from the earthquake epicentre, mud began to spill out onto the surface and Lusi was born. Eruption rates peaked at 180,000 cubic meters of mud per day, and continues today as a vigorous geyser system, with geochemistry studies showing that is a geologic rarity of a newborn tectonic-scale hydrothermal system linked to the nearby volcano complex. We are modelling this system to gain insight of its workings and the possible exploitation of geothermal energy.

Co-Authors: **Maïté Faubert** (University of Neuchatel, Switzerland); Reza Sohrabi (University of Neuchatel, Switzerland)

Modeling 3D THM Processes in Geothermics with Continuum Mechanics; Gunnar Jansen

(University of Neuchatel, Switzerland)

Monday, June 1, 2015

15:30 – 16:00
HG E22

The geothermal community is challenged by the Energy Strategy 2050 goal to uncover the potential of renewable energy resources in Switzerland. To this end we implement a novel finite element based simulation tool for rock and fluid physics. It efficiently couples the dominant processes in the subsurface, such as fracture nucleation and growth using continuum mechanics, anisotropic multiphase fluid flow and heat transfer to provide a deeper understanding. We aim at state of the art performance by using massively parallel tools and modern accelerator techniques. We present first results from 3D fully coupled THM-simulations and evaluate the performance from a series of benchmark simulations.

Co-Authors: **Reza Sohrabi** (University of Neuchatel, Switzerland); **Boris Galvan** (University of Neuchatel, Switzerland); **Stephen A. Miller** (University of Neuchatel, Switzerland)

Prediction of Elastostatic Friction for Rock-Like Surfaces with FEM; Alessandro Rigazzi

(Università della Svizzera italiana, Switzerland)

Monday, June 1, 2015

16:00 – 16:30
HG E22

We present the results of our recent work, in which we apply the Finite Element Method to study the frictional forces resulting from the elastostatic interactions of surface asperities. To do this, we generate several self-affine rough surfaces that are statistically similar to rock surfaces. Such surfaces are used as rigid obstacles onto which an elastic smooth cube is pushed and sheared to measure the maximal resistance opposed by the asperities. The contact problem gives rise to a huge nonsmooth system of equations. We solve this system with a solver based on our nonsmooth multigrid algorithm of optimal complexity for which we investigate scaling properties.

Co-Authors: **Rolf Krause** (Università della Svizzera italiana, Switzerland)

Modeling Induced Seismic Hazard During Geothermal Reservoir Creation; Joseph Doetsch

(ETH Zurich, Switzerland)

Monday,
June 1, 2015

16:30 – 17:00
HG E22

To enable the large-scale exploitation of deep geothermal energy for electricity generation in Switzerland, solutions must be found for two fundamental and coupled problems: (1) How to create an efficient heat exchanger in the hot underground that can produce energy for decades and (2) at the same time keeping the risk posed by induced earthquakes to acceptable levels' Numerical simulations of different complexity and physical detail are currently being developed for an Advanced Traffic Light System (ATLS) to predict the risk of in induces earthquakes in real-time. This contribution presents developments of the induced seismicity prediction codes towards high performance computing.

Co-Authors: **Valentin Gischig** (ETH Zurich, Switzerland); **Dimitrios Karvounis** (ETH Zurich, Switzerland); **Stefan Wiemer** (ETH Zurich, Switzerland)

Silt Erosion Simulation Using Finite Volume Particle Method; Ebrahim Jahanbakhsh

(EPFL, Switzerland)

Monday,
June 1, 2015

17:00 – 17:30
HG E22

Silt erosion is a destructive phenomenon that may occur in hydropower plants. This work presents a new erosion prediction model in which, fluid flow and solid deformation equations are discretized by Finite Volume Particle Method (FVPM), and silt contact forces are calculated according to Hertz contact theory. FVPM is a meshless method, which includes many of the desirable features of the mesh-based finite volume method. To obtain a more accurate and robust model, a new FVPM formulation is presented in which particle interaction integrals are evaluated exactly and efficiently. To validate the new silt erosion model, 2D and 3D erosion cases are simulated and compared with experimental data.

MS08

Scientific Libraries/Frameworks in Japan for Future HPC Systems

Organiser: *Kengo Nakajima (The University of Tokyo, Japan)*

Reliable software is the key technology for future HPC systems. In 2010, 'Development of System Software Technologies for Post-Peta Scale HPC (Post-Peta CREST)' was initiated by the Japan Science & Technology Agency. It aims at developing software exploiting maximum efficiency and reliability on future HPC systems in late 2010s. It includes 14 projects, which cover a wide range of research areas in software for HPC, such as system software, programming languages, compilers, numerical libraries, and application frameworks. This minisymposium offers an overview of recent activities of four projects in Post-Peta CREST related to scientific computing, and discusses future international/interdisciplinary collaborations.

ppOpen-HPC: Open Source Infrastructure for Development and Execution of Large-Scale Scientific Applications on Post-Peta Scale Supercomputers with Automatic Tuning (AT); Kengo Nakajima

(The University of Tokyo, Japan)

Monday,
June 1, 2015

13:00 – 13:30
HG F30

In this presentation, recent achievements and progress of the "ppOpen-HPC" project are discussed. ppOpen-HPC is an open source infrastructure for development and execution of optimized and reliable simulation code on post-peta-scale (pp) parallel computers based on many-core architectures with automatic tuning (AT), and it consists of various types of libraries, which cover general procedures for scientific computation. An example of automatic tuning by ppOpen-AT on 3D FDM code of seismic simulations (Seism3D) will be discussed. Moreover, recent achievements in the development of ppOpen-MATH/MG, which is a geometric multigrid solver in ppOpen-HPC, will be also presented.

Co-Authors: **Takahiro Katagiri** (University of Tokyo, Japan)

Domain-Specific Approaches in Scientific Computing; Naoya Maruyama

(RIKEN, Japan)

Monday,
June 1, 2015

13:30 – 14:00
HG F30

Parallel programming with low-level interfaces has been the most viable choice in scientific computing for a long time. In such models, different parallelisms require different parallel programming interfaces, e.g., message passing for parallelism across nodes, threading for intra-node parallelism, and vector processing for SIMD and GPUs. Often applications are confronted with these multiple interfaces to fully exploit the current and future large-scale machines. We present our work toward higher-level programming models, allowing for a single program to run on different parallel platforms without much human intervention, and at the same time to achieve close to hand-tuned performance.

A Scalable Parallel Eigensolver for Large-Scale Simulations in Post-Peta Scale Environments; Tetsuya Sakurai

(University of Tsukuba, Japan)

Monday, June 1, 2015

14:00 – 14:30
HG F30

Large-scale eigenvalue problems arise in wide variety of applications such as nano-scale materials simulation, vibration analysis of automobiles, big data analysis, etc., and high performance solvers are required to exploit distributed parallel computing environments. In this talk, we present a contour-integral based parallel eigensolver for interior eigenvalue problems. This method has a good parallel scalability according to a hierarchical structure of the method. We also present some efficient implementations of the method for large-scale simulations. We show performance evaluations on state-of-art supercomputers with some applications.

Co-Authors: **Yasunori Futamura** (University of Tsukuba, Japan); **Akira Imakura** (University of Tsukuba, Japan)

Development of a Numerical Library Based on Hierarchical Domain Decomposition; Daisuke Tagami

(Kyushu University, Japan)

Monday, June 1, 2015

14:30 – 15:00
HG F30

We have been developing an open source system software, ADVENTURE, which is a general-purpose parallel finite element analysis system and can simulate a large-scale analysis model with supercomputer like K-computer. In the system, HDDM (hierarchical domain decomposition method), which is a very effective technique to large-scale analysis, was developed. The aim of this project is to develop a numerical library based on HDDM that is extended to pre and post processing parts, including mesh generation and visualization of large-scale data, for the Post Petascale simulation.

Co-Authors: **Masao Ogino** (Nagoya University, Japan); **Hiroshi Kawai** (The University of Toyo, Japan); **Yasuhi Nakabayashi** (The University of Toyo, Japan)

MS09

Abstractions Interplay in Domain Frameworks to Tackle Heterogeneity

Organiser: *Anshu Dubey (Lawrence Berkeley National Laboratory, USA)*
Co-organiser: *Brian Van Straalen (Lawrence Berkeley National Laboratory, USA)*

Current generation of domain frameworks have componentization and composability implemented in a stable and portable programming model as their primary abstractions. As platforms began to become heterogeneous some domain frameworks added abstractions to tackle the performance-portability trade-offs, for which the current best practices are no longer adequate. However, there is a growing separation between the shortening life-cycles for future programming models and the life-cycle of a community software framework. This minisymposium seeks to collect and document the abstraction-lifting efforts of multiphysics frameworks with a hope of starting the discussion for closing this gap.

Tiling Abstraction for Data-Centric Computing; Didem Unat

(Koc University, Turkey)

Monday, June 1, 2015

15:30 – 16:00
HG E1.2

Programming models play a crucial role in providing the necessary tools to express locality and minimize data movement, while also abstracting complexity from programmers. Unfortunately, existing compute-centric programming environments provide few abstractions to manage data movement and locality, and rely on a large shared cache to virtualize data movement. We propose three programming abstractions, tiles, layout and loop traversal that address data locality and increased parallelism on emerging parallel computing systems. The TiDA library implements these abstractions in the data structures through domain decomposition and provides performance portable codes.

Co-Authors: **Tan Nguyen** (Lawrence Berkeley National Laboratory, USA); **Weiqun Zhang** (Lawrence Berkeley National Laboratory, USA); **John B. Bell** (Lawrence Berkeley National Laboratory, USA); **John Shalf** (Lawrence Berkeley National Laboratory, USA)

Using Abstractions in Heterogeneous Architectures for Scalable Thermal Radiation Calculations with AMR and the Uintah Framework; Martin Berzins

(University of Utah, USA)

Monday, June 1, 2015

16:00 – 16:30
HG E1.2

The use of abstractions in achieving performance portability for challenging petascale and beyond calculations is considered in the context of the Uintah framework applied to an engineering design study with one trillion variables that concerns a large 6000 cubic M clean coal-boiler currently under design for power generation. The role of task-based abstractions, runtime systems and portable execution layers such as Kokkos will be explored on heterogenous architectures consisting of CPUs GPUs and Xeon Phis. The success of this approach will be demonstrated through scalability results involving the most challenging part of the calculation involving a thermal radiation calculation that coupled all variables.

The GROMACS Road to Performance-Portable Programming Abstractions; Mark Abraham

(KTH, Sweden)

Monday, June 1, 2015

16:30 - 17:00
HG E1.2

Scientists' computing resources are often both scarce and expensive, so high absolute performance is an ongoing key development objective for the GROMACS molecular simulation package. The increasingly wide range and heterogeneity of HPC hardware adds considerably to this challenge, and doubly so when such high portability is also required. It is critical to choose algorithms that match the hardware well. It is also necessary to implement them via abstractions appropriate to the computational task at hand, if we are to do so for reasonable development costs. This talk will discuss recent work in GROMACS that lifts the abstraction level to permit ongoing high performance and high portability.

Co-Authors: **Roland Schulz** (Oak Ridge National Laboratory, USA); **Teemu Murtola** (Royal Institute of Technology, Sweden); **Berk Hess** (Royal Institute of Technology, Sweden); **Erik Lindahl** (Royal Institute of Technology, Sweden)

STELLA: Optimization of the COSMO Dynamical Core for Heterogeneous Platforms; Carlos Osuna Escamilla

(ETH Zurich, Switzerland)

Monday, June 1, 2015

17:00 – 17:30
HG E1.2

Regional weather and climate models typically solve Partial Differential Equations (PDEs) using compact stencils on structured grids. STELLA (Stencil Loop Language) is a DSL written in C++ for such stencil computations. It abstracts the underlying programming models and optimization techniques (loop tiling, loop fusion) for multiple hardware architectures. The STELLA language allows to describe stencils with a unique source code in a concise way, close to the mathematical description of the PDEs. We present the STELLA syntax and the performance results achieved for the dynamical core of an important community code (COSMO) for GPU (5.8x speedup) and CPU (1.8x speedup).

Co-Authors: **Tobias Gysi** (ETH Zurich, Switzerland); **Oliver Fuhrer** (MeteoSwiss, Switzerland); **Thomas Schulthess** (CSCS / ETH Zurich, Switzerland)

MS10

Emerging Applications of Computation in Economics

Organiser: *Simon Scheidegger (University of Zurich, Switzerland)*
Co-organiser: *Kenneth L. Judd (Stanford University, USA)*

Clearly, the world economy is an extremely complex system. Even when modeling only the most relevant features of a small part of this system, one easily ends up with a large and intricate formal structure. A further complication stems from the fact that human beings choose their actions based on expectations about an uncertain future. This feedback from the future makes economic modeling particularly difficult. This symposium provides an overview of recent developments in how state-of-the art computational economical modeling tackles these issues in the fields of macroeconomics, optimal taxation, game theory, climate change, and growth models.

An Agenda for Bringing Computational Science to Economics; Kenneth Judd

(Stanford University, USA)

Monday,
June 1, 2015

15:30 – 16:00
HG F30

Computational science is becoming the third pillar of science. Unfortunately, economics still largely relies on only two pillars - theory and observations. This can change but only after identifying the mathematical and computational methods that match the needs of economic modeling. I will point to the unique features of economics modeling, and illustrate how a combination of computational tools can be used to address a policy issue in the area of climate change.

Generational Policy and Aging in Closed and Open Dynamic General Equilibrium Models; Laurence Kotlikoff

(Boston University, USA)

Monday,
June 1, 2015

16:00 – 16:30
HG F30

This talk will review my recent co-authored work on generational policy and aging in closed and open dynamic general equilibrium models.

Does it Pay to Get a Reverse Mortgage?; Valentina Michelangeli

(Bank of Italy, Italy)

Monday, June 1, 2015

16:30 – 17:00
HG F30

This paper uses data on single households from the Health and Retirement Study (HRS) to study the economic gains or losses associated with reverse mortgages. These data are examined within a dynamic structural life-cycle model featuring consumption, housing, and mobility decisions with uncertainty about both life span and mobility. I develop and apply new methods for solution and estimation based on a combination of four state-of-the-art mathematical programming tools. I find that reverse mortgages provide liquidity and a form of longevity insurance; however, moving becomes a risky proposition.

DYNARE, a Toolbox for Solving and Estimating DSGE Models; Michel Juillard

(Banque de France, France)

Monday, June 1, 2015

17:00 – 17:30
HG F30

Dynare is a software tool to solve, simulate and estimate dynamic stochastic general equilibrium models. This requires heavy use of numerical methods: such as solving large sparse complementarity problems, function approximation with the perturbation approach or MCMC simulation of the posterior density. Dynare rests on a strict separation of the specification of a particular model and the use of standard software tools implied the development of a specificmodeling language. The numerical routines are provided as a Matlab/Octave toolbox. Dynare is open source so as to make used algorithms transparent. Challenges ahead include occasionally binding constraints and large shocks.

Scalable High-Dimensional Dynamic Stochastic Economic Modeling; Simon Scheidegger

(University of Zurich, Switzerland)

Tuesday, June 2, 2015

10:30 – 11:00
HG F1

I will present a highly parallelizable and flexible computational method to solve high-dimensional stochastic dynamic economic models. Solving such models often requires the use of iterative methods, like dynamic programming. The solution method I will present includes the use of a fully adaptive sparse grid algorithm and the use of a mixed MPI-Intel TBB-CUDA/Thrust implementation to improve the interprocess communication strategy on massively parallel architectures. Numerical experiments on 'Piz Daint' (Cray XC30) at the Swiss National Supercomputing Centre show that high-dimensional international real business cycle models up to at least 50 countries can be solved efficiently.

Co-Authors: **Johannes Brumm** (University of Zurich, Switzerland); **Dmitry Mikushin** (Università della Svizzera italiana, Switzerland); **Olaf Schenk** (Università della Svizzera italiana, Switzerland)

Dynamic Oligopoly with Uncertain Demand; Sevin Yeltekin

(Carnegie Mellon University, USA)

Tuesday, June 2, 2015

11:00 – 11:30
HG F1

The evolution of strategic interaction, competition, and market power have been some of the central issues in the field of industrial organization. However, most of the analysis has been confined to simplified models since solving dynamic models with heterogenous firms, market entry and exit, investment are quite difficult. In this paper we introduce a numerical method for computing equilibria of dynamic multi-firm competition game with endogenous productivity, uncertain demand and entry/exit.

Solving Optimal Taxation Models through Scalable, Reusable Simulation; Jeremiah Bejarano

(University of Chicago, USA)

Tuesday, June 2, 2015

11:30 – 12:00
HG F1

Mirrlees (1971) first formulated optimal taxation of a heterogeneous population as the solution to a bi-level optimization problem. This formulation is practical to solve only when people differ in a single dimension. The multidimensional problem lacks an organizing principle to simplify an otherwise enormous number of constraints, and solutions often do not satisfy constraint qualification. We present a method to circumvent these issues by decomposing the problem into two steps: one-time creation of a reusable sample of the impacts of various policies, and a quick search that takes an interchangeable distribution function over the heterogeneity and finds the corresponding optimal policy.

Co-Authors: **Christian Baker** (Brigham Young University, USA); **Richard W. Evans** (Brigham Young University, USA); **Kenneth L. Judd** (Stanford University, USA); **Kerk L. Phillips** (Brigham Young University, USA)

Polynomial Problems in Economics; Karl Schmedders

(University of Zurich, Switzerland)

Tuesday, June 2, 2015

12:00 – 12:30
HG F1

Economic models frequently lead to polynomial systems of equations or polynomial optimization problems. Although the literature on computational algebraic geometry has made great progress in solving polynomial systems of equations and polynomial optimization problems, many difficulties remain. In particular, currently we can only solve rather small problem instances on computers. In this talk, we will review some economic applications of polynomial methods and discuss some current technical limitations.

MS11

Large-Scale Scientific Computing with Julia

Organiser: *Lars Ruthotto (Emory University, USA)*
Co-organiser: *Eldad Haber (University of British Columbia, Canada)*

Julia is a new and emerging dynamic high-level programming language designed for high performance computing. Julia enables rapid development of expressive and easily extensible code and therefore becomes increasingly popular in science and engineering. It overcomes some limitations often associated with established dynamic languages, most importantly, large computational overhead and imperfect scaling on parallel computers. This mini symposium contains examples that outline Julia's potential for the solution of large-scale real-world problems.

A Subglacial Hydrology Model Embedding a 1D Channel Network in a 2D Model-Domain; Mauro Werder

(University of Zurich, Switzerland)

Monday, June 1, 2015

15:30 – 16:00
HG E21

I present the Julia implementation of GlaDS, a Glacier Drainage System model. It simulates the water flow at the ice-bedrock interface underneath a glacier or ice sheet, both in a channelized and a diffusive macro-porous system. Its most innovative feature is that the strictly 1D channel equations are embedded into the 2D model-domain by simulating them on the edges of the numerical grid. The equations are a non-linear reaction-diffusion equation coupled to two local ODEs. The model uses finite elements combined with a Rosenbrock-W time stepper. I will review some of the code in detail and highlight Julia specific implementation strategies, such as algebraic datatypes and multiple dispatch.

StochJuMP - Parallel Algebraic Modeling for Stochastic Optimization in Julia; Cosmin Petra

(Argonne National Lab, USA)

Monday, June 1, 2015

16:00 – 16:30
HG E21

We present scalable algebraic modeling software, StochJuMP, for stochastic optimization as applied to power grid economic dispatch. It enables the user to express the problem in a high-level algebraic format with minimal boiler-plate and allows efficient parallel model instantiation across nodes and efficient data localization. Computational results on up to 2048 cores of the Blues cluster of Argonne National Laboratory are presented showing that the model construction is both efficient and scalable. StochJuMP is configured with the parallel interior-point solver PIPS-IPM but is sufficiently generic to allow straightforward adaptation to other solvers.

Co-Authors: **Joey Huchette** (Massachusetts Institute of Technology, USA); **Miles Lubin** (Massachusetts Institute of Technology, USA)

On the Solution of Large-Scale Inverse Problems that "Cannot be Solved"; Eldad Haber

(University of British Columbia, Canada)

Monday, June 1, 2015

16:30 – 17:00
HG E21

Many problems in earth science involve with the solution of inverse problems on very large domains and with multiple sources and frequency. Solving such problems was considered to be impossible until recently. In this talk we explore algorithmic and software development that enable the solution of these problems. First, we explore the use of adaptive mesh refinement coupled with the use of direct solvers. Second, we discuss the use of stochastic programming techniques and finally we discuss the parallelization of the algorithm using Julia. We use the controlled source EM as a model problem and demonstrate how it can be solved using the above techniques.

Co-Authors: **Lars Ruthotto** (Emory University, USA)

Distributed and Parallel Algorithms for PDE Constrained Optimization in Julia; Lars Ruthotto

(Emory University, USA)

Monday, June 1, 2015

17:00 – 17:30
HG E21

This talk presents a Julia framework for the solution of large-scale PDE constrained optimization problems. It is based on a discretize-then-optimize approach, uses a (projected) Gauss-Newton method, and provides interfaces state-of-the-art linear solvers (both explicit and iterative). The framework uses Julia's potential for parallel and distributed computation. Being written in a dynamic language, it is easily extendable and yet fast as it will be outlined for a large electromagnetic test problem.

Co-Authors: **Eldad Haber** (University of British Columbia, Canada)

MS12

Bayesian Life Sciences Models

Organiser: *Linda Dib (University of Lausanne, Switzerland)*
Co-organiser: *Xavier Meyer (University of Lausanne, Switzerland; Swiss Institute of Bioinformatics, Switzerland; University of Geneva, Switzerland)*

The development of Bayesian methods in health sciences and biology has increased tremendously over the past decades since they learn about the data by exploring different hypothesis based on a priori knowledge. These models are computationally demanding and may require several million of iterations to reach convergence. Very few algorithms have explored the possibilities of using HPC approaches to speed up Bayesian methods. In this meeting we aim to provide an opportunity to bring together world experts in the fields of Bayesian statistics and HPC, to discuss the potential of new methodologies, and to investigate how to build Bayesian models that meet HPC platform requirements.

Bayesian Model for Decoding Organizational Principles of the Brain Anatomy; Lester Melie-Garcia

(Centre Hospitalier Universitaire Vaudois, Switzerland)

Tuesday,
June 2, 2015

10:30 – 11:00
HG E21

A Bayesian Model is proposed as framework to decode the organizational principles of the brain anatomy. This problem aims at investigating how tissue properties ('trait') in the brain manifold predict 'states' represented by clinical variables. Our Bayesian Model deals with the problem of mapping thousands of multivariate variables to a small dimensional space having different sets of data informing the same model. We used the idea of 'Streaming Variational Bayes' approach based on different model evidences to tackle this difficulty. This framework is ideal when Neuroimaging data coming from different Hospitals are not allowed to be used due to confidentiality reasons.

Co-Authors: **Ferath Kherif** (Centre Hospitalier Universitaire Vaudois, Switzerland)

Efficient Approaches to Model Evolution in Computational Biology; Nicolas Salamin

(University of Lausanne, Switzerland)

Tuesday,
June 2, 2015

11:00 – 11:30
HG E21

Biological modeling is important to study the evolution of genes and organisms. The increased availability of genomic data is pushing for the development of HPC approaches to model evolutionary processes. The availability of Bayesian approaches has been essential to extend the realism of the evolutionary models. The development of these methods based on MCMC techniques is computationally intensive and requires HPC approaches to deal with the computational complexity. I will present recent work to optimize and parallelize MCMC techniques. I will discuss our efforts to extend modeling of adaptation from genomic data to complex phenotypic traits using hierarchical Bayesian computations.

Bayesian Model in Medical Sciences; Linda Dib

(University of Lausanne, Switzerland)

Tuesday,
June 2, 2015

11:30 – 12:00
HG E21

Coevolving sites play a critical role the structure and function of a protein. I have recently developed two methods for the detection of such signature. The first method is a combinatorial and compares the homologous sequences whereas the other method is probabilistic and looks for the evolution of amino acids along the specie tree. The latter was implemented in a ML and Bayesian framework. I applied both methods on a large set of proteins. Among these proteins, I took particular care to analyze the Amyloid B protein that is implied in Alzheimer disease. The method revealed that well-known fragments of the protein are co-evolving revealing an evolutionary signature in this protein.

A Bayesian MCMC Method to Estimate Selection Coefficients from Mutagenesis Experiments: Insights in to Adaptation; Claudia Bank

(EPFL, Switzerland)

Tuesday,
June 2, 2015

12:00 – 12:30
HG E21

With the advent of next-generation sequencing technologies and advances in bioengineering, the field of experimental evolution is developing novel approaches that allow for unique opportunities to study adaptation. In particular, genetic mutations can be systematically engineered and tracked in bulk population competitions, allowing for the simultaneous assessment of hundreds of mutational effects. Here, we present a Bayesian Monte Carlo Markov Chain approach that allows for the estimation of fitness effects and experimental power from such large-scale data. Results are presented in the framework of classical evolutionary models, many of which can now be experimentally evaluated.

Co-Authors: **Sebastian Matuszewksi** (EPFL, Switzerland); Jeffrey D. Jensen (EPFL, Switzerland)

MS13

Increasing Computational Efficiency for Temporal Integration

Organiser: *Michael Minion (Lawrence Berkeley National Laboratory, USA)*
Co-organiser: *Daniel Ruprecht (Università della Svizzera italiana, Switzerland);*
Marcus Grote (University of Basel, Switzerland);
Rolf Krause (Università della Svizzera italiana, Switzerland)

The temporal integration of ordinary or partial differential equations is a fundamental computational problem in many application areas such as molecular dynamics, weather and climate, structural mechanics, combustion, cosmology, and many others. This minisymposium will present innovative strategies for realizing better computational efficiency in cases where the temporal direction creates a computational bottleneck. Topics include exploiting disparate time scales in the governing equations, applying techniques from multigrid in the time direction, and using time parallel algorithms like parareal and PFASST.

Multirate Infinitesimal Step Methods for the Compressible Euler Equations; Joerg Wensch

(Technische Universität Dresden, Germany)

Tuesday,
June 2, 2015

10:30 – 11:00
HG E22

The simulation of atmospheric dynamics relies on the numerical solution of the Euler equations. We consider here sound-advection systems for stratified fluids. These systems exhibit wave type solutions, which impose CFL-based restrictions on the time step size. Buoyancy, sound and advection cause separate restrictions each on their own scale. We develop Finite Volume Methods where a splitting approach allows different treatment of fast and slow waves. The methods are optimized with respect to order and maximum stable CFL numbers. Different scenarios for the scales of sound and advection are discussed.

Co-Authors: **Oswald Knoth** (Leibniz Institute of tropospheric research, Germany)

Adaptive Inexact Spectral Deferred Correction Methods for Long-Time Integration; Sunayana Ghosh

(Zuse Institute Berlin, Germany)

Tuesday,
June 2, 2015

11:00 – 11:30
HG E22

Inexact spectral deferred correction (SDC) method for solving non-stiff initial value problems (IVPs) are addressed. In many IVPs the approximate evaluation of the right hand side (rhs) is obtained much faster. This allows us to exploit the trade-off between accuracy and computational cost in evaluation of rhs. Error propagation in the SDC method is studied to obtain expressions of global errors w.r.t. local errors. Work models relating local errors to computational costs are derived. Error and work models are combined to obtain an adaptive tolerance selection by minimizing total work. Inexact SDC is then tested on long-time integration of damage evolution in oscillatory fatigue problems.

Co-Authors: **Martin Weiser** (Zuse Institute Berlin, Germany)

High-Order Temporal Integration Methods for Schroedinger Equations; Michael Minion

(Lawrence Berkeley National Laboratory, USA)

Tuesday, June 2, 2015

11:30 – 12:00
HG E22

I will report on the construction of a temporal integration scheme designed to be used with a higher-order finite-difference spatial approximation to the nonlinear Schroedinger equation with perfectly matched layer boundary conditions for the paraxial wave equation. The temporal method is based on a semi-implicit spectral deferred corrections approach coupled with an alternating direction implicit (ADI) approximation to the (linear) implicit terms. The accuracy and efficiency of the methods, as well as a discussion of space-time parallelization of the method will be presented.

Co-Authors: **Jeffrey Banks** (Rensselaer Polytechnic Institute, USA)

Load-Balanced Local Time Stepping for Large-Scale Wave Propagation; Max Rietmann

(ETH Zurich, Switzerland)

Tuesday, June 2, 2015

12:00 – 12:30
HG E22

Applications using finite element meshes often require regions of refinement to honor small-scale features. These localized smaller elements create a bottleneck for explicit time-stepping schemes due to the Courant-Friedrichs-Lewy stability condition. Recently developed local time stepping (LTS) algorithms reduce the impact of these small elements by locally adapting the time-step size to the size of the element. The multi-level nature of LTS introduces a strong load imbalance across processors. We examine the use of multi-constraint graph and hypergraph partitioning tools to achieve effective, load-balanced parallelization for CPUs and GPUs implemented in the seismology package SPECFEM3D.

Co-Authors: **Marcus Grote** (University of Basel, Switzerland); **Daniel Peter** (Università della Svizzera italiana, Switzerland); **Bora Ucar** (INRIA, France); **Olaf Schenk** (Università della Svizzera italiana, Switzerland)

Numerical Simulation of Skin Transport using Parareal; Rolf Krause

(Università della Svizzera italiana, Switzerland)

Tuesday, June 2, 2015

13:30 – 14:00
HG E22

The talk will present recent results on the applicability of the time-parallel Parareal algorithm to the in-silico modeling of permeation of chemicals through human skin. For our analysis we use a brick-and-mortar setup as a model problem. A C++ library implementing Parareal is combined with the ug4 simulation framework, which provides the spatial discretization and parallelization. By numerical examples, we investigate Parareal's performance on an anisotropic domain with large jumps in the diffusion coefficients. While speedup from the time parallelization is shown to be possible, load balancing is identified as an important aspect.

Co-Authors: **Andreas Kreienbuehl** (Università della Svizzera italiana, Switzerland); **Daniel Ruprecht** (Università della Svizzera italiana, Switzerland); **Robert Speck** (Università della Svizzera italiana, Switzerland); **Arne Naegel** (University of Frankfurt, Germany); **Gabriel Wittum** (University of Frankfurt, Germany)

Parallel-in-Time Simulation of Black Hole Formation; Andreas Kreienbuehl

(Università della Svizzera italiana, Switzerland)

Tuesday, June 2, 2015

14:00 – 14:30
HG E22

We present and discuss an application of the parallel-in-time integration method Parareal to the Einstein gravity equations for a collapsing massless scalar field in spherical symmetry. We show that Parareal captures the correct black hole formation event and generates the proper mass scaling law. Moreover, if the computational load is properly balanced in time, Parareal features speedup when compared to the serial two-step Lax-Wendroff Richtmyer scheme. As we are using a two-level approach in both space and time, we furthermore analyze the influence of the spatial interpolation. Finally, the efficiency of different Parareal implementations is compared with respect to energy consumption.

Co-Authors: **Pietro Benedusi** (Università della Svizzera italiana, Switzerland); **Daniel Ruprecht** (Università della Svizzera italiana, Switzerland); **Rolf Krause** (Università della Svizzera italiana, Switzerland)

Parallel Time Integration with Multigrid; Tzanio Kolev

(Lawrence Livermore National Laboratory, USA)

Tuesday,
June 2, 2015

14:30 – 15:00
HG E22

In this talk we examine an optimal-scaling parallel time integration method, multigrid-reduction-in-time (MGRIT). MGRIT applies multigrid to the time dimension by iteratively solving all time steps simultaneously. This results in a non-intrusive approach that wraps existing time evolution codes. MGRIT allows for various time integrators, adaptive refinement/coarsening in time and space and handles non-linear problems through FAS multigrid. Aspects of the theory, software implementation in the XBraid library (llnl.gov/casc/xbraid), and practical result for a variety of problems will be presented, e.g., explicit/implicit time integration, non-linear diffusion and compressible Navier-Stokes.

Co-Authors: **R. Falgout** (Lawrence Livermore National Laboratory, USA); **S. Friedhoff** (Tufts University, USA); **V. Dobrev** (Lawrence Livermore National Laboratory, USA); **S. MacLachlan** (Tufts University, USA); **N. A. Petersson** (Lawrence Livermore National Laboratory, USA); **U. Yang** (Lawrence Livermore National Laboratory, USA)

The Parallel-in-Time Integration Library PFASST++ Applied to Molecular Dynamics; Torbjörn Klatt

(Forschungszentrum Jülich, Germany)

Tuesday,
June 2, 2015

15:00 – 15:30
HG E22

Iterative parallel-in-time integration methods like the 'parallel full approximation scheme in space and time' (PFASST) provide parallelism along the temporal axis by integrating multiple time-steps simultaneously. Along the line of a high-order Boris-SDC integrator for charged particles in external magnetic fields we present the evolution of three implementations of PFASST. Starting from a prototyping Python framework, we explain different implementation strategies and conceptual challenges. We then present results using the HPC library libpfasst and describe our new, lightweight PFASST++ code, highlighting the lessons learned from the interplay with existing HPC applications.

Co-Authors: **Robert Speck** (Forschungszentrum Jülich, Germany); **Mathias Winkel** (Università della Svizzera italiana, Switzerland); **Daniel Ruprecht** (Università della Svizzera italiana, Switzerland); **Matthew Emmett** (Lawrence Berkeley National Laboratory, USA)

MS14

Radiative Transfer in Astrophysics; Methods and Applications to Multi-Scale Simulations

Organiser: *Lucio Mayer (University of Zurich, Switzerland)*
Co-organiser: *Romain Teyssier (University of Zurich, Switzerland)*

Our Mini-Symposium focuses on presenting and discussing methods and applications of radiative transfer in multi-scale simulations of astrophysical systems. The subject is timely as it reflects the main theme of the ongoing 'DIAPHANE' PASC project. Radiative transfer is the current bottleneck of multi-scale simulations across a wide range of scales and problems, from planet formation to galaxy formation and cosmological reionization. State-of-the-art methods employed in the major particle-based and grid-based codes worldwide will be presented and their range of application critically discussed. We will foster discussion of innovative algorithmic strategies.

Multifrequency Radiation Hydrodynamics on Adaptive-Mesh-Refinement Using the Flux-Limited Diffusion Approximation; Benoit Commercon

(CNRS, France)

Tuesday, June 2, 2015

10:30 – 11:00
HG E3

I will present our last developments to model multifrequency radiation hydrodynamics within the adaptive-mesh-refinement code RAMSES (Teyssier 2002). We employ the flux-limited-diffusion approximation and use a combination of explicit (for hydrodynamics) and implicit (for radiation transport) schemes, as well as an efficient scheme for adaptive-time-stepping. I will present our numerical implementation and the tests we have performed. Last, I will present an application to star formation problems (protostellar collapse).

Co-Authors: **M. Gonzalez** (ENS de Lyon, France); **N. Vaytet** (ENS de Lyon, France); **J. Masson** (ENS de Lyon, France); **V. Debout** (Université Paris-Diderot, France); **R. Teyssier** (University of Zurich, Switzerland)

Numerical Algorithms to Solve the Time-Dependent Radiative Transfer Equation Based on VET and Finite Volume Method; Yan-Fei Jiang

(Harvard-Smithsonian Center for Astrophysics, USA)

Tuesday, June 2, 2015

11:00 – 11:30
HG E3

Two algorithms to solve the time dependent radiation (magneto)hydrodynamic equations will be described. The first method solves the two radiation momentum equations, which are closed with the variable Eddington tensor based on time-independent radiative transfer equation using short characteristics. The second method solves the time-dependent radiative transfer equation for specific intensities directly based on finite volume method. Both methods are accurate for both optically thick and optically thin regimes and can be used to model both gas pressure and radiation pressure dominated flows. Application of both methods to study black hole accretion disks will also be described.

Co-Authors: **James Stone** (Princeton University, USA); **Shane Davis** (University of Virginia, USA)

Hybrid Radiation Transport Methods for Star and Planet Formation; Rolf Kuiper

(University of Tübingen, Germany)

Tuesday,
June 2, 2015

11:30 – 12:00
HG E3

Many astrophysical studies require a highly accurate treatment of radiation transport to properly determine heating and cooling timescales, observables, or dependent physical properties. At the same time the radiation transport algorithm should be as fast as possible to allow for an efficient usage of computing resources. Hybrid approaches try to combine the accuracy of a high-order radiation transport method with the speedup of sensible approximations. As an example, I will present the theory and numerics of our own hybrid radiation transport scheme developed for hydrodynamical studies of star formation and accretion disks. Benchmark tests and science applications will be addressed.

Chemistry-Coupled Radiative Transfer in Flash4: Towards Fully Self-Consistent Massive Stellar Feedback on the ISM; Christian Baczynski

(University Heidelberg, Germany)

Tuesday,
June 2, 2015

12:00 –12:30
HG E3

We present a chemistry-coupled radiative transfer scheme for the magnetohydrodynamical simulation code FLASH4. We briefly describe its design philosophy and implementation, and show how non-equilibrium effects captured by the on-the-fly solution of a fast hydrogen chemical network changes the expansion behavior of ionization fronts obtained from simpler approximations. We characterize the differences by modeling a massive star embedded in a molecular clump and furthermore look at the combined expansion of ionization- and photon dominated region (PDR) fronts. We find that the pre-heating by UV-photons changes the stability of the shell typically found around HII regions.

Co-Authors: **Simon C. O. Glover** (University of Heidelberg, Germany); **Ralf S. Klessen** (University of Heidelberg, Germany)

A New Method for Fast Approximate Radiative Transfer; James Wadsley

(McMaster University, Canada)

Tuesday, June 2, 2015

13:30 – 14:00
HG E3

We present a new scheme for radiative transfer. The goals are a fast approach (low cost, no timestep constraints) for an approximate radiation field to drive chemistry and heating for many potential applications. The method combines ray tracing and the tree method. It is flexible in terms of geometry and can use multiple wave-bands. It has been implemented in the GASOLINE2 code but is modular and could be added to different code types. The result scales well with source numbers and is cheap for sub-regions (i.e. multiple timesteps). We demonstrate test results for ionizing radiation (HII regions) and shadowing tests. We show first results on some astrophysical applications.

Co-Authors: **Rory Woods** (McMaster University, Canada); **Hugh Couchman** (McMaster University, Canada)

TRAPHIC: an Efficient Radiative Transfer Method for SPH Simulations with Many Sources; Alireza Rahmati

(University of Zurich, Switzerland)

Tuesday, June 2, 2015

14:00 – 14:30
HG E3

I will talk about the radiative transfer (RT) code TRAPHIC (TRAnsport of PHotons In Cones). TRAPHIC is a multi-frequency RT code for use in Smoothed Particle Hydrodynamics (SPH) simulations. It solves the time-dependent RT equation by tracing photon packets emitted by source particles at the speed of light and in a photon-conserving manner through the simulation box. While the unique design of TRAPHIC makes it ideal for cosmological simulations with large number of sources, it is a general purpose ionizing RT code, and as I will show with several examples, has already been successfully employed in a range of problems.

Galaxy Evolution with Radiation-Hydrodynamics in RAMSES-RT; Joakim Rosdahl

(Leiden University, Netherlands)

Tuesday,
June 2, 2015

14:30 – 15:00
HG E3

I present an implementation of radiation-hydrodynamics in the RAMSES code, which models the emission and propagation of radiation and its interaction with gas via ionisation, dissociation, heating, dust-scattering, and momentum transfer. We use moment-based radiative transfer, which has the advantage over ray-based implementations of handling an unlimited number of radiation sources without an effect on the computational load. I discuss the basic aspects of the implementation, highlighting advantages and disadvantages, and show examples where it has been used in studies of radiation feedback, the emission properties of the circum-galactic medium, and the escape of UV radiation from galaxies.

MS15

Recent Advances on Scalable High-Order Finite Element Type Schemes for PDEs

Organiser: *Stéphane Lanteri (INRIA, France)*
Co-organiser: *Peter Bastian (Universität Heidelberg, Germany)*

The availability of exaflop computers will enable the numerical treatment of more challenging physical problems. However, the simulation of such complex physical phenomena will require very accurate and scalable numerical schemes. In this context, the objective of this minisymposium is to address these needs for different types of PDE models underlying challenging physical problems from modern computational sciences. Related topics are among others, high-order or spectral accuracy, space and time adaptivity, finite element methods, finite volume methods, discontinuous Galerkin methods, multiscale methods, stencil codes, etc.

High-Performance Computing for Flows in Porous Media; Peter Bastian

(Universität Heidelberg, Germany)

Tuesday,
June 2, 2015

10:30 – 11:00
HG E1.2

This talk will focus on the efficient solution of porous media flow problems with discontinuous Galerkin methods. For the fast solution of the linear systems arising in the elliptic flow equation a hybrid preconditioner based on subspace correction in the conforming finite element subspace is employed. The transport equation is solved with explicit methods as part of an operator splitting scheme for the coupled system. The performance of the implementation based on the sum factorization approach is assessed on various architectures and computational results for density-driven flow and miscible displacement are presented.

Co-Authors: **Steffen Müthing** (Universität Heidelberg, Germany)

Scalable High-Order Finite Element Discretizations and Solvers with MFEM, Hypre and BLAST; Tzanio Kolev

(Lawrence Livermore National Laboratory, USA)

Tuesday,
June 2, 2015

11:00 – 11:30
HG E1.2

High-order (HO) finite element (FE) discretizations are a natural fit for future HPC hardware. In this talk we present our work on scalable HO FE software that combines the modular FE library MFEM (mfem.googlecode.com), the hypre library of linear solvers (llnl.gov/casc/hypre), and the HO shock hydrodynamics code BLAST (llnl.gov/casc/blast). We discuss the FE abstractions provided by MFEM, the use of hypre data structures/kernels for efficient parallel assembly, and demonstrate the benefits with respect to scaling/GPU acceleration in BLAST. We also consider HO adaptive refinement and present recent work on scalable algebraic multigrid for electromagnetic problems in this context.

Co-Authors: **J. Cerveny** (Lawrence Livermore National Laboratory, USA); **V. Dobrev** (Lawrence Livermore National Laboratory, USA); **A. Grayver** (Lawrence Livermore National Laboratory, USA); **R. Rieben** (Lawrence Livermore National Laboratory, USA); **I. Karlin** (Lawrence Livermore National Laboratory, USA); **M. Kumbera** (Lawrence Livermore National Laboratory, USA)

Scalable High-Order Finite Element Solvers for Computational Nanophotonics; Stéphane Lanteri

(INRIA, France)

Tuesday, June 2, 2015

11:30 – 12:00
HG E1.2

The numerical study of electromagnetic wave propagation in interaction with nanometer scale structures generally relies on the solution of the system of time-domain Maxwell equations, taking into account an appropriate physical dispersion model for characterizing the material properties of the involved nanostructures at optical frequencies. In this talk, we will present our recent efforts aiming at the design of high performance Discontinuous Galerkin Time-Domain (DGTD) methods for 3d nanophotonic applications. We will consider more particularly DGTD methods for solving the system of Drude-Maxwell equations.

Co-Authors: **Claire Scheid** (Université de Nice - Sophia Antipolis, France); **Jonathan Viquerat** (INRIA, France)

Minimizing Time- and Energy-to-Solution of SeisSol; Alexander Breuer

(Technische Universität München, Germany)

Tuesday, June 2, 2015

12:00 – 12:30
HG E1.2

This talk gives an overview of SeisSol's performance. SeisSol solves the elastic wave equations with a ADER-DG-FEM. Together with hardware-aware optimizations on three generations of CPUs and the Xeon Phi coprocessor, the talk covers a broad range of characteristics and strategies common to high-order DG-FEMs. At single-node level we present a detailed study including the cross-architecture influence of the convergence order, clock frequency and vector instruction set on time- and energy-to-solution. The second part shows our completely redesigned communication scheme aiming at overlapping communication and computation on homogeneous supercomputers in a very natural way.

Co-Authors: **Michael Bader** (Technische Universität München, Germany); **Alexander Heinecke** (Intel Corporation, USA)

Discontinuous Galerkin Approximations for Seismic Wave Propagation in a HPC Framework; Julien Diaz

(INRIA, France)

Tuesday,
June 2, 2015

13:30 – 14:00
HG E1.2

The accurate representation of the heterogeneities of the subsurface requires using high-order numerical methods based on unstructured meshes. Discontinuous Galerkin Methods (DGM) are becoming very popular in the geophysicist community, but they still have to be improved to tackle realistic 3D configurations. Issues are different regarding the equation regime. In time domain, stability depends on a penalization parameter and efficiency of the code requires task-based programming to take advantage of heterogeneous architecture. In harmonic domain, the size of the global DG linear system is huge and Hybridizable DG methods are a promising framework to reach reasonable dimensions.

Co-Authors: **Hélène Barucq** (INRIA, France); **Lionel Boillot** (INRIA, France); **Marie Bonnasse-Gahot** (INRIA, France); **Henri Calandra** (Total, France); **Stéphane Lanteri** (INRIA, France)

Shared Memory Parallelization Strategies for Matrix-Free Finite Element Operator Evaluation; Martin Kronbichler

(Technische Universität München, Germany)

Tuesday,
June 2, 2015

14:00 – 14:30
HG E1.2

Matrix-free finite element operator evaluation for quadratic and higher order hexahedral bases has been shown to be faster per degree of freedom than sparse matrix-vector products for linear elements. The key to success is substituting a memory intensive kernel by fast tensorial integration in a way that suits modern hardware. Our shared-memory implementation dynamically schedules integration tasks on non-conflicting cells and faces, offering coloring, partitioning, and more abstract flow graph concepts. Results show that hardware trends with a growing number of cores per memory controller and widening vector units require particular emphasis on memory access patterns into solution vectors.

Co-Authors: **Katharina Kormann** (Technische Universität München, Germany)

Asynchronous OpenCL/MPI Numerical Simulations of Conservation Laws; Philippe Helluy

(Université de Strasbourg, France)

Tuesday, June 2, 2015

14:30 – 15:00
HG E1.2

Hyperbolic conservation laws are important mathematical models for describing many phenomena in physics or engineering. The Discontinuous Galerkin (DG) method is a popular method for solving conservation laws. We present how we have implemented the DG method in the OpenCL/MPI framework in order to achieve high efficiency on recent GPU or multicore processors. The implementation relies on a splitting of the DG mesh into sub-domains and sub-zones. Different kernels are compiled according to the zones properties. In addition, we rely on the OpenCL asynchronous task graph in order to overlap OpenCL computations, memory transfers and MPI communications.

Co-Authors: **Thomas Strub** (Axessim, France)

High Performance Implementation of High-Order Finite Element Operations; Joachim Schoeberl

Vienna University of Technology, Austria)

Tuesday, June 2, 2015

15:00 – 15:30
HG E1.2

We discuss an object oriented design of finite element core functionality. It allows to separate the mathematical definition of the finite element basis functions, the efficient implementation of operations, and the calculation of stiffness matrices and residual vectors. We show how features of the C++11 programming language help to reduce code complexity and thus allow for additional performance optimization such as vectorization. The presented techniques are implemented in the open source finite element package NGSolve. We present examples including matrix-free solvers and high-order tent-pitching methods for conservation laws.

MS16

Software for Exascale Computing

Organiser: *Harald Koestler (University of Erlangen-Nuremberg, Germany)*
Co-organiser: *Matthias Bolten (University of Wuppertal, Germany)*

This minisymposium in centered around the German Priority Programme 'Software for Exascale Computing' (SPPEXA). SPPEXA addresses fundamental research on the various aspects of HPC software, which is particularly urgent against the background that we are currently entering the era of ubiquitous massive parallelism. It drives research towards extreme-scale computing in six areas or research directions: computational algorithms, system software, application software, data management and exploration, programming, and software tools.

EXASTENCILS - Advanced Stencil-Code Engineering; Harald Koestler

(University of Erlangen-Nuremberg, Germany)

Tuesday,
June 2, 2015

10:30 – 11:00
HG F3

The central goal of ExaStencils is to develop a radically new software technology for applications with exascale performance. To reach this goal, the project focuses on a comparatively narrow but very important application domain of stencil codes. The aim is to enable a simple and convenient formulation of problem solutions in this domain. The software technology developed in ExaStencils shall facilitate the highly automatic generation of a large variety of efficient implementations via the judicious use of domain-specific knowledge in each of a sequence of optimization steps such that, at the end, exascale performance results.

Co-Authors: **Christian Lengauer** (Universität Passau, Germany); **Armin Größlinger** (Universität Passau, Germany); **Sven Apel** (Universität Passau, Germany); **Jürgen Teich** (University of Erlangen-Nuremberg, Germany); **Frank Hannig** (University of Erlangen-Nuremberg, Germany); **Matthias Bolten** (University of Wuppertal, Germany); **Ulrich Rüde** (University of Erlangen-Nuremberg, Germany)

Highly Scalable and Robust Multi-Grid Solvers for Extreme Computing; Gabriel Wittum

(Universität Frankfurt, Germany)

Tuesday,
June 2, 2015

11:00 – 11:30
HG F3

Projected from today, exascale computers are characterized by billion-way parallelism. Computing on such extreme scale needs methods with perfect scaling and optimal complexity. The solver itself must be of optimal numerical complexity - a requirement becoming more and more severe with increasing problem size - and scale efficiently on extreme scales of parallelism. We will present a multigrid approach scaling efficiently unto the full size of the largest computers available and looking promising for even larger scales. We further show that robustness can be maintained during the scaling process for relevant application problems while still maintaining optimal complexity.

Co-Authors: **Ingo Heppner** (G-CSC, Germany); **Michael Hoffer** (G-CSC, Germany); **Arne Nägel** (G-CSC, Germany); **Raphael Prohl** (G-CSC, Germany); **Sebastian Reiter** (G-CSC, Germany); **Martin Rupp** (G-CSC, Germany); **Andreas Vogel** (G-CSC, Germany)

How Many Threads Will Be Too Many? On the Scalability of OpenMP Implementations; Christian Iwainsky

(Technische Universität Darmstadt, Germany)

Tuesday, June 2, 2015

11:30 – 12:00 HG F3

Exascale systems are expected to exhibit much higher degrees of parallelism in terms of number of cores per node. While OpenMP is used today for exploiting parallelism on the level of individual nodes, it is unclear how well OpenMP implementations will scale too much higher numbers of threads. In this work, we apply automated performance modeling to examine the scalability of OpenMP constructs across different compilers and platforms, such as Intel Xeon multi-board, Intel Xeon Phi, and Blue Gene with compilers from GNU, IBM, Intel, and PGI. The resulting models reveal a number of scalability issues in implementations of OpenMP constructs and show unexpected differences between compilers.

Co-Authors: **Sergei Shudler** (German Research School for Simulation Sciences, Germany); **Alexandru Calotoiu** (German Research School for Simulation Sciences, Germany); **Alexandre Strube** (Forschungszentrum Jülich, Germany); **Michael Knobloch** (Forschungszentrum Jülich, Germany); **Christian Bischof** (Technische Universität Darmstadt, Germany); **Felix Wolf** (Technische Universität Darmstadt, Germany)

Performance Engineering of the Kernel Polynomial Method on Large-Scale CPU-GPU Systems; Gerhard Wellein

(University of Erlangen-Nuremberg, Germany)

Tuesday, June 2, 2015

12:00 – 12:30 HG F3

The Kernel Polynomial Method (KPM) is a well-established scheme in quantum physics to determine eigenvalue density and spectral properties of large sparse matrices. We demonstrate the high performance potential of KPM on heterogeneous CPU-GPU supercomputers. At the node level we perform optimizations, which transform our sparse matrix problem towards pure data streaming with high computational intensity. All optimizations are guided by a performance modeling process that indicates how computational bottlenecks change. The optimized KPM code is embedded in a hybrid-parallel framework to perform large-scale KPM calculations on Piz Daint (Cray XC30) achieving 0.5 PF on 4096 nodes.

Co-Authors: **Moritz Kreutzer** (University of Erlangen-Nuremberg, Germany); **Georg Hager** (University of Erlangen-Nuremberg, Germany); **Andreas Pieper** (University of Greifswald, Germany); **Andreas Alvermann** (University of Greifswald, Germany); **Holger Fehske** (University of Greifswald, Germany)

EXASTEEL - Node Level Performance Analysis and Optimization in FETI-DP Methods; Holger Stengel

(University of Erlangen-Nuremberg, Germany)

Tuesday, June 2, 2015

13:30 – 14:00
HG F3

We present the performance engineering process for a FETI-DP application (2D nonlinear hyperelasticity) used in the SPPEXA project EXASTEEL. Starting from a pure MPI code we incrementally develop a hybrid MPI/OpenMP parallel approach that allows efficient utilization of current multi-core compute nodes. The PETSc+MPI-based finite element assembly is parallelized with OpenMP and as a multithreaded direct solver we have chosen Pardiso. This hybrid parallel approach can extend the scalability range of FETI-DP methods by up to a factor of four. Besides a multi-core scaling analysis each step is accompanied with single-core runtime analysis revealing relevant performance bottlenecks.

Co-Authors: **Axel Klawonn** (University of Cologne, Germany); **Martin Lanser** (University of Cologne, Germany); **Oliver Rheinbach** (Technische Universität Bergakademie Freiberg, Germany); **Gerhard Wellein** (University of Erlangen-Nuremberg, Germany)

EXA-DUNE - Flexible PDE Solvers, Numerical Methods and Applications; Jorrit Fahlke

(University of Münster, Germany)

Tuesday, June 2, 2015

14:00 – 14:30
HG F3

DUNE is a software framework for the flexible construction of solvers for PDEs. It has been used successfully on up to O(10^6) cores using MPI. In the EXA-DUNE project we make DUNE suitable for EXA-scale computing. This includes using shared-memory parallelism, wide SIMD units, and accelerator devices while requiring minimal changes in the way users of the framework implement their solvers. In addition, some applications require new numerical methods to overcome restrictions like limited memory and bandwidth. Solving these challenges gives us a set of methods, which we present here. They allow constructing applications that take advantage of EXA-scale computers.

Co-Authors: **Peter Bastian** (University of Heidelberg, Germany); **Christian Engwer** (University of Münster, Germany); **Dominik Göddeke** (University of Stuttgart, Germany); **Steffen Müthing** (University of Heidelberg, Germany); **Dirk Ribbrock** (Technische Universität Dortmund, Germany)

Algorithm-Based Fault Tolerance with the Plasma Physics Code GENE; Dirk Pflüger

(University of Stuttgart, Germany)

Tuesday,
June 2, 2015

14:30 – 15:00
HG F3

Massively parallel simulation codes will have to be able to handle faults in the coming age of exascale computing. Faults are predicted to occur in the time-span of minutes or even below. We employ the combination technique for the simulation of hot fusion plasmas. It numerically decomposes a single and huge problem into many, small partial problems that can be computed in parallel. This hierarchical splitting provides a new handle to treat faults without checkpoint-restart at the cost of slightly slower convergence or slightly higher error. Furthermore, our algorithm-based fault tolerance does not depend on expensive recomputations of missing solutions.

Co-Authors: **Alfredo Parra Hinojosa** (Technische Universität München, Germany); **Mario Heene** (University of Stuttgart, Germany)

ExaFSA -- Parallel Coupling of Structures, Turbulent Flow and Acoustics; Miriam Mehl

(University of Stuttgart, Germany)

Tuesday,
June 2, 2015

15:00 – 15:30
HG F3

Fluid-Structure-Acoustics Interactions are one example for multiphysics simulations featuring a high model accuracy but also high computational costs which requires the use of massively parallel computers. Whenever we want to ensure flexibility in adding or exchanging physical fields and solver or set up a new model combination in a short time range, such simulations use a partitioned approach combining independent existing single-physics solvers. We present functionalities, efficient numerics and parallelization strategies that we implemented in our coupling library preCICE comprising the complete functionality required to combine codes to a multiphysics simulation environment.

Co-Authors: **Florian Lindner** (University of Stuttgart, Germany); **Benjamin Uekermann** (Technische Universität München, Germany)

MS17

Big Data Analytics in Science

Organiser: *Costas Bekas (IBM Research, Switzerland)*

Big Data driven scientific discovery presents a new paradigm next to theory, experimentation and simulation. It relies on the foundational concept of discovery pipelines that start with data acquisition and curation, introduce knowledge representation and exploration and finally lead to scientific discovery. Thus, data flow, as well as advanced and deep analytic algorithms and new appropriate computer architectures will be central in our discussion. This new paradigm challenges the state of the art in Big Data and computing, as it demands unprecedented degrees of integration and interoperability, as well as new levels of combined computational and data-centric performance.

The ADES Model for Computational Science; Nicola Marzari

(EPFL, Switzerland)

Tuesday, June 2, 2015

10:30 – 11:00
HG F30

Computational science has seen a meteoric rise in the scope, breadth, and depth of its efforts. Notwithstanding this prevalence and impact, it is often still performed using the renaissance model of individual artisans gathered in a workshop, under the guidance of an established practitioner. Great benefits could follow from adopting concepts and tools coming from computer science to manage, preserve, and share these computational efforts. I will illustrate here our vision for the four pillars that should sustain such effort (the ADES model: Automation, Data, Environment, and Sharing) and discuss their implementation in the open-source AiiDA platform (http://www.aiida.net).

Co-Authors: **Giovanni Pizzi** (EPFL, Switzerland); **Andrea Cepellotti** (EPFL, Switzerland); **Andrius Merkys** (EPFL, Switzerland); **Nicolas Mounet** (EPFL, Switzerland); **Riccardo Sabatini** (EPFL, Switzerland); **Martin Uhrin** (EPFL, Switzerland); **Boris Kozinsky** (Robert Bosch RTC, Cambridge MA, USA)

Data Management in Climate Science - Cost-Benefit Considerations at DKRZ; Thomas Ludwig

(DKRZ, Germany)

Tuesday, June 2, 2015

11:00 – 11:30
HG F30

Climate science is highly data intensive and data is the raw material for the scientist for gaining new insights. The German Climate Computing Centre DKRZ stores dozens of Petabyte of modelling output on disks and tapes. Costs for this part of the infrastructure are increasing and we look into methods of how to reduce them. The talk will introduce the most important aspects of data management within climate science and cover various aspects during the lifecycle of data. We will explain how a well-balanced HPC system needs to be configured and which investment and operational costs are generated by it. A look at Exascale systems will conclude the presentation.

Big & Smart, High Energy Data; Maria Spiropulu

(California Institute of Technology, USA)

Tuesday,
June 2, 2015

11:30 – 12:00
HG F30

The raw data rate at the LHC is 1 Petabyte/sec. In terms of production, capturing, communicating, aggregating, storing and analyzing it this is arguably the biggest and most challenging science data frontier and one that offers solutions for other fields and affords innovation as we move to the next era of the High Luminosity LHC when the needs and requirements can be an order magnitude bigger. I will discuss Big and Smart Data and intelligent data handling systems in high energy physics as we move forward towards the High Luminosity LHC and beyond, and highlight the importance of validation and verification that we can afford in this science domain.

The Human Brain Project; Sean Hill

(EPFL, Switzerland)

Tuesday,
June 2, 2015

12:00 – 12:30
HG F30

The aim of the Human Brain Project (HBP) is to integrate global neuroscience knowledge and data into supercomputer-based models and simulations to accelerate our understanding of the human brain. To do this, HBP will deliver six collaborative ICT platforms: Neuroinformatics, Brain Simulation, High Performance Computing, Medical Informatics, Neuromorphic Computing, and Neurorobotics. The HBP will create new technologies for interactive supercomputing, visualization and big data analytics; federated analysis of globally distributed data; simulation of the brain; objective classification of disease; and neuromorphic computing systems based on brain-like principles.

Scientific Big Data Analytics at the John von Neumann-Institute for Computing (NIC); Thomas Lippert

(Forschungszentrum Jülich, Germany)

Tuesday,
June 2, 2015

13:30 – 14:00
HG F30

The importance of data analytics, management, sharing and preservation of very big, often heterogeneous or distributed data sets - besides the basic technical requirements transfer and storage - is of increasing significance for science, research and industry. The John von Neumann Institute for Computing, a joint institute by DESY, GSI and Forschungszentrum Jülich in Germany, is going to establish a call for project submission in the field of scientific big data analytics (SBDA). The goal is to extend and optimize the existing HPC and data services. A call for expressions of interest has been launched in order to identify and analyze the needs of the scientific communities.

Big Data Based Materials Discovery; Peter W. J. Staar

(IBM Research, Switzerland)

Tuesday,
June 2, 2015

14:00 – 14:30
HG F30

Traditionally, the discovery of new materials is extremely labor-intensive. This approach is not scalable and, as such, this field of research is ideally suited for a big data based cognitive computing approach. In this talk, we will present how this approach is applied in practice. We will discuss in detail the various aspects ranging from the used data-models to the algorithms applied. Special attention will be given to the design and construction of the knowledge graph, which encodes the underlying data and knowledge model. We will discuss in detail how the nodes and edges in the graph are designed and how the algorithms can be used to refine and optimize the edges of the graph.

Communication Efficient Distributed Training of Machine Learning Models; Martin Jaggi

(ETH Zurich, Switzerland)

Tuesday,
June 2, 2015

14:30 – 15:00
HG F30

Communication remains the most significant bottleneck in the performance of distributed optimization algorithms for large-scale machine learning. We propose a communication-efficient framework, COCOA, that uses local computation in a primal-dual setting to dramatically reduce the amount of necessary communication. We provide a strong convergence rate analysis for this class of algorithms, as well as experiments on real-world distributed datasets with implementations in Spark. In our experiments, we find that as compared to state-of-the-art mini-batch versions of SGD and SDCA algorithms, COCOA converges to the same .001-accurate solution quality on average 25× as quickly.

Co-Authors: **Virginia Smith** (UC Berkeley, USA); **Martin Takáč** (Lehigh University, USA); **Jonathan Terhorst** (UC Berkeley, USA); **Sanjay Krishnan** (UC Berkeley, USA); **Thomas Hofmann** (ETH Zurich, Switzerland); **Michael I. Jordan** (UC Berkeley, USA)

Hierarchical Bayesian Models on HPC Platforms; Panagiotis Hadjidoukas

(ETH Zurich, Switzerland)

Tuesday,
June 2, 2015

15:00 – 15:30
HG F30

Hierarchical Bayesian modeling provides an inference framework to fuse heterogeneous data into engineering applications. Hierarchical models suffer from extensive computational demands arising from multiple model evaluations and data intensity. We tackle both challenges using our parallel framework for uncertainty quantification. We combine state of the art parallelized sampling schemes to achieve multiple levels of nested parallelism and manage large data volumes generated by the simulations. We demonstrate our approach to the calibration of Pharmacokinetic models using heterogeneous experimental data measurements on supercomputing platforms.

Co-Authors: **Panagiotis Angelikopoulos** (ETH Zurich, Switzerland); **Steven Wu** (ETH Zurich, Switzerland); **Petros Koumoutsakos** (ETH Zurich, Switzerland)

MS18

Domain Specific Compilation for Scientific Computing

Organiser: *Tobias Grosser (ETH Zurich, Switzerland)*
Co-organiser: *Torsten Hoefler (ETH Zurich, Switzerland)*

Languages and compilation strategies that exploit domain specific knowledge are well known as effective tools for the automatic generation of optimized program code. However, the increasingly complex heterogeneous hardware at the core of todays HPC platforms, as well as the large base of existing HPC applications, make the use and integration of domain specific compilation techniques challenging. In this symposium, we present and discuss recent approaches that address the challenge of domain specific optimizations in the context of heterogeneous systems, scientific computing problems as well as the integration of domain specific languages with existing code bases.

MODESTO: Data-Centric Analytic Optimization of Complex Stencil Programs on Heterogeneous Architectures; Tobias Gysi

(ETH Zurich, Switzerland)

Tuesday,
June 2, 2015

13:30 – 14:00
HG F1

An efficient implementation of stencil computations requires code transformations such as loop tiling and loop fusion. In the course of the HP2C project we developed the STELLA stencil library that goes a long way in applying efficient code transformations for different target architectures. Nevertheless, STELLA still requires some manual tuning. In this talk, we introduce MODESTO, a model-driven stencil optimization framework, that for a stencil program suggests program transformations optimized for a given target architecture. Using a compile-time performance model and mathematical optimization we successfully tune example stencils of the COSMO atmospheric model.

Co-Authors: **Tobias Grosser** (ETH Zurich, Switzerland); **Torsten Hoefler** (ETH Zurich, Switzerland)

A Basic Linear Algebra Compiler; Daniele Spampinato

(ETH Zurich, Switzerland)

Tuesday,
June 2, 2015

14:00 – 14:30
HG F1

Many applications in media processing, control, graphics, and other domains require efficient small-scale linear algebra computations. However, most existing high performance libraries for linear algebra, such as ATLAS or Intel MKL, are geared towards large problems (matrix sizes in the hundreds and larger). We present LGen: a compiler for small-scale, basic linear algebra computations. The input to LGen is a fixed-size linear algebra expression; the output is a corresponding C function optionally SIMD-vectorized. We show benchmarks against libraries (e.g., Intel MKL) and alternative generators (e.g., C++ template-based Eigen). The typical speedup is about a factor of two to three.

Co-Authors: **Markus Püschel** (ETH Zurich, Switzerland)

AnyDSL: A Compiler-Framework for Domain-Specific Libraries; Richard Membarth

(German Research Center for Artificial Intelligence, Germany)

Tuesday,
June 2, 2015

14:30 – 15:00
HG F1

In this talk, we present AnyDSL, a compiler-framework that allows to define arbitrary domain-specific abstractions in the form of a library. AnyDSL allows to express hierarchies of abstractions and efficient transformation to lower-level abstractions through refinement. At the lowest level, the code can be optimized via exposed compiler functionality such as partial evaluation or target code generation. Further, we will present a DSL for stencil codes that achieves the same performance as hand-optimized implementations on CPUs, as well as on GPUs.

ExaStencils: Domain-Specific Stencil Code Generation and Optimization; Armin Größlinger

(Universität Passau, Germany)

Tuesday,
June 2, 2015

15:00 – 15:30
HG F1

Project ExaStencils aims to develop a code generator, which generates high performance multigrid stencil codes for a certain class of problems. Going from the continuous mathematical high-level description of the problem down to highly optimized low-level code requires making choices that make the description more concrete and, in the end, yield a fast code. ExaStencils has defined 4 layers of domain-specific languages at different levels of abstractions to express these choices. In this talk, we give an overview of the current state of the language layers, the code generator and the use of domain knowledge in the code transformations and optimizations.

MS19

Accelerating Scientific Computing with FPGAs

Organiser: *Christian Plessl (University of Paderborn, Germany)*
Co-organiser: *Heiner Giefers (IBM Research, Switzerland)*

Since the performance of CPUs started to stagnate, computing with field-programmable gate arrays (FPGAs) has attracted significant interest. FPGAs not only provide massive parallelism but also allow for fully customizing the processing architecture to the application through a software programming process. As a result, FPGAs can outperform CPUs in speed and energy-efficiency by orders of magnitude for many applications. In this symposium we will bring together leading experts in FPGA computing with computational scientists with a selection of talks that elaborate on the foundations, programming approaches and case studies of the applications of FPGAs for scientific computing.

Examples of Accelerating Algorithms with FPGAs; Christof Sidler

(Supercomputing Systems AG, Switzerland)

Tuesday, June 2, 2015

13:30 – 14:00
HG E1.1

FPGAs can dramatically speed-up certain algorithms. This presentation will show some practical examples of algorithms accelerated by FPGAs.

Enabling Energy-Efficient Exascale Computing: Acceleration of HPC Kernels with Reconfigurable Hardware; Heiner Giefers

(IBM Research, Switzerland)

Tuesday, June 2, 2015

14:00 – 14:30
HG E1.1

Recent studies have shown that arising big data analytics problems cannot be performed at economically affordable energy if we rely on the traditional scaling of Von-Neumann microprocessors based on Moore's law. A drastic reduction of energy consumption requires the transition from the current computing-centric model to a more data-centric model in which data is pushed to functional units tailored to the specific workload requirements. In this talk, we present an architecture for such a near-data processing approach and show initial results that unveil the energy-efficiency of custom processing pipelines implemented in reconfigurable hardware.

Co-Authors: **Raphael Polig** (IBM Research, Switzerland); **Jan van Lunteren** (IBM Research, Switzerland); **Christoph Hagleitner** (IBM Research, Switzerland)

Custom Data-Flow Engines for Computational Nanophotonics; Christian Plessl

(University of Paderborn, Germany)

Tuesday,
June 2, 2015

14:30 –15:00
HG E1.1

Finite difference methods are widely used, highly parallel algorithms for solving differential equations. While simple from a computational point of view, these algorithms are hard to implement efficiently because their performance is essentially memory-bound. In this talk we discuss how the finite difference time domain (FDTD) method for solving Maxwell's equations can be translated to custom data-flow engines implemented on FPGAs. We evaluate our work with a case study from the computational nanophotonics domain and show that the resulting solution provides both, performance and energy-efficiency benefits over CPU and GPU implementations.

Reconfigurable Computing for All: Efficient Use of FPGAs for Non-Hardware Experts; David Novo

(EPFL, Switzerland)

Tuesday,
June 2, 2015

15:00 – 15:30
HG E1.1

Field-Programmable Gate Arrays (FPGAs) can achieve significant acceleration over traditional processor-based solutions. Unfortunately, their inaccessible programming model, which is inherited from circuit design and far from software-like productivity, is probably the main reason for many users to stay away from FPGAs. In this talk, I will present a cost-effective approach to develop domain-specific high-level synthesis tools. In particular, we leverage domain-specific languages (i.e., designed to specify applications within a particular domain, e.g., machine learning) to express the application at a high abstraction level while enabling the automatic generation of efficient hardware.

Co-Authors: **Nithin George** (EPFL, Switzerland); **Mohsen Owaida** (EPFL, Switzerland); **Paolo Ienne** (EPFL, Switzerland)

MS20

Integrating Resilience and Communication Hiding/Avoiding in a Extreme Scale Preconditioned Krylov Solver

Organiser: *Wim Vanroose (University Antwerpen, Netherlands)*
Co-organiser: *Olaf Schenk (Università della Svizzera italiana, Switzerland)*

We report the progress of the Exascale Algorithms and Advanced Computational Techniques (Exa2CT) project funded by the European Union. In this project resilience and communication avoiding/hiding techniques are integrated in a preconditioned Krylov solver for exascale applications. We use the pipelining to hide the latencies of the global reductions, stencil compilers to increase the arithmetic intensity and avoid communication at the level of the preconditioner. Resiliency to soft errors is also discussed. We report initial benchmarks of the components and the integrated prototypes on various proto applications ranging from combustion to mechanics.

ExaShark: A Scalable Hybrid Array Kit for Exascale Simulation; Tom Vander Aa

(IMEC, Belgium)

Tuesday, June 2, 2015

13:30 – 14:00
HG E21

Design and implementation of solvers that scale to large HPC systems is not only a challenge from a numerical point of view, but also - and even more so - from an implementation and verification point of view. To estimate how a newly developed solver would behave on modern heterogeneous HPC architectures, knowledge of many different programming paradigms and libraries is needed. ExaShark's goal is to reduce the increasing programming burden while still offering good performance.

Co-Authors: **Imen Chakroun** (IMEC, Belgium); **Bram Reps** (University Antwerpen, Belgium); **Wim Vanroose** (University Antwerpen, Belgium); **Roel Wuyts** (IMEC, Belgium)

On Resilience in Krylov Subspace Solvers; Luc Giraud

(INRIA, France)

Tuesday, June 2, 2015

14:00 – 14:30
HG E21

In this talk we will discuss possible numerical remedies to survive data loss in some numerical linear algebra solvers namely Krylov subspace linear solvers and some widely used eigensolvers. Assuming that a separate mechanism ensures fault detection, we propose numerical algorithms to extract relevant information from available data after a fault. After data extraction, well-chosen part of missing data is regenerated through interpolation strategies to constitute meaningful inputs to numerically restart. We will also present some preliminary investigations to address soft error detection again at the application level in the conjugate gradient framework.

Co-Authors: **E. Agullo** (INRIA, France); **L. Giraud** (INRIA, France); **P. Salas** (University of Sherbrooke, Canada); **E.F. Yetkin** (INRIA, France); **M. Zounon** (INRIA, France)

Improving the Applicability of Highly Efficient Compilers to a Wider Class of Problems; Simplice Donfack

(Università della Svizzera italiana, Switzerland)

Tuesday,
June 2, 2015

14:30 – 15:00
HG E21

We propose an approach that allows current solvers to adapt to future architectures and continue to scale at exascale, and this by removing the bottleneck introduced in the communication process. Our objective is to increase the arithmetic intensity, that is the number of floating-point operations performed per bytes fetched in the memory during the execution of the solvers, indeed reduce the number and the volume of the data exchanged among the processors and the memory. We use the help of efficient stencil compilers such as PLUTO and PATUS to increase the arithmetic intensity of these solvers.

Co-Authors: **Olaf Schenk** (Università della Svizzera italiana, Switzerland); **Bram Reps** (University of Antwerpen, Belgium); **Wim Vanroose** (University of Antwerpen, Belgium); **Drosos Kourounis** (Università della Svizzera italiana, Switzerland)

Parallel Implementation of Hybrid FETI Solver with Communication Hiding Techniques; Alexandros Markopoulos

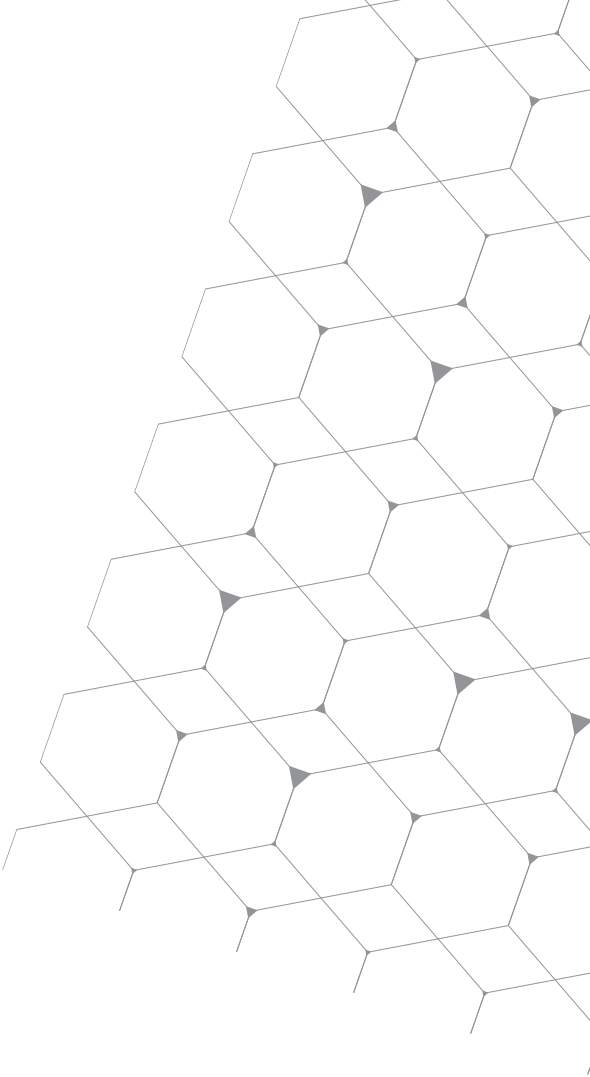
(Technical University of Ostrava, Czech Republic)

Tuesday,
June 2, 2015

15:00 – 15:30
HG E21

We would like to present a massively parallel implementation of the Hybrid Total Finite Element Tearing and Interconnecting (FETI) method, which is designed to solve extremely large problems using multilevel decomposition combined with communication hiding techniques. In Hybrid FETI a relatively small number of neighboring subdomains is aggregated into clusters and each cluster is processed by a single compute node. This method significantly reduces main bottleneck of the two level FETI caused by solving the coarse problem. As of now the solver is able to solve problems larger than 4.3 billions of unknowns using 720 compute nodes with 64 GB of RAM.

Co-Authors: **Lubomir Riha** (University of Ostrava, Czech Republic); **Tomas Brzobohaty** (University of Ostrava, Czech Republic); **Tomas Kozubek** (University of Ostrava, Czech Republic)



CTS

Contributed Talks

CTS01

Climate & Weather

Co-Designing a System for Regional Weather and Climate Prediction;

Oliver Fuhrer (MeteoSwiss, Switzerland)

Wednesday, June 3, 2015

10:30 – 10:50
HG E21

Chair:
Isabelle Bey
(ETH Zurich, Switzerland)

Adapting weather and climate models to current and emerging hardware architectures is a formidable challenge. We present the design decisions, implementation, performance results and learnings from an effort to re-design an existing, widely used community code (COSMO) to hybrid architectures. Using the concrete example of MeteoSwiss' next-generation operational forecasting system, we illustrate the gains in scientific possibilities, time-to-solution and energy-to-solution.

Co-authors: **Xavier Lapillonne** (MeteoSwiss, Switzerland); **Carlos Osuna** (ETH Zurich, Switzerland); **Andrea Arteaga** (ETH Zurich, Switzerland); **Stefan Ruedisuehli** (ETH Zurich, Switzerland); **Thomas Schulthess** (CSCS / ETH Zurich, Switzerland)

Is Convection-Resolving Resolution Necessary for Climate Simulations?;

Nikolina Ban (ETH Zurich, Switzerland)

Wednesday, June 3, 2015

10:50 – 11:10
HG E21

Chair:
Isabelle Bey
(ETH Zurich, Switzerland)

Convection-resolving models (CRMs) operate at very high resolution (grid spacing between 1 and 3km) where convective processes (i.e., thunderstorms and rain showers) can be explicitly represented. The use of CRMs is feasible in numerical weather prediction since recently, but is computationally challenging in climate applications. Here we present pilot CRM climate simulations at horizontal resolution of 2.2km across a greater Alpine region conducted on a Cray XE6 system using a setup with 2000 cores on a grid of 500x500x60 points. The results demonstrate the importance of high resolution in climate simulations for assessing short-term precipitation events.

Co-authors: **Jürg Schmidli** (ETH Zurich, Switzerland); **Christoph Schär** (ETH Zurich, Switzerland)

Towards Continental-Scale Convection-Resolving Climate Simulations on GPUs;

David Leutwyler (ETH Zurich, Switzerland)

Wednesday, June 3, 2015

11:10 – 11:30
HG E21

Chair:
Isabelle Bey
(ETH Zurich, Switzerland)

Climate simulations using horizontal resolution of O(1km) allow to explicitly resolve deep convection. Precipitation processes are then represented much closer to first principles and allow for an improved representation of the water cycle. We present a set of convection-resolving simulations covering the European-scale using a COSMO-model prototype enabled for GPUs, integrated on a computational mesh of 1536x1536x60 grid points. Results illustrate the interactions between synoptic-scale and meso-scale atmospheric circulations, and the initiation of new convective cells by propagating cold pools. Furthermore we discuss computational benefits from using GPUs for climate simulations.

Co-authors: **Oliver Fuhrer** (MeteoSwiss, Switzerland); **Daniel Lüthi** (ETH Zurich, Switzerland); **Christoph Schär** (ETH Zurich, Switzerland)

CTS02

Life Sciences

Off-Limits Modeling for Biological Systems;

Valery Weber (IBM Research, Switzerland)

Wednesday, June 3, 2015

10:30 – 10:50
HG E22

Chair:
Maria Grazia Giuffreda
(CSCS / ETH Zurich, Switzerland)

Reliable atomistic modeling of complex life-science systems has so far been limited by the sizes and time scales accessible by molecular simulations. In this talk, we will present a radical and innovative approach to enable the application of quantum simulations to biological domains typical of classical Hamiltonians. Our approach will merge the extensive knowledge accumulated in the field of semi-empirical quantum simulation and the latest development in low-complexity and scalable algorithms, allowing us to exploit modern supercomputers efficiently and to achieve high scalability and low time to solution. Details of the methodology and efficiency will be discussed.

Co-authors: **Teodoro Laino** (IBM Research, Switzerland); **Alessandro Curioni** (IBM Research, Switzerland)

Modelling and Simulation of Branching Morphogenesis;

Roberto Croce (ETH Zurich, Switzerland)

Wednesday, June 3, 2015

10:50 – 11:10
HG E22

Chair:
Maria Grazia Giuffreda
(CSCS / ETH Zurich, Switzerland)

Organogenesis is a dynamic, self-organizing process. Many of the individual regulatory components, e.g. signaling molecules and their regulatory interactions, have been identified in experiments. However, an integrative mechanistic understanding of the regulatory processes is missing. Computational modeling provides a formalism to formulate and test hypotheses. We present and discuss an according Turing model for the simulation of branching morphogenesis and focus on its numerical challenges. Finally, we show a quantitative comparison between simulated- and real branching morphogenesis in vitro, acquired at the D-BSSE Single Cell Facility.

Co-authors: **Dzianis Menshykau** (ETH Zurich, Switzerland); **Tamas Kurics** (ETH Zurich, Switzerland); **Dagmar Iber** (ETH Zurich, Switzerland)

Experiment-Based Simulations of Interacting Swimmers;

Siddhartha Verma (ETH Zurich, Switzerland)

Wednesday,
June 3, 2015

11:10 – 11:30
HG E22

Chair:
Maria Grazia Giuffreda
(CSCS / ETH Zurich, Switzerland)

Large groups of fish in the ocean often swim in recognizable patterns. One line of thought identifies 'schooling' as an evolutionary means to dissuade attacks from predators. There is also speculation that such behavior may bestow a hydrodynamic advantage to swimmers. The mechanism of reduction in the required energy input may arise from interactions between the leaders' wake, and the undulatory motion of the following-swimmers. The goal of this study is to probe this possibility, by numerically re-creating swimming behavior observed in experiments. In preliminary studies, both the leader, as well as the follower, have been observed to experience an increase in swimming efficiency.

Co-authors: **Sergey Ivannikov** (ETH Zurich, Switzerland); **Petros Koumoutsakos** (ETH Zurich, Switzerland)

CTS03

Materials 1

Double Counting Problem in DFT+DMFT Method: A Study in the Exact Limit;

Andrei Plamada (ETH Zurich, Switzerland)

Wednesday, June 3, 2015

10:30 – 10:50
HG F1

Chair:
Markus Meuwly
(University of Basel, Switzerland)

The combination of density functional theory (DFT) with dynamical mean field (DMFT) has become a popular method for first principles studies of strongly correlated materials. Yet, one of the most severe drawbacks of the method is the double counting of correlations that have been included in both, DFT and DMFT, and that so far could be removed only by introducing an empirical parameter. Assuming that DFT and DMFT produce the exact density, we devise a method to derive the double counting correction from first principles. We validate it on metals, charge transfer and Mott insulators, and find that in all cases the predicted correction is in agreement with the accepted values.

Co-authors: **Peter Staar** (IBM Research, Switzerland); **Anton Kozhevnikov** (CSCS / ETH Zurich, Switzerland); **Thomas Schulthess** (CSCS / ETH Zurich, Switzerland)

Formation of Defects and Self-Healing Processes in Single Layer Hexagonal Boron Nitride Supported on Rh(111);

Marcella Iannuzzi (University of Zurich, Switzerland)

Wednesday, June 3, 2015

10:50 – 11:10
HG F1

Chair:
Markus Meuwly
(University of Basel, Switzerland)

The Nanomesh (nm) is the Moire-like structure formed by a single hBN layer grown on Rh. It can be functionalized by sputtering ions, while the pristine form can be recovered by annealing. Argon implantation leads to the formation of vacancy and interstitial defects. The interstitials are atoms trapped beneath the sp2 layer. The vacancies are formed when B and N atom are kicked out by Ar ion impact. DFT-based optimizations and MD provide better understanding of the observed phenomena. We go beyond the static picture and address the defect formation kinetics, their mobility, leading to aggregation and eventually the self-healing of the sp2 lattice. H.Y. Cun et al. ACS Nano 8 (2014).

Solid State Electrolyte Transporter from Ab-Initio, Machine Learning and Data Mining Techniques;

Ivano Tavernelli (IBM Research, Switzerland)

Wednesday, June 3, 2015

11:10 – 11:30
HG F1

Chair:
Markus Meuwly
(University of Basel, Switzerland)

Solid state electrolyte transporter for Lithium ions are of great importance in the design of highly efficient batteries. In this study we investigate the static and dynamical properties of a new class of ceramic electrolytes based on the Garnet structure that exhibits the unprecedented combination of high ionic conductivity and chemical stability. Using data from ab-initio metadynamics combined with thermodynamic integration we parametrized a kinetic Monte Carlo model for the characterization of the transport properties at ambient conditions. This model is the starting point for the design of better performing materials using machine learning and data mining techniques.

Co-authors: **Matthieu Mottet** (IBM Research, Switzerland); **Teodoro Laino** (IBM Research, Switzerland); **Alessandro Curioni** (IBM Research, Switzerland)

CTS04

Materials 2

High-Throughput Computational Screening of Rare-Earth Perovskite Oxides for Light Harvesting Applications;

Ivano E. Castelli (EPFL, Switzerland)

Wednesday, June 3, 2015

10:30 – 10:50
HG E1.2

Chair:
Nicola Marzari
(EPFL, Switzerland)

Many codes and pseudopotentials (PP) are available and attempts to evaluate errors inside simulations have been made. We compare equations of state (EOS) using various libraries of PP inside the DFT code QUANTUM Espresso with all-electron data. A PP is considered good when the squared deviation of the two EOS is small. Using these values, together with the energy cutoffs required to converge phonons, heats of formation, and computational costs, we propose two libraries, called Standard Solid State Pseudopotentials (SSSP), with focus on efficiency and accuracy. We use the SSSP and a screening technique based on stability and bandgap to search for novel light harvesting rare-earth perovskites.

Co-authors: **Nicola Marzari** (EPFL, Switzerland)

Lithiation / Delithiation of Tin-Oxide;

Andreas Pedersen (ETH Zurich, Switzerland)

Wednesday, June 3, 2015

10:50 – 11:10
HG E1.2

Chair:
Nicola Marzari
(EPFL, Switzerland)

Based on first-principles calculations, we propose a microscopic model that explains the reversible lithiation/delithiation of tin-oxide anodes in Li-ion batteries. At the point when the irreversible regime ends, the anode is ordered and consists of layers of Li-oxide separated by Sn bilayers. During the following reversible lithiation, the Li-oxide undergoes two-phase transformations, which give rise to a Li-enrichment of the oxide and the formation of a SnLi composite. The predicted anode volume expansion and voltage profile agree well with experiments, as opposed to existing models.

Co-authors: **Petr A. Khomyakov** (ETH Zurich, Switzerland); **Mathieu Luisier** (ETH Zurich, Switzerland)

Molecular-Dynamics Simulations of Resistance Switch in Amorphous Carbon;

Federico Zipoli (IBM Research, Switzerland)

Wednesday,
June 3, 2015

11:10 – 11:30
HG E1.2

Chair:
Nicola Marzari
(EPFL, Switzerland)

Diamond-like carbon films are considered very promising materials for resistive random access memories. The information is stored by setting different levels of electric resistance in amorphous carbon (a-C). An electric pulse is used to switch between the low and the high resistance states. The current challenge is to ensure reversible switch in a-C. We use atomistic simulations at the realistic device sizes to find which structural changes produce the resistance switch and its associated optimal process conditions. This work is funded by the EU research & innovation project CareRAMM, N. 309980.

Co-authors: **Alessandro Curioni** (IBM Research, Switzerland)

CTS05

Computer Science & Mathematics

Core Algorithms for High-Performance, Interactive Rendering of Large-Scale Scientific Data;

Valentin Fütterling (Fraunhofer, Germany)

Wednesday, June 3, 2015

10:30 – 10:50
HG E1.1

Chair:
Torsten Hoefler
(ETH Zurich, Switzerland)

The efficient analysis of large-scale scientific data demands interactive rendering techniques unconstrained by bus bottlenecks or memory limits. This favors CPU-based solutions over accelerators (GPUs). Ray-tracing provides the ideal method, supporting a variety of primitives and naturally incorporating ambient occlusion as a view-point neutral lighting strategy. Our contributions are novel algorithms for coherent and incoherent ray-traversal that significantly outperform previous solutions. We demonstrate the efficiency of our core algorithms implemented in shared and distributed memory rendering systems with the capability of rendering billions of primitives interactively.

Co-authors: **Carsten Lojewski** (Fraunhofer Institute for Industrial Mathematics, Germany); **Franz-Josef Pfreundt** (Fraunhofer Institute for Industrial Mathematics, Germany); **Achim Ebert** (Technische Universität Kaiserslautern, Germany)

A Communication Avoiding Scheme for Sparse Matrix Multiplication;

Alfio Lazzaro (ETH Zurich, Switzerland)

Wednesday, June 3, 2015

10:50 – 11:10
HG E1.1

Chair:
Torsten Hoefler
(ETH Zurich, Switzerland)

DBCSR is a sparse matrix library designed to efficiently perform sparse matrix-matrix multiplication, among other operations. It is MPI and OpenMP parallel, and can exploit accelerators. It is developed as part of CP2K, where it provides core functionality for linear scaling electronic structure theory. The multiplication algorithm is based on Cannon's algorithm, whose scalability is limited by the MPI communication time. We present a novel implementation based on a 2.5D algorithm, which takes in account the sparsity of the problem in order to reduce the MPI communication.

Co-authors: **Ole Schuett** (ETH Zurich, Switzerland); **Florian Schiffmann** (ETH Zurich, Switzerland); **Joost VandeVondele** (ETH Zurich, Switzerland)

Scientific Computing Based on Mobile Embedded Technology;

Filippo Mantovani (Barcelona Supercomputing Center, Spain)

Wednesday, June 3, 2015

11:10 – 11:30
HG E1.1

Chair:
Torsten Hoefler
(ETH Zurich, Switzerland)

In the late 1990s, mostly economic reasons led to the adoption of commodity processors in high-performance computing. This transformation has been so effective that in 2015 the TOP500 list is still dominated by x86-based supercomputers. In 2015, the largest commodity market is the one of smartphones and tablets, most of which are built with ARM-based SoCs. This leads to the suggestion that once mobile SoCs deliver sufficient performance, mobile SoCs can help reduce the cost of HPC. In view of the experiences within the Mont-Blanc project, this talk will describe possibilities, results and challenges raised when developing HPC platforms from mobile embedded technology.

CTS06

Physics

Electromagnetic Turbulence Simulations of the Tokamak Scrape-Off Layer;

Federico Halpern (EPFL, Switzerland) Abstract

Wednesday, June 3, 2015

10:30 – 10:50
HG E3

Chair:
Laurent Villard
(EPFL, Switzerland)

We present the new version of the Global Braginskii Solver (GBS) a code addressing tokamak boundary turbulence. GBS employs a 3D cartesian communicator and a parallel multigrid Poisson/Ampere solver, achieving excellent parallel scalability, and it is being ported into manycore and hybrid architectures. Two new capabilities resulted from improved algorithms: the inclusion of electromagnetic fluctuations at realistic plasma size, and a non-Boussinesq Poisson operator for the electrostatic potential. Simulations of the turbulent plasma dynamics are benchmarked against state-of-the-art imaging diagnostics in tomakak experiments, showing remarkable agreement in many observables.

Co-authors: **Trach-Minh Tranh** (EPFL, Switzerland); **Felix Musil** (EPFL, Switzerland); **Paolo Ricci** (EPFL, Switzerland); **Fabio Riva** (EPFL, Switzerland); **Christoph Wersal** (EPFL, Switzerland)

Towards Petascale Particle-In-Cell (PIC) Simulations and Beyond;

Farah Hariri (EPFL, Switzerland)

Wednesday, June 3, 2015

10:50 – 11:10
HG E3

Chair:
Laurent Villard
(EPFL, Switzerland)

Our focus is to port Particle-In-Cell (PIC) codes applied for studying turbulence in magnetic fusion relevant plasmas to various computational platforms equipped with GPUs and MICs. To this end, a so-called 'PIC ENGINE' framework containing the main features of the PIC algorithm has been designed and implemented with different approaches ensuring the locality of the method. Our implementation on the GPU is done using the OpenACC parallel programming standard. The algorithmic performance is tested on the Cray XC30 - Piz Daint - platform. Results show that our optimizations lead to significant performance improvements and will be compared to a reference parallel OpenMP implementation.

Co-authors: **T. M. Tran** (EPFL, Switzerland); **A. Jocksch** (CSCS / ETH Zurich, Switzerland); **S. Brunner** (EPFL, Switzerland); **C. Gheller** (CSCS / ETH Zurich, Switzerland); **L. Villard** (EPFL, Switzerland)

Upgrading Smoothed Particle Hydrodynamics Calculations;

Rubén Cabezón (University of Basel, Switzerland)

Wednesday,
June 3, 2015

11:10 – 11:30
HG E3

Chair:
Laurent Villard
(EPFL, Switzerland)

In the last years there has been a change of paradigm within the SPH calculations. What was considered as 'standard' in SPH has been renewed by a set of recent formalisms that have helped to overcome various long-lasting inherent problems of this numerical technique. These new additions include, among others, the use of new kernels resistant against pairing instability, and more accurate gradient calculation via an integral approach. In this talk I will focus on how these simple changes can substantially improve our SPH calculations at almost no cost.

Co-authors: **Domingo García-Senz** (Universitat Politècnica de Catalunya, Spain)

CTS07

Engineering

High-Fidelity Aeroelasticity;

Marcello Righi (Zurich University of Applied Sciences, Switzerland)

Wednesday, June 3, 2015

10:30 – 10:50
HG F3

Chair:
Satoshi Matsuoka
(Tokyo Institute of Technology, Japan)

Aeroelasticity considers the joint effects of aerodynamic, elastic and inertial forces. This discipline initially relied on analytical methods to model the underlying physics. Later on, low-fidelity methods such as doublet-lattice became the standard. High-fidelity, CFD-based approaches are of course possible but demanding, as, unlike most engineering disciplines, they require time-accurate simulations, often used to feed convenient Reduced-Order-Models. Availability of HPC might soon allow practitioners to systematically capture flow non-linearities in full. We would like to present the state-of-art and the current trends.

Co-authors: **Jan Koch** (Zurich University of Applied Sciences, Switzerland)

Large-Eddy Simulation of Turbulent Combustion with Finite Rate Chemistry Model;

Tulin Kaman (ETH Zurich, Switzerland)

Wednesday, June 3, 2015

10:50 – 11:10
HG F3

Chair:
Satoshi Matsuoka
(Tokyo Institute of Technology, Japan)

We present Large-Eddy simulations (LES) of the combustion chamber of a scram jet experiment with finite rate chemistry, using only the fundamental chemical reaction equations. The main focus of this work is to provide necessary guidance to the mesh resolution needed to perform a full-domain numerical simulation of a three-dimensional scram jet, which is M=7 experimental aircraft. The combustion process modeled by the finite rate chemistry is based on the notion that it can be resolved on a larger scale than the levels needed to resolve turbulence.

Co-authors: **Xiaoxue Gong** (Stony Brook University, USA); **Ying Xu** (Stony Brook University, USA); **James Glimm** (Stony Brook University, USA)

Petascale Simulations of Cloud Cavitation Collapse;

Jonas Sukys (ETH Zurich, Switzerland)

Wednesday, June 3, 2015

11:10 – 11:30
HG F3

Chair:
Satoshi Matsuoka
(Tokyo Institute of Technology, Japan)

Simulation of cloud cavitation collapse pertains to the erosion of liquid-fuel injectors, hydropower turbines and ship propellers, or can even be harnessed in treating kidney stones by shock wave lithotripsy. Cavities undergo a collapse at higher pressure regions inside the flow and produce extreme pressure spots, possibly causing erosion. Numerical simulations of cloud cavitation collapse require two-phase flow solvers capable of capturing interactions between multiple deforming bubbles. We present the two-phase flow simulations enabling quantitative prediction of cavitation of clouds containing up to 50'000 vapor bubbles on unprecedented resolution of up to 1 trillion grid points.

Co-authors: **Panagiotis Hadjidoukas** (ETH Zurich, Switzerland); **Diego Rossinelli** (ETH Zurich, Switzerland); **Fabian Wermelinger** (ETH Zurich, Switzerland); **Babak Hejazialhosseini** (ETH Zurich, Switzerland); **Petros Koumoutsakos** (ETH Zurich, Switzerland)

Solid Earth Dynamics
Climate & Weather
Life Sciences
Materials
Physics
Computer Science & Mathematics
Engineering
Emerging Domains

Poster Session

Solid Earth Dynamics

EAR-01
Advection of Material Interfaces via a Two-Way Particle Level Set Approach;
Henri Samuel (CNRS, France)

EAR-02
High-Fidelity Aeroelasticity;
Patrick Sanan (Università della Svizzera italiana, Switzerland)

EAR-03
Discontinuous Galerkin Methods for Variable Viscosity Stokes;
Dominic Etienne Charrier (ETH Zurich, Switzerland)

EAR-04
Forward and Adjoint Spectral-Element Simulations of Seismic Wave Propagation Using Hardware Accelerators;
Daniel Peter (Università della Svizzera italiana & ETH Zurich, Switzerland)

EAR-05
From Capillary to Bubbly Flow: the Fate of Low Reynolds Number, Buoyancy Driven Fluids Transport at Strong Porosity Transition;
Andrea Parmigiani (ETH Zurich, Switzerland)

EAR-06
Large-Scale Geo-Electromagnetic Modeling with Adaptive High-Order FEM;
Alexander Grayver (ETH Zurich, Switzerland)

EAR-07
Towards a Data-Comprehensive Earth Model Across the Scales;
Michael Afanasiev (ETH Zurich, Switzerland)

EAR-08
Use of High Performance and Massively Parallel GPU Computing to Resolve Nonlinear Waves in Poromechanics;
Ludovic Räss (University of Lausanne, Switzerland)

Climate & Weather

CLI-01
Alternate Direction Implicit Preconditioning for Geophysical Applications on CPU and GPU;
Zbigniew Piotrowski (Institute of Meteorology and Water Management, Poland)

CLI-02
Computational and Energy Efficiency Optimizations of the Air Quality Prediction Model COSMO-ART;
Joseph Charles (CSCS / ETH Zurich, Switzerland)

CLI-03
Ensemble Kalman Particle Filter for Convective Scale Data Assimilation;
Sylvain Robert (ETH Zurich, Switzerland)

CLI-04
GridTools: A Tool for Stencil Methods on Grids;
Mauro Bianco (CSCS / ETH Zurich, Switzerland)

CLI-05
Modifications of the Atmospheric Moisture Field as a Result of Cold-Pool Dynamics;
Linda Schlemmer (ETH Zurich, Switzerland)

CLI-06
Tuning a Global Climate Model - a Costly Hunt in Parameter Space;
Doris Folini (ETH Zurich, Switzerland)

Life Sciences

LS-01
A Parallel Block Preconditioner for Fluid-Structure Interaction Problems in Hemodynamics;
Davide Forti (EPFL, Switzerland)

LS-02
Agent-Based Modeling of Hunter-Gatherer Populations;
Natalie Tkachenko (University of Zurich, Switzerland)

LS-03
Backbone Hydration Determines the Folding Signature of Amino Acid Residues;
Olivier Bignucolo (University of Basel, Switzerland)

LS-04
FEM/FD Immersed Boundary FSI Simulations;
Barna Becsek (Universiy of Bern, Switzerland)

LS-05
HPC-ABGEM: Simulating Population Dynamics and Genetics of the Worldwide Human Dispersal;
Simone Callegari (University of Zurich, Switzerland)

LS-06
Image-Based Computation of in Vivo Bone Loading History in Patients
Patrik Christen (ETH Zurich, Switzerland)

LS-07
Investigation of the Effect of Ca2+ Binding on Tissue Transglutaminase;
Lukas Braun (ETH Zurich, Switzerland)

LS-08
Needle in a Bloody Haystack;
Diego Rossinelli (ETH Zurich, Switzerland)

LS-09
Novel Semi-Implicit Approach and Platform for Personalized Fluid-Structure Interaction Modeling;
Frederico Teixeira (ETH Zurich, Switzerland)

LS-10
Standardization of Efficient Genomic Data Representation and Processing;
Daniel Zerzion (Swiss Institute of Bioinformatics, Switzerland)

LS-11
Structural Insights into Phosphoinositide 3-Kinase Alpha (PI3Ks) Regulation Using Molecular Dynamics Simulations;
Ilias Patmanidis (University of Geneva, Switzerland)

LS-12
Tumor Induced Brain Deformations;
Jana Lipkova (Technische Universität München, Germany)

Materials

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A Hybrid OpenMP/MPI Solver for First-principles Plane Wave Materials Science Codes;
Andrew Canning (Lawrence Berkeley National Laboratory, USA)

MAT-02
A Solver for the Generalized Poisson Equation in Wet-Environments Electronic-Structure Calculations;
Giuseppe Fisicaro (University of Basel, Switzerland)

MAT-03
A Spherical P-Method for Full-Potential Electronic Structure Problems;
Lukas Drescher (Technische Universität Berlin, Germany)

MAT-04
Accelerating Nano-Device Simulations with Extreme-Scale Algorithms and Software Co-Integration;
Mathieu Luisier (ETH Zurich, Switzerland)

MAT-05
Achieving Linear Scaling in Computational Cost for a Fully Polarizable MM/Continuum Embedding;
Louis Lagardère (UPMC, France)

MAT-06
Computer Simulation and Neutron Scattering Investigations of Phospholipid Bilayers in Water Solutions of Room-Temperature Ionic Liquids;
Antonio Benedetto (Paul Scherrer Institut, Switzerland)

MAT-07
DBCSR: Accelerated Sparse Matrix Multiplication Library;
Andreas Glöss (ETH Zurich, Switzerland)

MAT-08
Developing Experimental and Theoretical Crystallography Open Databases;
Andrius Merkys (EPFL, Switzerland)

MAT-09
DFT+DMFT Study of Strain and Interface Effects in D1 and D2 T2g-Perovskites;
Gabriele Sclauzero (ETH Zurich, Switzerland)

MAT-10
Direct Path Integral Estimators for Isotope Fractionation Ratios;
Bingqing Cheng (EPFL, Switzerland)

MAT-11
EXAFS Spectra Interpretation Using Molecular Dynamics and DFT Simulations;
Dmitry Bocharov (Paul Scherrer Institut, Switzerland)

MAT-12
Large Scale Density Matrix Renormalization Group Calculations;
Michele Dolfi (ETH Zurich, Switzerland)

MAT-13
Local Density Fitting within a Gaussian and Plane Waves Approach;
Dorothea Golze (University of Zurich, Switzerland)

MAT-14
New Spectroscopic Approaches for Periodic Systems;
Sandra Luber (University of Zurich, Switzerland)

MAT-15
Pyrphyrin Adsorption on Reconstructed and Ideal Au(111) Surface;
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MAT-16
Recognizing Molecular Patterns by Machine Learning: An Agnostic Structural Definition of the Hydrogen Bond;
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MAT-18
Solvation Effects on Electronic Energy Differences of a Co-Cubane;
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MAT-19
The Computational Design of Pb Free and Stable Hybrid Materials for Solar Cells;
Fadwa El Mellouhi (Qatar Environment and Energy Research Institute, Qatar)

MAT-20
Towards an Ab Initio Electronic Transport Model for Photovoltaic Materials Design;
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MAT-21
Understanding Enantioselectivity of PdGa High-Symmetry Surfaces;
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MAT-22
Liquid Layering Effects on the Kapitza Resistance Between Few-Layer Graphene and Water;
Dmitry Alexeev (ETH Zurich, Switzerland)

Physics

PHY-01
3-D Radiation Magnetohydrodynamic Simulations of the Near Surface Layers of the Sun;
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PHY-02
A Bucketsort Algorithm on GPUs for the Particle-In-Cell (PIC) Method;
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PHY-03
Ab Initio Atomic Heat Transport Via Green-Kubo Formalism;
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Adopting CERN SixTrack Fortran Legacy Modeling Code to Perform Ensemble Simulations on GPU;
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PHY-05
Chaos in Terrestrial Planet Formation;
Volker Hoffmann (University of Zurich, Switzerland)

PHY-06
DIAPHANE: Building a Library for Radiation and Neutrino Transport in Hydrodynamic Simulations;
Darren Reed (University of Zurich, Switzerland)

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High-Temperature Series Expansions for Quantum Lattice Models;
Andreas Hehn (ETH Zurich, Switzerland)

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Polarizable Coarse-Grained Water and Protein Models for Dissipative Particle Dynamics;
Emanuel Peter (Università della Svizzera italiana, Switzerland)

PHY-09
Polarized Radiative Transfer in Discontinuous Media;
Oskar Steiner (Istituto Ricerche Solari Locarno, Switzerland)

PHY-10
The Bulk Monopolization in Diagonal Magnetoelectrics;
Florian Thöle (ETH Zurich, Switzerland)

PHY-11
Topological Quantum Computation and Fractional Quantum Hall: Phase Diagram of the 5/2 State;
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Computer Science & Mathematics

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Sandie Moody (University of Geneva, Switzerland)

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Uldis Locans (University of Latvia & Paul Scherrer Institute, Switzerland)

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Energy Efficiency of Parareal;
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HPC.m - the MATLAB HPC Compiler and its Use for Solving 3D Poromechanics on Supercomputers;
Samuel Omlin (University of Lausanne, Switzerland)

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Time and Energy to Solution Study of the Generalized Eigenvalue Solver;
Raffaele Solcà (ETH Zurich, Switzerland)

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Parallel Solver for the Space Inhomogeneous and Time Dependent Boltzmann Equation;
Simon Pintarelli (ETH Zurich, Switzerland)

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Pipelined Flexible Krylov Subspace Methods for Large-Scale Computing;
Sascha Schnepp (ETH Zurich, Switzerland)

CSM-11
Simulating Large-Scale Scattering Phenomena with the Open-Source Boundary Element Library BEM++;
Elwin van 't Wout (University College London, United Kingdom)

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Snowball Sampling for Modeling Large Networks;
Alberto Caimo (Università della Svizzera italiana, Switzerland)

CSM-13
Stencil-Based Exascale Simulations Using an N-Dimensional Array Toolkit;
Imen Chakroun (IMEC, Belgium)

Engineering

ENG-01
OpenGeoSys-GEM: A Coupled Thermo-Hydro-Chemical (-mechanical) Code THC(M) for Geoscientific and Engineering Applications;
Georg Kosakowski (Paul Scherrer Institut, Switzerland)

Emerging Domains

EMD-01
Computing Stationary Markov Equilibria with Heterogeneity;
Elisabeth Proehl (University of Geneva, Switzerland)

EMD-02
Towards the HPC-Inference of Causality Networks from Multiscale Economical Data;
William Sawyer (CSCS / ETH Zurich, Switzerland)


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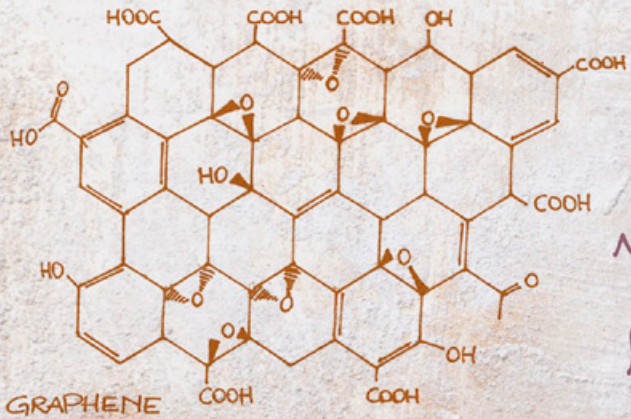


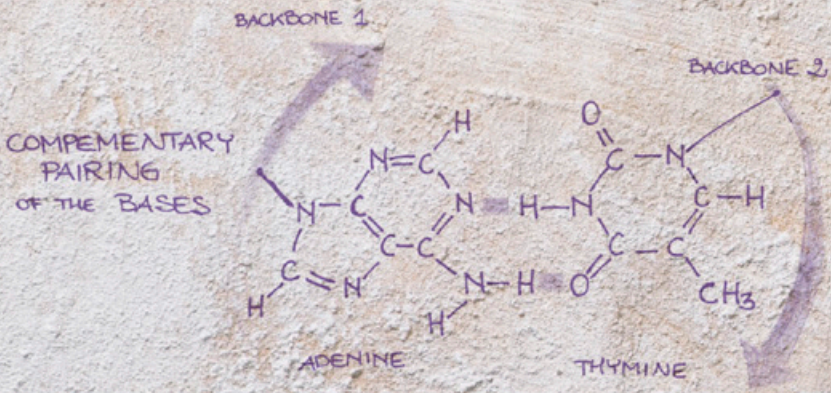
GRAPHENE OXIDE

NAVIER-STOKES EQUATION

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v}\right) =$$

$$= -\nabla p + \mu\nabla^2\mathbf{v} + \mathbf{f}$$

$\mathbf{f}$ - body forces (gravity or centrifugal)



METROPOLIS ALGORITHM

initialize x_1, n and s
for $i = 1 : (n-1)$ do
  while x_{i+1} not assigned do
    draw $z \in [0,1]$ and $u_i \in [-1,1]^d$
    $x_{new} = x_i + u_i s$
    if $f(x_{new})/f(x_i) \geq z$ then $x_{i+1} = x_{new}$
  end while
end for

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