TALKS PROGRAM

Booth 396

SC15

Austin

ENABLING SCIENCE
DRIVING INNOVATION

Tuesday 17

11:30 **hpc-ch – How to create a community to support HPC activities in your country** // Michele De Lorenzi, CSCS // 1

13:30 **Scientific Benchmarking of Parallel Computing Systems** // Torsten Hoefler, ETH Zurich // 2

16:30 **User Lab at CSCS and PASC16 Conference** // Maria Grazia Giuffreda, CSCS // 3

Wednesday 18

11:30 **Efficient Implementation of Quantum Materials Simulations on Dist. CPU-GPU Systems** // Anton Kozhevnikov, CSCS & Raffaele Solcà, ETH Zurich // Best Paper Finalist // 4

13:30 **Interactive weather models on GPU accelerated systems** // Peter Messmer, NVIDIA & NVIDIA Co-Design Lab for Hybrid Multicore Computing @ ETH Zurich // 5

16:30 **Pushing Back the Limit of Ab-initio Quantum Transport Simulations on Hybrid Supercomputers** // Mauro Calderara, ETH Zurich // ACM Gordon Bell Finalist // 6

Thursday 19

11:30 **MeteoSwiss and CSCS pave the way for more detailed weather forecasts** //Sadaf Alam, CSCS // 7

14:00 **The In-Silico Lab-on-a-Chip: Petascale and High-Throughput Simulations of Microfluidics at Cell Resolution** // Christian Conti, ETH Zurich // ACM Gordon Bell Finalist // 8

1 . *The goal of hpc-ch is to support and foster the knowledge exchange between providers of HPC systems in Switzerland. We will show how to create a community to support and foster the knowledge exchange between providers of HPC systems in a country. A case study of professionals which decided to create a community in order to know the offering and organization of Swiss HPC providers, exchange best practices, co-ordinate activities and discuss developments in HPC will be presented.*

2. *Measuring and reporting performance of parallel computers constitutes the basis for scientific advancement of HPC. Most scientific reports show performance improvements of new techniques and are thus obliged to ensure reproducibility or at least interpretability. Our investigation of a stratified sample of 120 papers across three top conferences in the field shows that the state of the practice is not sufficient. For example, it is often unclear if reported improvements are in the noise or observed by chance. In addition to distilling best practices from existing work, we propose statistically sound analysis and reporting techniques and simple guidelines for experimental design in parallel computing. We aim to improve the standards of reporting research results and initiate a discussion in the HPC field. A wide adoption of this minimal set of rules will lead to better reproducibility and interpretability of performance results and improve the scientific culture around HPC.*

3. *CSCS is run as User Lab, promotes and encourages top-notch research, and operates cutting-edge computer systems as an essential service facility for Swiss researchers. These computers aid scientists with diverse issues and requirements. We will give an overview of the services offered at CSCS, the allocation schemes, as well as who can apply, how and when. We will also present the PASC16 Conference a leading event for researchers in computational science and HPC. From 2016, the PASC Conference will be co-sponsored by the Association for Computing Machinery's (ACM) Special Interest Group on High Performance Computing (SIGHPC).*

4. *We present a scalable implementation of the Linearized Augmented Plane Wave method for distributed memory systems, which relies on an efficient distributed, block-cyclic setup of the Hamiltonian and overlap matrices and allows us to turn around highly accurate 1000+ atom all-electron quantum materials simulations on clusters with a few hundred nodes. The implementation runs efficiently on standard multi-core CPU nodes, as well as hybrid CPU-GPU nodes. Key for the latter is a novel algorithm to solve the generalized eigenvalue problem for dense, complex Hermitian matrices on distributed hybrid CPU-GPU systems.*

5. *We show the GPU accelerated weather simulation code COSMO running in live at CSCS with immediate visualization of the ongoing simulation. The simulation runs about 20x faster than real time with grid cells of 1km. The simulation makes it possible to modify the surface temperature and the wind direction in areas of the simulation domain.*

6. *The capabilities of CP2K, a density-functional theory package and OMEN, a nano-device simulator, are combined to study transport phenomena from first-principles in unprecedentedly large nanostructures. Based on the Hamiltonian and overlap matrices generated by CP2K for a given system, OMEN solves the Schrödinger equation with open boundary conditions (OBCs) for all possible electron momenta and energies. To accelerate this core operation a robust algorithm called SplitSolve has been developed. It allows to simultaneously treat the OBCs on CPUs and the Schr"odinger equation on GPUs, taking advantage of hybrid nodes. Our key achievements on the Cray-XK7 Titan are (i) a reduction in time-to-solution by more than one order of magnitude as compared to standard methods, enabling the simulation of structures with more than 50000 atoms, (ii) a parallel efficiency of 97% when scaling from 756 up to 18564 nodes, and (iii) a sustained performance of 14.1 DP-PFlop/s.*

7. *At CSCS, the new "super weather computer" of the Swiss Federal Office of Meteorology and Climatology has started its operation. MeteoSwiss is the first meteorological service which has switched to a new GPU based computer architecture. Thus, the new supercomputer is able to calculate weather models with a resolution twice as high more efficiently and quicker than before.*

8. *We present simulations of blood and cancer cell separation in complex microfluidic channels with subcellular resolution, demonstrating unprecedented time to solution and performing at 42% of the nominal 39.4 Peta-instructions/s on the 18'688 nodes of the Titan supercomputer. These simulations outperform by one to three orders of magnitude the current state-of-the-art in terms of numbers of cells and computational elements. We demonstrate an improvement of up to 30X over competing state-of-the-art solvers, thus setting the frontier of particle based simulations. The simulation setup follows the realism of the conditions and the geometric complexity of microfluidic experiments, and our results confirm the experimental findings. These simulations redefine the role of computational science for the development of microfluidic devices -- a technology that is becoming as important to medicine as integrated circuits have been to computers.*