CSCS

Annual Report **2017**

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

Annual Report 2017

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

The photographers Alessandro Della Bella, Thomas Angus and Panayiotis Kyriacou, have portrayed five scientists of different scientific fields who use CSCS supercomputers for their research work: Sandra Luber (University of Zurich), David Leutwyler & Nikolina Ban (ETH Zurich), Martina Messmer (University of Bern), Peter Vincent (Imperial College London), Constantia Alexandrou (University of Cyprus and the Cyprus Institute).

The photographer Stefano Spinelli presents his work **Transcriptions** – ***The Medium Is the Message (2017)*** based on images collected during visits at CSCS. The images are rendered using sentences from science fiction novels written in very small characters (author and novel name are indicated for every work). Transcriptions is a reflection on the need to include an analysis of critical aspects both at individual and societal level in discussions related to state-of-the-art technology.

Welcome from the Director

Thomas Schulthess, Director of CSCS.

It strikes me as such a short time since I last welcomed you to read our annual report. But in fact, yet another dynamic, eventful and successful year lies behind us. And for this I would like to thank my staff, ETH Zurich, the ETH Board and indeed all who made it possible.

During 2017, we were able to initiate many new and exciting European and Swiss collaborations at CSCS. With the "Piz Daint" supercomputer, we have now become a Hosting Member of the Partnership for Advanced Computing in Europe (PRACE). In this way, we can ensure that our researchers have access to diverse computing architectures across Europe and are able to make use of whichever architecture is best suited to solving their specific problems.

Moreover, major developments in 2017 have confirmed that Switzerland is on the right track with CSCS and the High-Performance Computing and Networking (HPCN) initiative: Long-held hopes of simply being able to continue the strategy of incrementally porting old codes to newer supercomputing architectures have been shattered by Intel discontinuing the Xeon Phi processor line. As a result, massive investments in software development are now required in other European countries and in the USA to get application codes in many fields of computer-aided sciences in shape for new computer architectures. In comparatively small Switzerland meanwhile, the HPCN initiative now gives us a structural advantage from having systematically invested in HPC software development for new architectures since 2010. This is an advantage to be exploited, without losing the focus on scientific goals.

Let me illustrate briefly with an example from the field of climatology and meteorology: Although resolving convective currents in the atmosphere dramatically improves the quality of weather and climate models, a test we ran on "Piz Daint" in early 2017 showed that such high-resolution simulations are about 100 times too slow to be productive. Thus, it is important to ensure that such calculations become productive on future supercomputers. However, it is unfortunate that such goals run contrary to ambitions of attaining a high ranking on the TOP500 list. According to the High-Performance Linpack (HPL) benchmark on which the list is based, "Piz Daint" has only one-fifth the speed of the computer currently in first place. And yet, the climate benchmark runs two to three times faster on "Piz Daint" than it does on the top-ranked TaihuLight[1]. There could well be an order of magnitude discrepancy between the objectives set by policymakers in some places, and the resulting scientific benefits. That is why it is important for the sciences to maintain their independence when it comes to developing future computing infrastructures.

In supporting research at CSCS, we can look back on a successful 2017: With the help of "Piz Daint", an international team of researchers accomplished a decisive step in solving what is known as the proton spin puzzle. Results achieved by an ETH research group impressively demonstrated how simulations pay off; their insights gained from simulations have led to nanosensors being developed that are of great interest to medicine and pharmacology and are now entering clinical research. These are but a few examples. We invite you to form your own impressions from taking a look at the reading material which follows, where we also present exciting research projects by renowned and up-and-coming young scientists.

Prof. Thomas Schulthess
Director of CSCS

[1] Fuhrer et al. 2017

Content

“HPC provides an unprecedented tool to advance the understanding of the quantum nature of our universe. With large scale computational resources at hand we are able to zoom in and get new angles on processes that underpin our life on earth on a molecular level, paving the way for informed design of advanced materials and processes for various purposes.”

Sandra Luber, University of Zurich

Name
Sandra Luber

Position
SNSF professor

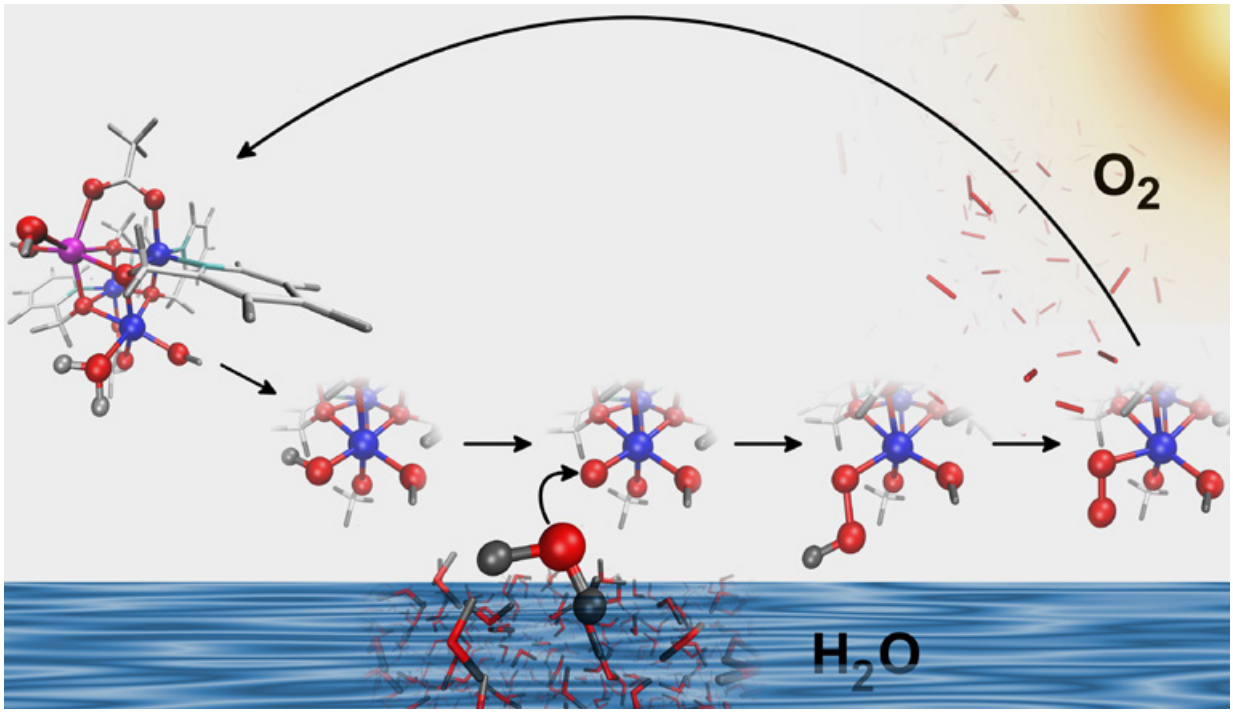
Institution
University of Zurich

Background
2001-2004 Diploma in chemistry, University of Erlangen-Nuremberg, Germany
2004-2005 Exchange Student, ETH Zurich
2005-2007 BSc/MSc in chemistry, ETH Zurich
2007-2009 PhD in theoretical chemistry, ETH Zurich
2010 Post-doctoral researcher at Biozentrum, University of Basel
2010-2011 Post-doctoral researcher, Yale University, USA
2012 Start-in program for young talents, BASF SE, Ludwigshafen, Germany
2012-2017 Project group leader, University of Zurich
2016 Habilitation thesis, University of Zurich
Since 2017 SNSF professor, University of Zurich

Area of research
Development and application of theoretical methods derived from quantum mechanics for chemistry and materials science.

Specialised in
Ab-initio methods for highly-accurate study of functional systems and spectroscopy, catalysis, in silico design of novel materials and processes.

HPC means for me
An exciting combination of excellent computational resources and forefront computational methods, which allows us to explain and predict properties of challenging chemical systems and complex processes.



Using sunlight to produce energy from water

Photosynthesis is one of the most common and fundamental life processes on Earth, and its complex sequence of events has been a topic of research for decades. Achieving artificial photosynthesis would not only address many environmental issues but could also solve our energy problems in a single stroke. High-performance computers are playing a crucial role in this research. Sandra Luber takes the natural photosynthetic process as the basis for her computer-aided research on catalysts for water splitting for hydrogen production.
(Image: Sandra Luber)

KEY INFORMATION

Founded in 1991, CSCS develops and provides the key supercomputing capabilities required to solve challenging problems in science and/or society. The centre enables world-class research with a scientific user lab that is available to domestic and international researchers through a transparent, peer-reviewed allocation process. CSCS's resources are open to academia, and are available as well to users from industry and the business sector.

Production Machines

Piz Daint, Cray XC50, 25.3 PFlops
Piz Daint, Cray XC40, 2.2 PFlops

Granted Resources for User Lab

2017: 43 451 090 node h
2016: 43 446 610 node h

User Community

2017: 116 Projects, 1 213 Users
2016: 109 Projects, 1 190 Users

Employees

2017: 92
2016: 79

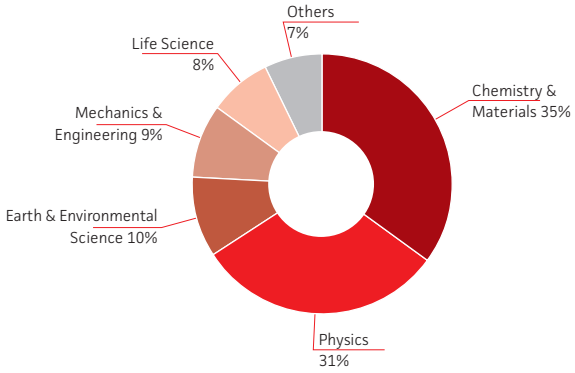
Investments

2017: 4.2 Mio CHF
2016: 40 Mio CHF

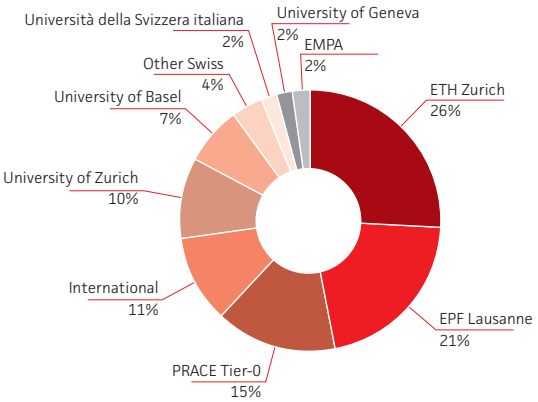
Operational Costs

2017: 16.4 Mio CHF
2016: 14.6 Mio CHF

User Lab Usage by Research Field



User Lab Usage by Institution



Computing Systems Overview

Name	Model	Installation/Upgrades	Owner	TFlops
Piz Daint	Cray XC50/Cray XC40	2012 / 13 / 16	User Lab, UZH, NCCR Marvel	25 326 + 2 193
Blue Brain BG/Q	IBM BG/Q	2013	EPF Lausanne	839
Blue Brain Viz	IBM Cluster	2013	EPF Lausanne	13
Monch	NEC Cluster	2013 / 14	ETH Zurich	132
Phoenix	x86 Cluster	2007 / 12 / 14 / 15 / 16	CHIPP (LHC Grid)	86
Piz Kesch	Cray CS-Storm	2015	MeteoSwiss	196
Piz Escha	Cray CS-Storm	2015	MeteoSwiss	196
Monte Leone	HP Cluster	2015	User Lab	7 + 15
Grand Tavé	Cray X40	2017	Research & Development	437

“Already envisioned back in 1922 by L. F. Richardson, numerical simulation of weather and climate has been among the success stories of supercomputing. Today we witness another major step forward as our models become capable of explicitly resolving thunderstorms and rain showers. These developments are rather exciting because they allow addressing key uncertainties in our understanding of the climate system.”
David Leutwyler and Nikolina Ban, ETH Zurich

Name
David Leutwyler

Position
Post-doctoral researcher

Institution
ETH Zurich

Background
2006-2009 Bachelor in Environmental Sciences, ETH Zurich
2010-2013 Master in Environmental Sciences, ETH Zurich
2013-2016 Doctor of Science, ETH Zurich
Since 2016 Post-doctoral researcher, ETH Zurich

Area of research
Weather and climate.

Specialised in
Convection-resolving climate modelling.

HPC means for me
A key research tool, helping us to understand how a warmer Planet Earth might look like.

Name
Nikolina Ban

Position
Post-doctoral researcher

Institution
ETH Zurich

Background
2004-2010 Study of Physics and Meteorology, University of Zagreb, Croatia
2011-2014 Doctor of Science, ETH Zurich
Since 2015 Post-doctoral researcher, ETH Zurich

Area of research
Weather and climate.

Specialised in
Convection-resolving climate modelling and extreme precipitation.

HPC means for me
To understand Earth's weather and climate, and to understand how it might change in the future.

Convection-resolving simulation over Europe

When the hybrid supercomputer "Piz Daint" came online in 2014, one of the first science projects that it ran was a convection-resolving simulation of the climate over Europe between 1999 and 2008. Now the researchers have compared and evaluated those simulations against real-world observations and measurement data. It was apparent that the high-resolution simulations far outstripped conventional models at reproducing diurnal cycles of precipitation over the decade, especially in summer. This tells the researcher that simulations like these are not only useful for early warning of storms, but also for long-term climate scenarios and adaptation strategies in the wake of climate change.
(Image: Kurt Abderhalden, 27 April 2016, Lake Constance)

February

27

Introduction to programming Pascal (P100) GPUs with CUDA 8

After upgrading the GPUs of "Piz Daint" to Nvidia Pascal, a three-day course was organised for the user community, intended to offer an introduction to the new GPU model using CUDA 8.

March

20

CSCS becomes PRACE's fifth hosting member

Since the inception of the Partnership for Advanced Computing in Europe (PRACE), Switzerland has been actively represented by ETH Zurich and its affiliated CSCS. Seven years later in 2017, CSCS became the fifth hosting member with "Piz Daint", Europe's most powerful supercomputer.

20 / 23

SOS21

SOS (Sandia, Oak Ridge National Laboratories, Switzerland) is a series of invitation only, highly interactive workshops on distributed supercomputing. CSCS hosted the 21st edition of this series in Davos with more than 82 international participants, focusing on the topic "Convergence with data science: A new beginning for HPC".

April

05 / 07

Intel KNL: Best practices and experiences

CSCS organised a three-day course to introduce the Intel Knights Landing (KNL) architecture. Attendees had access to the test and development system "Grand Tavé", a Cray XC40 featuring Intel KNL compute nodes.

10 / 12

HPC Advisory Council Switzerland Conference 2017

More than 120 professionals attended the eighth Switzerland Conference of the HPC Advisory Council in Lugano. Co-sponsored by CSCS, the conference delved into a wide range of best practices-in applications, tools, techniques, trends, technologies and collaborative partnerships-fostering this expert community and robust research ecosystem.

24

New tape library in production

To cover the increasing archival needs, the existing tape library was replaced by a new IBM TS4500 tape library with an initial potential capacity of 120 PB.

May

08

Webinar on "National and Tier-0 Calls for proposals"

A webinar was organised to help Swiss scientists submit to the National Call and the PRACE Tier-0 Call.

29 / 31

Workshop on directive based GPU programming: OpenACC and OpenMP

A three-day course with lectures and exercises was offered to introduce the two most promising directive based programming models for GPU accelerated architectures: OpenACC and OpenMP.

June

19 / 21

CSCS at ISC17

CSCS and the Swiss HPC community hpc-ch had a brand-new booth at ISC17 in Frankfurt. Attendees could ask about the latest news about CSCS, meet HPC specialists and scientists from different Swiss universities, and get the latest news about HPC in Switzerland.

26 / 28

Fourth PASC Conference in Lugano

Scientists from a wide range of disciplines gathered at the congress centre in Lugano for the fourth annual PASC Conference, locally hosted by the Università della Svizzera italiana. PASC17 grew yet again with a total of 65 sessions and about 400 participants.

28

CSCS Director meets the scientific community in Lugano

At the close of PASC17, CSCS invited the user community to a short User Assembly. The talk, given by CSCS Director Thomas Schulthess, mainly focused on a presentation of Tier-0 and Tier-1 application processes.

July

05

Introduction of the cscs2go platform

A new platform named cscs2go was launched in order to lower barriers and simplify access to world-class HPC compute and storage resources without having to go through any peer-review process.

16/28

CSCS-USI Summer School 2017

CSCS collaborated with the Institute of Computational Science at the Università della Svizzera italiana to organise a summer school dedicated to HPC, which was attended by around 30 students.

August

11

CERN visits CSCS

CERN Director General Fabiola Gianotti and other representatives from CERN and PSI visited CSCS and drafted new plans for further collaborations.

September

03/08

Third EuroHack

The third edition of the GPU programming hackathon in Lugano (EuroHack) allowed 10 development teams, for a total of 50 participants, three days to port their scalable applications to GPU accelerators, or optimize existing GPU-enabled applications, on a state-of-the-art GPU system.

04/06

CSCS-ICS-DADSi Summer School

CSCS, the Institute of Computational Sciences at the Università della Svizzera italiana, and the Data Analytics and Data-Driven Simulations program organised a summer school focused on "Accelerating Data Science with HPC", which took place at CSCS.

22

CSCS staff and user community at the Planetarium

Every year, CSCS organizes an excursion for all its employees. This year the staff spent an entire day in Lucerne and visited the Swiss Museum of Transport. While at the museum, employees as well as members of the user community were invited to a special private session at the Planetarium.

October

02/04

Workshop on advanced C++ for HPC

A three-day workshop gave attendees the opportunity to learn the principles of modern C++ programming for producing type-safe, efficient and portable code.

05/10

Workshop on task-based programming with HPX

A two-day workshop taught participants about programming with HPX. The aim of this course was to introduce students to the HPX library and demonstrate its use in writing task-based programs. The HPX library implements a lightweight threading model that allows concurrent, asynchronous, parallel and distributed programming constructs to coexist within the same application, with a consistent API based on C++ standards and using features to synchronize between tasks.

19

Best IT apprentice

CSCS apprentice David Isztl won 1st prize for the best IT apprentice of the year in Ticino in the System Administrator category.

November

03

Director-General of the European Commission at CSCS

Visit of the Director-General Robert-Jan Smits, the Directorate General for Research and Innovation of the EC and representatives of the Swiss State Secretariat for Education, Research and Innovation: Mauro Dell'Ambrogio, State Secretary for Education, Philipp Langer and Peter Brönnimann; together with Nicoletta Casanova, CEO, Femtoprint.

13/16

CSCS at Supercomputing 2017

CSCS and the Swiss HPC community hpc-ch had a booth at the world's largest supercomputing conference, SC17 in Denver, Colorado, where they presented the latest HPC developments in Switzerland.

23

Two new cabinets for "Piz Daint"

Two additional Cray XC40 multicore cabinets for "Piz Daint" were installed and made available for production computing.

December

04

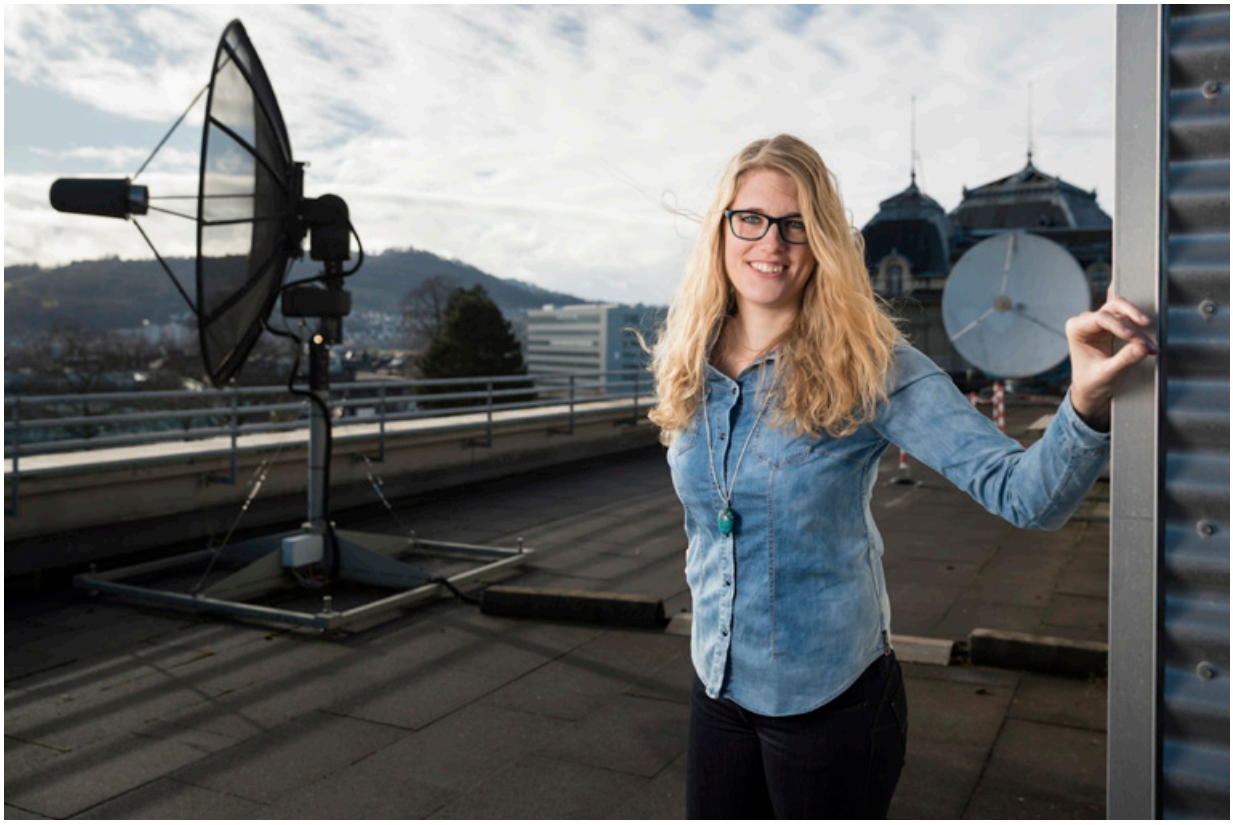
PetaByte Archive service for PSI

A new service for the Paul Scherrer Institute (PSI) has been launched that will allow the long-term storage of large quantities of scientific data produced at PSI in experiments like the SwissFEL or the Swiss Light Source.

12

New website cscs.ch

The CSCS website was fully updated with a new layout and a review of the contents. Accessibility from different devices was improved.



“The modelling of atmospheric dynamics and thermodynamics over the Alpine region, where high mountain peaks overlook deep valleys, heavily depends on the access to supercomputers to obtain high-resolution simulations. Thanks to ‘Piz Daint’ we have the exceptional opportunity to investigate extreme events and the associated underlying mechanisms in the past climate, but even more we can explore changes in the mechanisms of extreme events induced by future changes in climate.”
Martina Messmer, University of Bern

Name
Martina Messmer

Position
Post-doctoral researcher

Institution
University of Bern

Background
2007-2011 Bachelor in Environmental Science, ETH Zurich
2010-2013 Master in Environmental Science, ETH Zurich
2013-2017 PhD in Climate Sciences, University of Bern
Since 2017 Post-doctoral researcher, University of Bern

Area of research
Extratropical cyclones, high-impact weather events and regional climate modelling.

Specialised in
Running regional climate model experiments and analysing the output to understand the underlying processes involved in extratropical cyclones which are associated with high-impact weather events and to investigate possible changes in a warmer climate.

HPC means for me
Having the possibility to increase the resolution of the atmospheric processes not only spatially but also temporally, while the run-time of the simulations is still comparably short, allowing us to perform research beyond state-of-the-art.

Scientists use “Piz Daint” simulations to track heavy summer precipitation from the Mediterranean

Low-pressure weather systems in summer, that move northwards from Italy to central Europe are leading to extreme weather events every few years. The torrential precipitation on the northern side of the Alps and in central Europe often causes the Elbe, Danube and Rhine rivers to swell and flood their respective regions. But from where do they pick up this destructive moisture? The answer to that question has been clarified by climate scientists in Bern by means of simulations they ran on CSCS’s “Piz Daint” supercomputer: most of the moisture derives from the Mediterranean. (Image: Thomas Wüthrich)

Calls and Projects Overview

CSCS being part of PRACE has opened exciting possibilities to scientists in Switzerland and all over the world to address new challenging scientific problems on the top supercomputers in Europe. At the same time, the analysis of CSCS User Lab also confirmed the Swiss research is healthy and roaring.

"Piz Daint": Europe's most powerful supercomputer

CSCS has become the fifth hosting member of the European PRACE alliance, which dedicates large shares of supercomputing resources to the best and most ambitious computational projects pursued at European institutions. PRACE, the Partnership for Advanced Computing in Europe, was initiated in 2009, and has gained significant momentum since it went into its second phase in 2017. As a hosting member, CSCS contributes 15 million node hours per year, all on its flagship computer "Piz Daint", which at 19.59 Petaflops sustained performance currently is the most powerful supercomputer of all Europe.

In spring 2014, CSCS split its program into regular and extreme-scale allocations. The former are still maintained in the national program, but the latter ones, so far known under the name of CHRONOS, have been replaced by large-scale allocations through the PRACE program. The national (Tier-1) program awards allocations of up to 1 million node hours per year while the PRACE (Tier-0) program solicits proposals that request at least 1 million node hours per year and demonstrate the need for accelerated (GPU) computing.

Having CSCS in PRACE is of great advantage to the computational science community in Switzerland. The scientists can choose among different types of extreme-scale computing resources and apply for those best suited to the needs of the project.

These include, among others, the hybrid CPU/GPU architecture available at CSCS, Intel Xeon-Phi accelerated nodes at CINECA (Italy), or large multi-core systems at GENCI (France) and GCS (Germany). Visibility and quality of the Swiss Tier-0 program have much improved since it changed from national (CHRONOS) to European (PRACE) access. The User Lab benefits from additional Level-2 and -3 support for Tier-0 allocations; in particular Level-3 support helps scientists in Switzerland and elsewhere in Europe to achieve more ambitious goals at scale.

Resources allocated in 2017

Analysis of usage statistics shows that Chemistry & Materials remains the most compute-intensive community at CSCS, using 35% of the total allocation. Physics has become a close runner-up, however, at 31% utilization. Earth & Environmental Science have used 10% of the share, almost unchanged from 2016 (11%). Life Science and Mechanics & Engineering, together have used 17%, substantially more than in 2016 (11%), each gaining 3%.

ETH Zurich and EPF Lausanne have still remained the heaviest users at 26% and 21%, respectively. Beyond, however, the usage by institution statistics reflects the growing involvement of CSCS in the PRACE program: A total of 15% of the resources went to European Tier-0 projects of PRACE, including three projects pursued by Swiss scientists. The universities of Zurich, Basel, and Geneva have largely maintained their utilization, at 10, 7, and 2%, respectively. The remaining 20% of the resources have been distributed among other Swiss institutions or went to international groups that applied in the national calls of CSCS because of their need for GPU accelerated architectures.

List of CHRONOS Projects Renewals

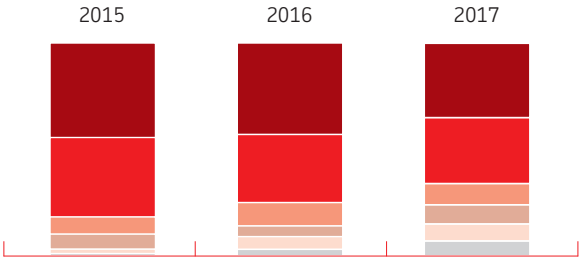
Principal Investigator	Organisation	Research Field	Project Title	Node h
Petros Koumoutsakos	ETH Zurich	Others	Simulation of microfluidics for mechanical cell separation: Building the in-silico lab-on-a-chip	2 150 000
Constantia Alexandrou	University of Cyprus & Institute of Cyprus	Physics	The neutron electric dipole moment and proton charge radius using lattice QCD simulations at physical pion mass	2 000 000

List of PRACE Tier-0 Projects

Principal Investigator	Organisation	Research Field	Project Title	Node h
Xavier Barril	University of Barcelona	Life Science	Understanding TET2 regulation and development of chemical probes that control its function	1 004 410
Richard Bower	Durham University	Physics	EAGLE-XL	441 180
Pino D'Amico	Consiglio Nazionale delle Ricerche Modena	Chemistry & Materials	SIDEX - SIze DEpendence of the EXcitonic properties of MoS2 nanoribbons from many-body perturbation theory	867 650
Ilian T. Iliev	University of Sussex	Physics	Multi-scale simulations of cosmic reionization	500 000
Javier Jimenez	Technical University of Madrid	Mechanics & Engineering	TREC - Time resolved evolution of the energy-containing scales in turbulent channel flow at Ret=5000	1 800 000
Olaf Kaczmarek	University of Bielefeld	Physics	The pseudo-critical line in the QCD phase diagram	980 000
Himanshu Khandelia	University of Southern Denmark	Life Science	FLEXO: The relationship between electrostatic potential and curvature in biomembranes, and its impact on membrane transport	265 000
Thomas Kluge	Helmholtz-Zentrum Dresden-Rossendorf	Physics	Radiation imprint of ultra-intense laser heating of solids	1 602 950
Vittorio Limongelli	Università della Svizzera italiana	Life Science	Homo- and heterodimerization mechanism of chemokines receptors CCR5 and CXCR4 investigated by Coarse-Grained Metadynamics simulations	233 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	High-throughput simulations of transistors based on 2D materials	1 044 120
Nicola Marzari	EPF Lausanne	Chemistry & Materials	Mapping the structures and properties of all bulk forming binary systems: A high-throughput study	1 253 000
Modesto Orozco	Institute for Research in Biomedicine Barcelona	Life Science	Understanding of the molecular basis of the decoding process in prokaryotic and eukaryotic ribosomal A-sites	468 369
Christoph Schär	ETH Zurich	Earth & Environ. Science	Convection-resolving Climate on GPUs (gpuCLIMATE)	1 352 420
Ilpo Vattulainen	Tampere University of Technology	Life Science	Activation mechanism of the beta2-adrenergic receptor	529 200
Gabriel Wlazlowski	University of Warsaw	Physics	Non-equilibrium dynamics in strongly interacting and superfluid Fermi systems	925 000

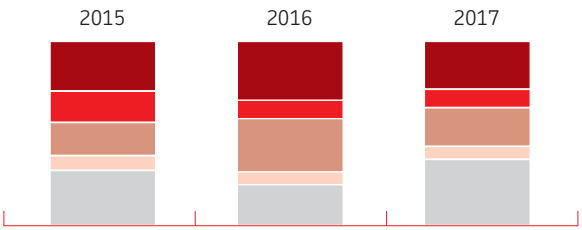
Usage by Research Field (%)

Research Field	2015	2016	2017
Chemistry & Materials	44	43	35
Physics	37	32	31
Earth & Environ. Science	8	11	10
Mechanics & Engineering	7	5	9
Life Science	3	6	8
Others	1	3	7
Total Usage	**100**	**100**	**100**



Usage by Institution (%)

Institution	2015	2016	2017
ETH Zurich	27	32	26
University of Zurich	17	10	10
EPF Lausanne	18	29	21
University of Basel	8	7	7
Others	30	22	36
Total Usage	**100**	**100**	**100**



Largest Projects (> 500 000 Node h)

Principal Investigator	Organisation	Research Field	Project Title	Node h
Stefan Goedecker	University of Basel	Chemistry & Materials	Structure prediction of solids, surfaces and clusters	1 000 000
Nicola Spaldin	ETH Zurich	Chemistry & Materials	Coupled and competing instabilities in complex oxides	1 000 000
Andrew Jackson	ETH Zurich	Earth & Environ. Science	Beyond conventional planetary dynamo models	800 000
Matthias Liebendörfer	University of Basel	Physics	The isotropic diffusion source approximation for the simulation of faint and failed supernova explosions with additional degrees of freedom in the equation of state	750 000
Ulrike Lohmann	ETH Zurich	Earth & Environ. Science	The impact of aerosols in the past, present, and future climate	737 530
Sandra Luber	University of Zurich	Chemistry & Materials	Advancing biomimetic water oxidation catalysis via novel Co(II)-based cubanes	679 000
Carlo Pignedoli	EMPA	Chemistry & Materials	Screening of the electronic and optical properties of carbon based 1D heterostructures	602 000
Franco Vazza	Hamburg Observatory	Physics	Studying extragalactic magnetic field amplifications with the largest MHD cosmological simulation	600 000
Sandra Luber	University of Zurich	Chemistry & Materials	Advancing electronic structure calculations for complex nature-inspired systems	599 000
Jürg Hutter	University of Zurich	Chemistry & Materials	Properties of liquids, solutions, and interfaces from density functional theory	590 000
Martin Kunz	University of Geneva	Physics	Relativistic cosmological simulations with gevolution	504 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	First-principles simulation of van der Waals homo- and hetero-junctions for optoelectronic applications	504 000
Ursula Röthlisberger	EPF Lausanne	Chemistry & Materials	Computational modeling and design of halide perovskites with optimal electronic structures for solar cell applications	501 110
Carlo Massimo Casciola	University of Rome "La Sapienza"	Mechanics & Engineering	Simulations of hydrophobic nanoporous materials immersed in water for energy storage and dissipation	500 000
Dimitri Komatitsch	CNRS Marseille	Earth & Environ. Science	The «CLEAR IMAGE» Project	500 000
Lucio Mayer	University of Zurich	Physics	Mass evolution and collapse of protoplanets in massively parallel radiation-hydro simulations of disk instability with "protoplanet feedback"	500 000
Richard Sandberg	University of Melbourne	Mechanics & Engineering	High-resolution simulations of low-pressure and high-pressure turbine end wall flows	500 000

Transcriptions – *The Medium Is the Message*
William Gibson, Mona Lisa Overdrive (1988)

List of Projects by Institution

CNRS Marseille

The «CLEAR IMAGE» project, Dimitri Komatitsch (Earth & Environmental Science, 500 000 node h)

EMPA

Effect of saccharides on the association of calcium and phosphate ions in solution, Riccardo Innocenti Malini (Chemistry & Materials, 100 000 node h)

Screening of the electronic and optical properties of carbon based 1D heterostructures, Carlo Pignedoli (Chemistry & Materials, 602 000 node h)

EPF Lausanne

Mechanical properties of hybrid halide perovskite photovoltaics: Monitoring humidity-induced degradation with computer simulations, Wanda Andreoni (Chemistry & Materials, 350 000 node h)

Biocompatibility of inorganic biomaterials (in vitro bioactivity protocols for prediction of in vivo implant viability) Paul Bowen (Chemistry & Materials, 38 000 node h)

Local and global gyrokinetic GENE simulations of turbulent transport mechanisms, Stephan Brunner (Physics, 250 000 node h)

CFD study of a trileaflet mechanical heart valve, Angelo Casagrande (Life Science, 48 000 node h)

Towards an accurate, high-throughput framework for the prediction of anharmonic free energies in molecular crystals, Michele Ceriotti (Chemistry & Materials, 90 000 node h)

Molecular dynamics simulation of the nucleation of amorphous sodium chloride in a microfluidic spray dryer, Bingqing Cheng (Chemistry & Materials, 99 100 node h)

Computational design of epitope-focused immunogens for vaccine development, Bruno Correia (Life Science, 100 000 node h)

Cardiac and vascular numerical simulations, Simone Deparis (Computer Science, 350 000 node h)

Simulation of scrape-off-layer plasma turbulence in the TCV tokamak, Ivo Furno (Physics, 420 000 node h)

Energetic particle physics, in magnetically confined configurations, Jonathan Graves (Physics, 174 300 node h)

Simulation of plasma turbulence in the periphery of tokamak devices, Paolo Ricci (Physics, 450 000 node h)

Computational modeling and design of halide perovskites with optimal electronic structures for solar cell applications, Ursula Röthlisberger (Chemistry & Materials, 501 110 node h)

Nanoporous materials genome in action, Berend Smit (Chemistry & Materials, 450 000 node h)

ORB5 – Core and pedestal turbulence, Laurent Villard (Physics, 300 000 node h)

ETH Zurich

Reduction of losses of steam turbine's last stage through stator redesign using high fidelity CFD, Reza Abhari (Mechanics & Engineering, 55 440 node h)

Ultrasound tomography for early breast cancer detection, Christian Boehm (Life Science, 36 000 node h)

Land-climate feedbacks in a changing climate, Edouard Davin (Earth & Environmental Science, 42 000 node h)

Multiscale global Earth model, Andreas Fichtner (Earth & Environmental Science, 470 000 node h)

Investigation of prechamber-induced ignition of natural gas using direct numerical simulations, Christos Frouzakis (Mechanics & Engineering, 400 000 node h)

Advancing electronic structure calculations for complex nature-inspired systems, Chiara Gattinoni (Chemistry & Materials, 200 000 node h)

Aerosol cloud interactions and cloud variability on the regional scale, Jan Henneberger (Earth & Environmental Science, 180 000 node h)

Drops bouncing off macro-textures: Designing surfaces with extreme wettability, Ilya Karlin (Mechanics & Engineering, 100 000 node h)

Cloud cavitation collapse in turbulent flows, Petros Koumoutsakos (Mechanics & Engineering, 320 000 node h)

Hydrated electron's cavity: There and back again, Vladimir Rybkin (Chemistry & Materials, 200 000 node h)

High-resolution glacier modelling with PISM, Julien Seguinot (Earth & Environmental Science, 32 500 node h)

High-frequency Green's function databases for the Mars InSight mission, Martin van Driel (Earth & Environmental Science, 41 600 node h)

Focal adhesion proteins at the membrane, Viola Vogel (Life Science, 180 000 node h)

Hamburg Observatory

Studying extragalactic magnetic field amplifications with the largest MHD cosmological simulation, Franco Vazza (Physics, 600 000 node h)

Hellenic National Metreological Service

Optimization of a calibration procedure for weather prediction model, Antigoni Voudouri (Earth & Environmental Science, 400 000 node h)

Helmholtz-Zentrum Dresden-Rossendorf

Ab-initio simulation of a traveling-wave optical free-electron laser, Alexander Debus (Physics, 350 000 node h)

Imperial College London

Unraveling the microscopic details of ice formationon organic crystals, Gabriele Sosso (Chemistry & Materials, 195 000 node h)

Identifying the Eigenmodes of small averaged perturbations of turbulent channel flow using PyFR, Arvind Iyer (Mechanics & Engineering, 500 000 node h)

IRB Bellinzona

Computational design of ERG inhibitors, Andreas Cavalli (Life Science, 35 800 node h)

IRSOL

Magnetohydrodynamic processes in the solar atmosphere, Oskar Steiner (Physics, 25 000 node h)

Paul Scherrer Institute

Mechanistic understanding of uranium adsorption on clay minerals obtained by combining atomistic simulations and X-ray spectroscopy studies, Sergey Churakov (Earth & Environmental Science, 140 000 node h)

Dissolution, growth and ion uptake at phyllosilicate surfaces: Coupling atomistic interactions at the mineral-water interface with Kinetic Monte Carlo model, Sergey Churakov (Earth & Environmental Science, 160 000 node h)

Computational investigation of extended defects in UO2, Matthias Krack (Chemistry & Materials, 400 000 node h)

Generation-IV European sodium fast reactor: Computation of the core parameters using a high-fidelity Monte Carlo code, Konstantin Mikityuk (Physics, 100 000 node h)

Modelling of conversion of methane to methanol over Cu-exchanged zeolites, Dennis Palagin (Chemistry & Materials, 36 000 node h)

University of Rome "La Sapienza"

Simulations of hydrophobic nanoporous materials immersed in water for energy storage and dissipation, Carlo Massimo Casciola (Mechanics & Engineering, 500 000 node h)

Stanford University

Scaling the legion programming system, Alex Aiken (Computer Science, 50 000 node h)

SUPSI

STORM - Sirna polycaTion cOmplex foRMation, Marco Deriu (Life Science, 51 200 node h)

Univeristy of Geneva

Numerical relativistic cosmological simulation, David Daverio (Physics, 400 000 node h)

Università della Svizzera italiana

Cell biomechanics in flow: Parallel simulations, Igor Pivkin (Life Science, 70 420 node h)

Kinetics of urea decomposition in aqueous solution via enhanced ab-initio molecular dynamics, Daniela Polino (Chemistry & Materials, 270 000 node h)

University of Twente

Sheared Rayleigh-Benard convection, Detlef Lohse (Mechanics & Engineering, 300 000 node h)

University of Basel

Structural insights to combat colistin antibiotic resistance in human pathogens, Olivier Bignucolo (Life Science, 34 280 node h)

Doped insulators at high pressure as the new high temperature superconductors, José Flores-Livas (Chemistry & Materials, 350 000 node h)

University of Bern

Advancing electronic structure calculations for complex nature-inspired systems, Donat Adams (Earth & Environmental Science, 50 000 node h)

Surface structure and water oxidation chemistry on oxynitride surfaces, Ulrich Aschauer (Chemistry & Materials, 300 000 node h)

Virtual laboratories of hot jupiters: Shocks, shear instabilities and how dynamics, chemistry and radiation interact, Kevin Heng (Physics, 96 000 node h)

University of Fribourg

An atomistic view of intracellular lipid droplets and their interactions with proteins, Stefano Vanni (Life Science, 345 000 node h)

University of Latvia

First-principles molecular dynamics simulations of ZnO, Dmitry Bocharovs (Chemistry & Materials, 36 000 node h)

University of Lausanne

Elucidating the closed conformation and protonation sites of acid-sensing ion channel 1, Stephan Kellenberger (Life Science, 35 970 node h)

University of Melbourne

High-resolution simulations of low-pressure and high-pressure turbine end wall flows, Richard Sandberg (Mechanics & Engineering, 500 000 node h)

University of Parma

Ab-initio estimation of contact hyperfine fields in muon spin rotation spectroscopy: Towards a new DFT assisted method for long-range magnetic structure determination, Roberto De Renzi (Chemistry & Materials, 22 480 node h)

University of Rome "Tor Vergata"

Co-translocational unfolding of globular protein through biological nanopores, Mauro Chinappi (Life Science, 34 700 node h)

University of Zurich

The formation of dust in galaxies during the epoch of reionization, Robert Feldmann (Physics, 36 000 node h)

The galactic fountain in Milky Way-type galaxies: Positive feedback and the role of magnetohydrodynamics, Alexander Hobbs (Physics, 60 000 node h)

Computing renal oxygenation in realistic vascular networks for improved treatment of anemia associated with chronic kidney disease, Kartik Jain (Mechanics & Engineering, 36 000 node h)

Advancing electronic structure calculations for complex nature-inspired systems, Sandra Luber (Chemistry & Materials, 599 000 node h)

Solving large-scale public finance models on emerging HPC systems, Simon Scheidegger (Others, 129 000 node h)

Gas in galaxies: Bridging the gap between circum-nuclear and circum-galactic scales at the cosmic noon, Robert Feldmann (Physics, 100 000 node h)

Advancing biomimetic water oxidation catalysis via novel Co(II)-based cubanes, Sandra Luber (Chemistry & Materials, 679 000 node h)

Mass evolution and collapse of protoplanets in massively parallel radiation-hydro simulations of disk instability with "protoplanet feedback", Lucio Mayer (Physics, 500 000 node h)

High-resolution cosmological hydrodynamical simulations of neutral hydrogen in the CMG of massive galaxies, Alireza Rahmati (Physics, 200 000 node h)

Supermassive black hole growth and feedback in high-redshift galaxies, Romain Teyssier (Physics, 200 000 node h)

Renewals

EPF Lausanne

Large-scale atomic simulations of dislocation plasticity and fracture in magnesium and alloys, William Curtin (Chemistry & Materials, 252 000 node h)

Defect and band-edge levels through GW and hybrid functionals, Alfredo Pasquarello (Chemistry & Materials, 270 000 node h)

Novel topological electronic phases of materials, Oleg Yazyev (Chemistry & Materials, 120 000 node h)

THEOS NANO: Thermal, electrical, and optical properties of nanoscale materials, Nicola Marzari (Chemistry & Materials, 400 000 node h)

Halide perovskites for solar cells: In silico design of novel materials, Ursula Röthlisberger (Chemistry & Materials, 200 000 node h)

Study on snow precipitation and accumulation over complex alpine terrain, Michael Lehning (Earth & Environmental Science, 150 000 node h)

Multiscale simulations of biological systems and bioinspired devices, Ursula Röthlisberger (Life Science, 370 000 node h)

Application of Large-Eddy simulation to atmospheric boundary layer flows and transports of scalars above urban surfaces, Wai-Chi Cheng (Mechanics & Engineering, 150 000 node h)

ETH Zurich

Coupled and competing instabilities in complex oxides, Nicola Spaldin (Chemistry & Materials, 1 000 000 node h)

First-principles simulation of van der Waals homo- and heterojunctions for optoelectronic applications, Mathieu Luisier (Chemistry & Materials, 504 000 node h)

Ab-initio simulations of conductive bridging memristors for application as plasmonic optical switches, Mathieu Luisier (Chemistry & Materials, 385 000 node h)

Massively parallel computations for quantifying uncertainity in fluid flows, Siddhartha Mishra (Computer Science, 100 000 node h)

The impact of aerosols in the past, present, and future climate, Ulrike Lohmann (Earth & Environmental Science, 737 530 node h)

Beyond conventional planetary dynamo models, Andrew Jackson (Earth & Environmental Science, 800 000 node h)

Implementation of immersive boundary conditions for modeling, inversion, and imaging: Applications to a wave propagation laboratory, Filippo Broggini (Earth & Environmental Science, 100 000 node h)

Numerical modeling of seismic response of unstable rock slopes, Jan Burjánek (Earth & Environmental Science, 303 000)

The role of mechanics in fracture healing and bone turnover, Harry van Lenthe (Life Science, 70 000 node h)

Learning and optimization for collective swimming, Petros Koumoutsakos (Mechanics & Engineering, 300 000 node h)

Bayesian uncertainty quantification for large-scale predictive simulations in nanotechnology and life sciences, Petros Koumoutsakos (Others, 150 000 node h)

Rice University

High-temperature electronic structure by a novel Monte Carlo method for the warm dense electron gas and plasmonic catalysis, James Shepherd (Chemistry & Materials, 150 000 node h)

Università della Svizzera italiana

Homo- and heterodimerization mechanism of chemokines receptors CCR5 and CXCR4 investigated by coarse-grained metadynamics simulations, Vittorio Limongelli (Life Science, 180 000 node h)

University of Basel

The isotropic diffusion source approximation for the simulation of faint and failed supernova explosions with additional degrees of freedom in the equation of state, Matthias Liebendörfer (Physics, 750 000 node h)

Structure prediction of solids, surfaces and clusters, Stefan Goedecker (Chemistry & Materials, 1 200 000 node h)

University of Bern

Extreme events and underlying mechanisms in the last millennium and implications for the future, Christoph Raible (Earth & Environmental Science, 234 100 node h)

ISOTOPE (modelling ISOTOPEs in the Earth system), Fortunat Joos (Earth & Environmental Science, 29 250 node h)

University of Geneva

Quantum systems with strong correlations: Materials and novel computational approach, Antoine Georges (Chemistry & Materials, 347 000 node h)

Relativistic cosmological simulations with gevolution, Martin Kunz (Physics, 500 000 node h)

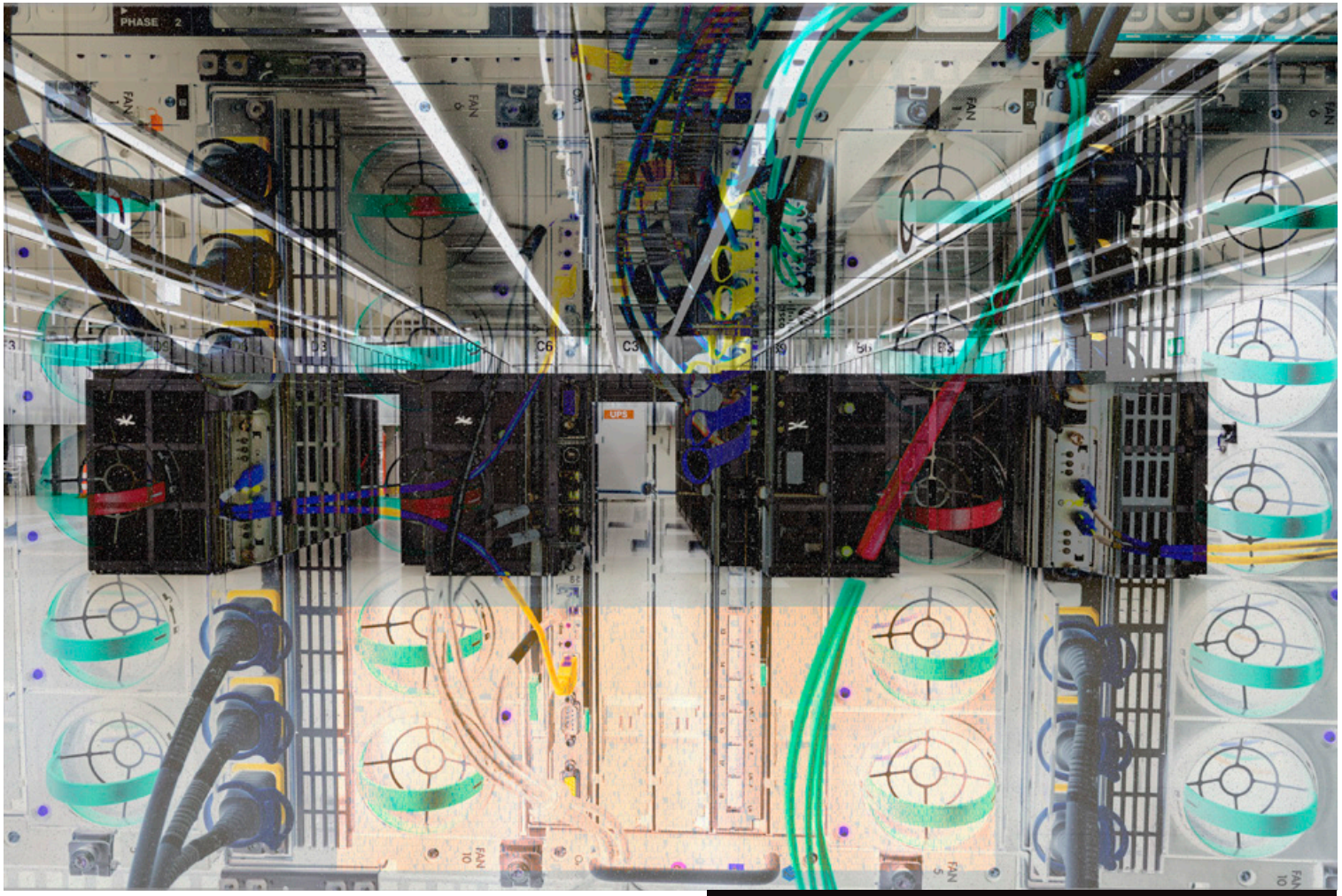
University of Heidelberg

Neutrinos in the aftermath of neutron star mergers, Albino Perego (Physics, 90 000 node h)

University of Zurich

Properties of liquids, solutions, and interfaces from density functional theory, Jürg Hutter (Chemistry & Materials, 590 000 node h)

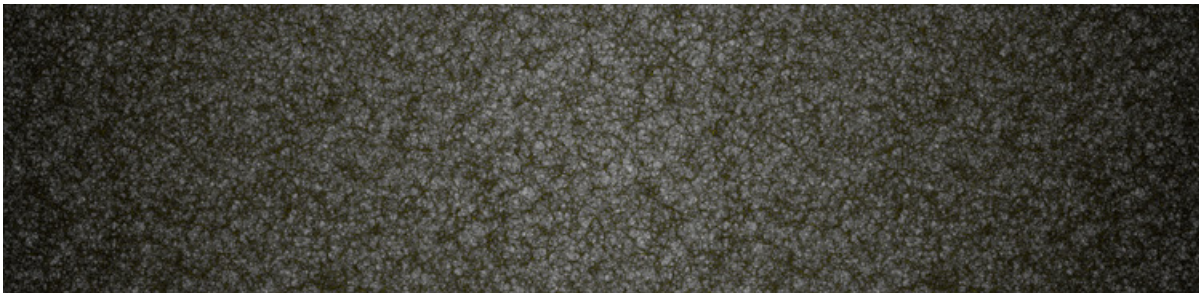
CP2K program development, Jürg Hutter (Chemistry & Materials, 96 000 node h)



Transcriptions – *The Medium Is the Message*
Stanislaw Lem, Solaris (1961)

Ground-breaking simulation for researching the "dark" Cosmos

For the first time, scientists from the University of Zurich have succeeded in carrying out a cosmological simulation with several trillion particles. The simulation on "Piz Daint" provides an important basis for researching the Universe with the Euclid satellite, which will be launched into space in 2021.



A slice through the invisible universe of dark matter: extending from the present, located at the centre, to the most distant regions observable by the Euclid satellite, 10 billion light years to the left and right. The Universe in the past looked considerably smoother. Large empty regions, known as voids, are much more prominent at the present. (Image: Joachim Stadel)

The Universe is a cradle of the unknown. Twenty-three per cent of it is made up of dark matter, while 72 per cent is dark energy, the source and composition of which remains an unsolved mystery for science. Dark energy is thought to influence the formation of structures in the Cosmos and cause the Universe to expand at an ever-increasing rate. The Euclid satellite is set to lift off into space in 2021 and gather data over a period of around six years. New ground-breaking simulations by astrophysicists at the Center for Theoretical Astrophysics and Cosmology at the University of Zurich carried out on "Piz Daint" supercomputer will provide an important basis for the mission. The objective is to research the development of the Universe over the past 10 billion years, uncover the source of dark energy and find out why it is accelerating the expansion of the Universe.

Catalogue of theoretical galaxies

Based on the findings from the simulation of two trillion (2 followed by 12 zeros) particles on "Piz Daint" supercomputer, a theoretical but realistic galaxy catalogue will be created with around 25 billion galaxies from the Universe. This will initially be used to calibrate what the satellite should focus on and measure. As soon as the satellite is active in space, the simulations will be supplemented with additional simulations. The results of the simulations gathered will then be compared against the data measured by the satellite in order to shed light on the sources, composition and effects of the Universe's "dark" components.

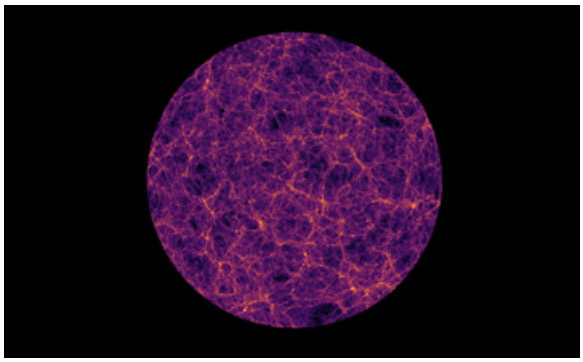
To perform the simulations, the astrophysicists at the University of Zurich spent three years revising a code (PKDGRAV3) that now simulates the accumulations of dark matter – known as halos – in a very precise manner. Galaxies reside within these halos and the density of the dark matter decreases outwards from the centre of each galaxy. At the same time, depending on the galaxy, the mass of the dark matter is 10 to 20 times higher than that of the stars and gases in the galaxy belonging to the halo. In their paper recently published in *Computational Astrophysics and Cosmology*, the researchers explain that the important factors are high-precision in the gravity calculation, a high-degree of accuracy in the different time steps in the simulation and keeping the statistical errors below 1 per cent.

The aim of the scientists Joachim Stadel, Douglas Potter and Romain Teyssier at the University of Zurich was to simulate trillions of particles within a useful timescale that facilitate the creation of the galaxy catalogue necessary for the project. According to the researchers, the code had to be optimised in detail and adjusted for this purpose in such a way as to exploit memory and computing processors in the best possible way. And they succeeded: in just 80 hours, which the researchers say is the fastest time-to-solution simulation with such a high number of particles, the astrophysicists used "Piz Daint" to simulate halos of the dark matter from one tenth of the Milky Way mass. Using another computer model, the researchers in the Euclid consortium then calculated, purely statistically, the galaxies that should be located in the halos.

Simulation as a basis for calibration

"Euclid will make a kind of tomography of the Universe from the dark ages, when the first stars and structures began to form in the Universe around 400 million years after the Big Bang, right up to the present day", explains Joachim Stadel. The galaxy catalogue created will be used beforehand to optimise the observation strategy of the satellite and quantify any sources of error. He explains that the primary function of the present highly precise and large simulations is to calibrate the entire "Euclid pipeline" because one problem is that the processes taking place after the dark period are no longer linear. "When we receive the measurement data, we have to be able to use the simulations to understand the non-linear effects and adjust the parameters accordingly."

On very large length scales, the Universe appears homogeneous, but the smaller the scales, the more inhomogeneous the Universe is, and the processes taking place are no longer linear. Both galaxies and dark matter clump together. This creates fluctuations in the density of the matter. In general, Stadel emphasises that the fluctuations of the mass density react very sensitively to the parameters of the fundamental physics of dark matter and dark energy. As a result, simulations are the only way to create this connection.



Simulation of the complex formed by the dark matter through the action of gravity and the expansion of the Universe. It measures 2.5 billion light years across. Dark regions are voids, bright yellow concentrations are halos, where the density of dark matter is the lowest and highest respectively. Both extremes are delineated and connected by filaments. The bright yellow coloured dark matter halos host the galaxies in our Universe. The simulation is the largest of its kind to date (using 2 trillion particles or resolution elements) and required almost all of the CPU, GPU, memory, network and disk resources of "Piz Daint" during its execution. The data produced has been used to create a giant simulated sky of 50 billion galaxies in order to prepare the Euclid space telescope mission (launch in 2021) to unravel the mysteries of dark matter and dark energy in the Universe. (Image: Joachim Stadel & Doug Potter)

Researchers use weak lensing to measure the material density, and through this also the percentage of dark matter. Weak lensing is the very subtle distortion of the light from background galaxies through the fluctuations in mass density, mainly of dark matter, taking place in the foreground. "It is comparable with the distortion you would see through a glass pane that is not quite even", Stadel says. The notion that mass can affect light in the same way as a lens (gravitational lensing) was one of the predictions made by Albert Einstein in his Theory of General Relativity. As Stadel explains, it is very difficult to determine this distortion in the picture of the galaxies with high precision. However, this is essential in order to determine the fundamental properties of dark matter and dark energy, which is why Euclid has to observe lots of galaxies across large areas of the sky.

In addition to weak lensing, Euclid also uses the effect of what is known as galaxy clustering. The new simulations conducted by the researchers at the University of Zurich will also be used for this method. As Stadel explains, however, these measurements are less direct and based on more assumptions.

Besides the simulation on "Piz Daint", the researchers also tested their new code on the US supercomputer Titan at Oak Ridge National Laboratory in Oak Ridge, Tennessee. Like "Piz Daint", the system is a hybrid supercomputer with graphics processors (GPUs) and traditional processors (CPUs) but is more powerful at the time of simulation. Here, the researchers succeeded in getting the newly revised code for the simulation of no less than eight trillion particles to run on up to 18 000 compute nodes with a peak performance of 10 Petaflops.

Beginning of a paradigm shift

For the scientists at the University of Zurich, the new simulation means the beginning of a paradigm shift in the field of simulations. In another decade, they expect to be able to carry out simulations like this in eight hours or less instead of in 80. It will then no longer be possible to store data and process it later. Stadel and his colleagues believe that analysis instruments would have to practically be installed in the code and used on the fly.

Reference: D. Potter, J. Stadel & R. Teyssier, PKDGRAV3: Beyond trillion particle cosmological simulations for the next era of galaxy surveys, Computational Astrophysics and Cosmology (2017), DOI 10.1186/s40668-017-0021-1

Nano-sensor measures tension of tissue fibres

Computer simulations have helped a team of researchers led by ETH Zurich professor Viola Vogel to develop a peptide that is able to detect the tensional state of tissue fibres. This paves the way for completely novel research approaches in medicine and pharmacology.

Bacteria are able to attach themselves to tissue fibres with the aid of a 'nano-adhesive'. Just how they achieve this was investigated a few years ago by Viola Vogel, Professor of Applied Mechanobiology at ETH Zurich, using computer simulations at CSCS. The researchers simulated how the bacterial nano-adhesive – a peptide thread with several binding sites strung together like pearls – adheres to what are called fibronectin fibres. These form part of the fibrous network in which cells are embedded. Where there is a lesion, the fibronectin fibres become severed.

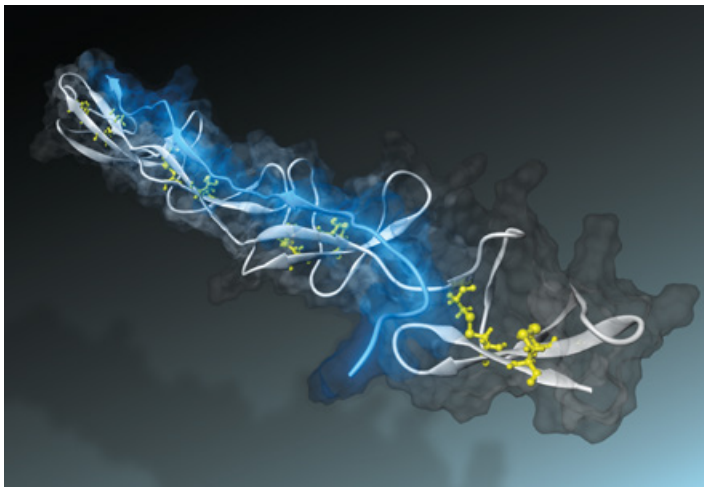
Bacterium senses tensional state of tissue fibres

Intact tissue fibres are held under tension by the pulling force from cells in the fibrous network. When fibronectin fibres are stretched by forces, simulations of this process showed that the distances between the individual binding sites on fibronectin, as bridged by the bacterial peptide, grow too large and hence the bacterial nano-adhesive becomes largely detached.

At the time, the researchers had not expected such results. These suggested that the staphylococcus aureus bacterium, whose adhesion was used in the simulation, might in the course of its evolution have developed a nano-sensor to detect the tensional state of fibronectin fibres. In order to 'successfully' infect a lesion, the dreaded bacterium probably binds itself to severed and therefore structurally relaxed fibres.

However, little is known about the tensional state of tissue fibres and their effect on physiological processes in degenerative changes in tissue, for example. There is also a lack of methods suitable for measuring the minuscule forces that cells exert on tissue fibres.

Viola Vogel and her research group are therefore working on nano-sensors that can do the job: inspired by the simulations, they developed a bacterial peptide able to recognise the tensional states of fibronectin in tissue. Such a peptide could be used both in therapy and diagnostics.



The bacterial peptide (blue) attaches to a fibronectin fibre (white) over several binding sites. (Graphics: Samuel Hertig)

Supercomputer-predicted nano-sensors were tested successfully in animals

Now, tests on the synthetically produced peptide in cell cultures as well as in tumour tissue from animal models have given the researchers positive results. Because the peptide binds to un-tensioned fibres only, it can visibly reveal which tumour tissue fibres are under tension. The research findings were published today in the scientific journal Nature Communications.

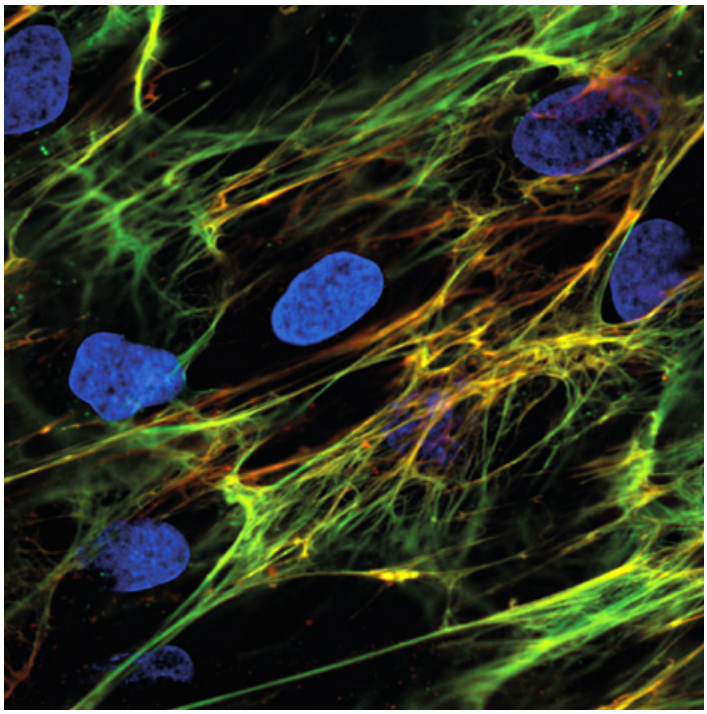
In order to test whether the peptide indeed binds only to un-tensioned fibres, the researchers added to the cell culture medium a special optical 'nano-probe' they had developed. This probe is only usable in cell cultures, where it changes colour to indicate the tensional state of the fibres. In addition, the researchers tagged the synthetically produced peptide with an additional fluorophore in order to visualize where it binds in cell culture.
Furthermore, tumour tissues were stained with special colour-tagged peptide and antibodies that bind to all fibronectin, where they rendered visible all fibronectin fibres in the tumour versus the relaxed fibres as marked by the peptide.

Not every fibre is under tension

Detailed examination of the tumour revealed to the scientists' astonishment that the peptides did not bind to all of the fibronectin fibres, though – a sign that not every fibre in the tumour is under tension. "However, we cannot yet say why tensioned fibronectin is more abundant in some areas of the tumour than in others," says Vogel.

In order to find out whether the bacterial adhesive is suitable for diagnostic purposes as well, researchers at the Paul Scherrer Institute led by Martin Behé and Roger Schibli injected radioactively tagged peptides into the animal model. This enabled the scientists to identify where the peptide binds in the organism. “Besides the well-perfused organs such as kidneys, liver and spleen, the peptide mainly accumulated in tumour tissue,” says Viola Vogel. This was also where it remained the longest.

The scientists hope that the peptides will be able to serve as diagnostic markers of tumour tissues and of other degenerative diseases. The peptides could be used for radiation therapy or for delivering active pharmaceutical ingredients to the diseased site, for example by binding an active ingredient to the bacterial peptide, whereupon the peptide’s binding sensors bring the active ingredient straight to its target. The great advantage of peptides is that they are much smaller than nanoparticles and antibodies. “These little molecules can therefore penetrate much better and deeper into dense tumour tissue,” says Vogel.



Cells are surrounded by extracellular matrix fibres, which they stretch and thereby change their functionality. The cell nuclei (blue) are shown together with fibronectin fibres (green), whereby the relaxed fibres are stained with a bacterial peptide (red). (Image: Viola Vogel group)

Examining possible applications

Both the results and Vogel’s novel research approach in the quest for new methods of diagnostics and therapy have attracted attention: in addition to an ERC and a recently awarded SNF grant, the renowned Charité university hospital in Berlin has conferred on Viola Vogel an Einstein Professorship that will enable her to fund two positions, making it possible to combine the new technique with clinical research. In cooperation with Paul Scherrer Institute, Vogel also intends to investigate which types of tissues and diseases can be best targeted by the peptide.

It has been a long road from the first simulations at CSCS and laboratory tests to animal models, Viola Vogel points out. The experimental sciences routinely take a critical view of research based on simulations. But the ETH professor refutes this perception: “Through simulations we try to sharpen our thinking about molecular processes.” The researcher is convinced that the present findings could not have been achieved without simulations. “This brings us clearly to the point where simulations have predictive value,” says Vogel.

Reference: Arnoldini et al., Novel peptide probes to assess the tensional state of fibronectin fibres in cancer, Nature Communications (2017), DOI 10.1038/s41467-017-01846-0.

Papers with Highest Journal Impact Factor[1)]

Nature
Impact Factor: 40.14

W. Karim, C. Spreafico, A. Kleibert, J. Gobrecht, J. VandeVondele, Y. Ekinci, J. A. van Bokhoven, Catalyst support effects on hydrogen spillover, Nature, DOI 10.1038/nature20782.

Nature Nanotechnology
Impact Factor: 38.99

E. R. Cruz-Chú, E. Papadopoulou, J. H. Walther, A. Popadić, G. Li, M. Praprotnik, P. Koumoutsakos, On phonons and water flow enhancement in carbon nanotubes, Nature Nanotechnology, DOI 10.1038/nnano.2017.234.

Science
Impact Factor: 37.21

V. L. Sushkevich, D. Palagin, M. Ranocchiari, J. A. Van Bokhoven, Selective anaerobic oxidation of methane enables direct synthesis of methanol, Science, DOI 10.1126/science.aam9035.

ACS Nano
Impact Factor: 13.94

M. Schwarz, A. Riss, M. Garnica, J. Ducke, P. S. Deimel, D. A. Duncan, P. K. Thakur, T.-L. Lee, A. P. Seitsonen, J. V. Barth, F. Allegretti, W. Auwärter, Corrugation in the weakly interacting hexagonal-BN/Cu(111) system: Structure determination by combining noncontact atomic force microscopy and X-ray standing waves, ACS Nano, DOI 10.1021/acsnano.7b04022.

M.-W. Chen, D. Ovchinnikov, S. Lazar, M. Pizzochero, M. B. Whitwick, A. Surrente, M. Baranowski, O. L. Sanchez, P. Gillet, P. Plochocka, O. V. Yazyev, A. Kis, Highly oriented atomically thin ambipolar $MoSe_2$ grown by molecular beam epitaxy, ACS Nano, DOI 10.1021/acsnano.7b02726.

G. E. Pacchioni, M. Pivetta, L. Gragnaniello, F. Donati, G. Autès, O. V. Yazyev, S. Rusponi, H. Brune, Two-orbital kondo screening in a self-assembled metal–organic complex, ACS Nano, DOI 10.1021/acsnano.6b07431.

L. Talirz, H. Sode, T. Dumslaff, S. Y. Wang, J. R. Sanchez-Valencia, J. Liu, P. Shinde, C. A. Pignedoli, L. Liang, V. Meunier, N. C. Plumb, M. Shi, X. Feng, A. Narita, K. Müllen, R. Fasel, P. Ruffieux, On-surface synthesis and characterization of 9-atom wide armchair graphene nanoribbons, ACS Nano, DOI 10.1021/acsnano.6b06405.

Journal of the American Chemical Society
Impact Factor: 13.86

F. Y. Song, R. Moré, M. Schilling, G. Smolentsev, N. Azzaroli, T. Fox, S. Luber, G. R. Patzke, $\{Co_4O_4\}$ and $\{CoxNi_{4-x}O_4\}$ cubane water oxidation catalysts as surface cut-outs of cobalt oxides, Journal of the American Chemical Society, DOI 10.1021/jacs.7b07361.

R. Casasnovas, V. Limongelli, P. Tiwary, P. Carloni, M. Parrinello, Unbinding kinetics of a p38 MAP kinase Type II inhibitor from metadynamics simulations, Journal of the American Chemical Society, DOI 10.1021/jacs.6b12950.

J. I. Urgel, H. Hayashi, M. Di Giovannantonio, C. A. Pignedoli, S. Mishra, Deniz, O. M. Yamashita, T. Dienel, P. Ruffieux, H. Yamada, R. Fasel, On-surface synthesis of heptacene organometallic complexes, Journal of the American Chemical Society, DOI 10.1021/jacs.7b05192.

G. Bauer, D. Ongari, X. Y. Xu, D. Tiana, B. Smit, M. Ranocchiari, Metal-organic frameworks invert molecular reactivity: Lewis acidic phosphonium zwitterions catalyze the Aldol-Tishchenko reaction, Journal of the American Chemical Society, DOI 10.1021/jacs.7b10928.

Physical Review X
Impact Factor: 12.79

Q. N. Meier, M. Lilienblum, S. M. Griffin, K. Conder, E. Pomjakushina, Z. Yan, E. Bourret, D. Meier, F. Lichtenberg, E. K. H. Salje, N. A. Spaldin, M. Fiebig, A. Cano, Global formation of topological defects in the multiferroic hexagonal manganites, Physical Review X, DOI 10.1103/PhysRevX.7.041014.

Nano Letters
Impact Factor: 12.71

J. Gooth, M. Borg, H. Schmid, V. Schaller, S. Wirths, K. E. Moselund, M. Luisier, S. Karg, H. Riel, Ballistic one-dimensional InAs nanowire cross-junction interconnects, Nano Letters, DOI 10.1021/acs.nanolett.7b00400.

S. N. Raja, R. Rhyner, K. Vuttivorakulchai, M. Luisier, D. Poulikakos, Length scale of diffusive phonon transport in suspended thin silicon nanowires, Nano Letters, DOI 10.1021/acs.nanolett.6b04050.

A. Cepellotti, N. Marzari, Boltzmann transport in nanostructures as a friction effect, Nano Letters, DOI 10.1021/acs.nanolett.7b01202.

[1)] 2017 JCR Science Edition, ISI Web of Knowledge℠

R. U. Chandrasena, W. B. Yang, Q. Y. Lei, M. U. Delgado-Jaime, K. D. Wijesekara, M. Golalikhani, B. A. Davidson, E. Arenholz, K. Kobayashi, M. Kobata, F. M. F. de Groot, U. Aschauer, N. A. Spaldin, X. X. Xi, A. X. Gray, Strain-engineered oxygen vacancies in $CaMnO_3$ thin films, Nano Letters, DOI 10.1021/acs.nanolett.6b03986.

Advanced Functional Materials

Impact Factor: 12.12

S. Ohno, S.; U. Aydemir, M. Amsler, J.-H. Pöhls, S. Chanakian, A. Zevalkink, M.A. White, S. K. Bux, C. Wolverton, G. J. Snyder, Achieving zT > 1 in inexpensive Zintl phase $Ca_9Zn^{4+x}Sb_9$ by phase boundary mapping, Advanced Functional Materials, DOI 10.1002/adfm.201606361.

Nature Communications

Impact Factor: 12.12

S. Arnoldini, A. Moscaroli, M. Chabria, M. Hilbert, S. Hertig, R. Schibli, M. Béhé, V. Vogel, Novel peptide probes to assess the tensional state of fibronectin fibers in cancer, Nature Communications, DOI 10.1038/s41467-017-01846-0.

I. Piquero-Zulaica, J. Lobo-Checa, A. Sadeghi, Z. M. Abd El-Fattah, C. Mitsui, T. Okamoto, R. Pawlak, T. Meier, A. Arnau, J. E. Ortega, J. Takeya, S. Goedecker, E. Meyer, S. Kawai, Precise engineering of quantum dot array coupling through their barrier widths, Nature Communications, DOI 10.1038/s41467-017-00872-2.

Proceedings of the National Academy of Sciences of the United States of America

Impact Factor: 9.66

F. Moraca, J. Amato, F. Ortuso, A. Artese, B. Pagano, E. Novellino, S. Alcaro, M. Parrinello, V. Limongelli, Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1612627114.

M. Invernizzi, O. Valsson, M. Parrinello, Coarse graining from variationally enhanced sampling applied to the Ginzburg-Landau model, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1618455114.

E. Caldarulo, A. Barducci, K. Wüthrich, M. Parrinello, Prion protein $\beta 2$- $\alpha 2$ loop conformational landscape, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1712155114.

Chemistry of Materials

Impact Factor: 9.47

H. A. Eivari, S. A. Ghasemi, H. Tahmasbi, S. Rostami, S. Faraji, R. Rasoulkhani, S. Goedecker, M. Amsler, Two-dimensional hexagonal sheet of TiO_2, Chemistry of Materials, DOI 10.1021/acs.chemmater.7b02031.

M. Amsler, S. M. Clarke, J. P. S. Walsh, T. Yu, Y. Wang, Y. Meng, S. D. Jacobsen, C. Wolverton, D. E. Freedman, Creating binary Cu–Bi compounds via high-pressure synthesis: A combined experimental and theoretical study, Chemistry of Materials, DOI 10.1021/acs.chemmater.7b01418.

M. Graužinytė, S. Goedecker, J. A. Flores-Livas, Computational screening of useful hole electron dopants in SnO_2, Chemistry of Materials, DOI 10.1021/acs.chemmater.7b03862.

S. M. Griffin, M. Reidulff, S. M. Selbach, N. A. Spaldin, Defect chemistry as a crystal structure design parameter: Intrinsic point defects and Ga substitution in $InMnO_3$, Chemistry of Materials, DOI 10.1021/acs.chemmater.6b04207.

Journal of Physical Chemistry Letters

Impact Factor: 9.35

S. R. Jensen, S. Saha, J. A. Flores-Livas, W. Huhn, V. Blum, S. Goedecker, L. Frediani, The elephant in the room of density functional theory calculations, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b00255.

F. Palazzesi, O. Valsson, M. Parrinello, Conformational entropy as collective variable for proteins, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b01770.

G. Piccini, J. J. McCarty, O. Valsson, M. Parrinello, Variational flooding study of a SN2 reaction, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.6b02852.

G. Piccini, D. Polino, M. Parrinello, Identifying slow molecular motions in complex chemical reactions, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b01889.

F. Ambrosio, G. Miceli, A. Pasquarello, Electronic levels of excess electrons in liquid water, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b00699.

J. Wiktor, U. Röthlisberger, A. Pasquarello, Predictive determination of band gaps of inorganic halide perovskites, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b02648.

O. A. Syzgantseva, M. Saliba, M. Grätzel, U. Röthlisberger, Stabilization of the perovskite phase of formamidinium lead triiodide by methylammonium, Cs, and/or Rb Doping, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.6b03014.

N. J. Browning, R. Ramakrishnan, O. A. von Lilienfeld, U. Röthlisberger, Genetic optimization of training sets for improved machine learning models of molecular properties, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b00038.

V. V. Rybkin, J. VandeVondele, Nuclear quantum effects on aqueous electron attachment and redox properties, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b00386.

Journal of Materials Chemistry A

Impact Factor: 8.87

S. Saedy, D. Palagin, O. Safonova, J. A. Van Bokhoven, A. A. Khodadadi, Y. Mortazavi, Understanding the mechanism of synthesis of Pt3Co intermetallic nanoparticles via preferential chemical vapor deposition, Journal of Materials Chemistry A, DOI 10.1039/C7TA06737B.

Chemical Science

Impact Factor: 8.67

J. Li, B. Zhang, G. Médard, A. P. Seitsonen, F. Haag, F. Allegretti, J. Reichert, B. Kuster, J. V. Barth, A. C. Papageorgiou, N-heterocyclic carbenes on the close packed coinage metal surfaces: Bis-carbene metal adatom bonding scheme of monolayer films on Au, Ag and Cu, Chemical Science, DOI 10.1039/C7SC03777E.

Physical Review Letters

Impact Factor: 8.46

S. Groth, T. Dornheim, T. Sjostrom, F. D. Malone, W. M. C. Foulkes, M. Bonitz, Ab-initio exchange-correlation free energy of the uniform electron gas at warm dense matter conditions, Physical Review Letters, DOI 10.1103/PhysRevLett.119.135001.

D. M. Juraschek, M. Fechner, N. A. Spaldin, Ultrafast structure switching through nonlinear phononics, Physical Review Letters, DOI 10.1103/PhysRevLett.118.054101.

D. Montanino, F. Vazza, A. Mirizzi, M. Viel, Enhancing the spectral hardening of cosmic TeV photons by mixing with axionlike particles in the magnetized cosmic web, Physical Review Letters, DOI 10.1103/PhysRevLett.119.101101.

N. Xu, G. Autès, C. E. Matt, B. Q. Lv, M. Y. Yao, F. Bisti, V. N. Strocov, D. Gawryluk, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, T. Qian, O. V. Yazyev, J. Mesot, H. Ding, M. Shi, Distinct evolutions of Weyl fermion auasiparticles and Fermi arcs with bulk band topology in Weyl semimetals, Physical Review Letters, DOI 10.1103/PhysRevLett.118.106406.

Transcriptions – *The Medium Is the Message*
Ray Bradbury, Fahrenheit 451 (1953)

Transcriptions – *The Medium Is the Message*
William Gibson, Neuromancer (1984)

Papers Published in 2017 by Principal Investigator[1)]

Reza S. Abhari, ETH Zurich

I. Papagiannis, A. Raheem, A. Basol, A. Kalfas, R. Abhari, H. Fukushima, S. Senoo, Unsteady flow mechanisms in the last stage of a transonic low pressure steam turbine-multistage effects and tip leakage flows, Journal of the Global Power and Propulsion Society, DOI 10.22261/F4IW8S.

Alex Aiken, Stanford University

A. Heirich, E. Slaughter, M. Papadakis, W. Lee, T. Biedert, A. Aiken, In situ visualization with task-based parallelism, ISAV' 17, Proceedings of the In Situ Infrastructures on Enabling Extreme-Scale Analysis and Visualization, DOI 10.1145/3144769.3144771.

Sebnem Aksoyoglu, Paul Scherrer Institute

S. Aksoyoglu, G. Ciarelli, I. El-Haddad, U. Baltensperger, A. S. H. Prévôt, Secondary inorganic aerosols in Europe: Sources and the significant influence of biogenic VOC emissions, especially on ammonium nitrate, Atmospheric Chemistry and Physics, DOI 10.5194/acp-17-7757-2017.

G. Ciarelli, S. Aksoyoglu, I. El Haddad, E. A. Bruns, M. Crippa, L. Poulain, M. Äijälä, S. Carbone, E. Freney, C. O'Dowd, U. Baltensperger, A. S. H. Prévôt, Modelling winter organic aerosol at the European scale with CAMx: Evaluation and source apportionment with a VBS parameterization based on novel wood burning smog chamber experiments, Atmospheric Chemistry and Physics, DOI 10.5194/acp-17-7653-2017.

Constantia Alexandrou, University of Cyprus and the Cyprus Institute

C. Alexandrou, M. Constantinou, K. Hadjiyiannakou, K. Jansen, C. Kallidonis, G. Koutsou, A. Vaquero Aavilés-Casco, C. Wiese, Nucleon spin and momentum decomposition using lattice QCD simulations, Physical Review Letters, DOI 10.1103/PhysRevLett.119.142002.

C. Alexandrou, M. Constantinou, K. Hadjiyiannakou, K. Jansen, C. Kallidonis, G. Koutsou, A. Vaquero Avilés-Casco, Nucleon electromagnetic form factors using lattice simulations at the physical point, Physical Review D, DOI 10.1103/PhysRevD.96.034503.

C. Alexandrou, M. Constantinou, K. Hadjiyiannakou, K. Jansen, C. Kallidonis, G. Koutsou, A. Vaquero Avilés-Casco, Nucleon axial form factors using $N_f = 2$ twisted mass fermions with a physical value of the pion mass, Physical Review D, DOI 10.1103/PhysRevD.96.054507.

C. Alexandrou, C. Kallidonis, Low-lying baryon masses using $N_f = 2$ twisted mass clover-improved fermions directly at the physical pion mass, Physical Review D, DOI 10.1103/PhysRevD.96.034511.

C. Alexandrou, M. Constantinou, P. Dimopoulos, R. Frezzotti, K. Hadjiyiannakou, K. Jansen, C. Kallidonis, B. Kostrzewa, G. Koutsou, M. Mangin-Brinet, A. Vaquero Avilès-Casco, U. Wenger, Nucleon scalar and tensor charges using lattice QCD simulations at the physical value of the pion mass, Physical Review D, DOI 10.1103/PhysRevD.96.099906, 10.1103/PhysRevD.95.114514.

C. Alexandrou, Novel applications of lattice QCD: Parton distributions, proton charge radius and neutron electric dipole moment, EPJ Web of Conferences, XIIth Quark Confinement & the Hadron Spectrum, DOI 10.1051/epjconf/201713701004.

N. G. Stefanis, C. Alexandrou, T. Horn, H. Moutarde, I. Scimemi, Round table: Nucleon tomography. What can we do better today than Rutherford 100 years ago? EPJ Web of Conferences, XIIth Quark Confinement & the Hadron Spectrum, DOI 10.1051/epjconf/201713701003.

C. Alexandrou, M. Constantinou, K. Hadjiyiannakou, K. Jansen, H. Panagopoulos, C. Wiese, Gluon momentum fraction of the nucleon from lattice QCD, Physical Review D, DOI 10.1103/PhysRevD.96.054503.

Maximilian Amsler, Northwestern University

H. A. Eivari, S. A. Ghasemi, H. Tahmasbi, S. Rostami, S. Faraji, R. Rasoulkhani, S. Goedecker, M. Amsler, Two-dimensional hexagonal sheet of TiO_2, Chemistry of Materials, DOI 10.1021/acs.chemmater.7b02031.

M. Amsler, C. Wolverton, Dense superconducting phases of copper-bismuth at high pressure, Physical Review Materials, DOI 10.1103/PhysRevMaterials.1.031801.

R. Rasoulkhani, H. Tahmasbi, S. A. Ghasemi, S. Faraji, S. Rostami, M. Amsler, Energy landscape of ZnO clusters and low-density polymorphs, Physical Review B, DOI 10.1103/PhysRevB.96.064108.

G. Fisicaro, M. Sicher, M. Amsler, S. Saha, L. Genovese, S. Goedecker, Surface reconstruction of fluorites in vacuum and aqueous environment, Physical Review Materials, DOI 10.1103/PhysRevMaterials.1.033609.

[1)] Citations based on ISI Web of Knowledge℠

M. Amsler, S. M. Clarke, J. P. S. Walsh, T. Yu, Y. Wang, Y. Meng, S. D. Jacobsen, C. Wolverton, D. E. Freedman, Creating binary Cu–Bi compounds via high-pressure synthesis: A combined experimental and theoretical study, Chemistry of Materials, DOI 10.1021/acs.chemmater.7b01418.

S. Ohno, U. Aydemir, M. Amsler, J.-H. Pöhls, S. Chanakian, A. Zevalkink, M. A. White, S. K. Bux, C. Wolverton, G. J. Snyder, Achieving zT > 1 in inexpensive Zintl phase Ca_9Zn_{4+x} Sb_9 by phase boundary mapping, Advanced Functional Materials, DOI 10.1002/adfm.201606361.

M. Amsler, S. S. Naghavi, C. Wolverton, Prediction of superconducting iron–bismuth intermetallic compounds at high pressure, Chemical Science, DOI 10.1039/C6SC04683E.

S. Faraji, S. A. Ghasemi, S. Rostami, R. Rasoulkhani, B. Schaefer, S. Goedecker, M. Amsler, High accuracy and transferability of a neural network potential through charge equilibration for calcium fluoride, Physical Review B, DOI 10.1103/PhysRev B.95.104105.

Wanda Andreoni, EPF Lausanne

M. Spina, A. Karimi, W. Andreoni, C. A. Pignedoli, B. Náfrádi, L. Forró, E. Horváth, Mechanical signatures of degradation of the photovoltaic perovskite $CH_3NH_3PbI_3$ upon water vapor exposure, Applied Physics Letters, DOI 10.1063/1.4978687.

Hartwig Anzt, University of Tennessee

H. Anzt, T. K. Huckle, J. Bäckle, J. Dongarra, Incomplete sparse approximate inverses for parallel preconditioning, Parallel Computing, DOI 10.1016/j.parco.2017.10.003.

H. Anzt, G. Collins, J. Dongarra, G. Flegar, E. S. Quintana-Ortí, Flexible batched sparse matrix-vector product on GPUs, ScalA'17, Proceedings of the 8th Workshop on Latest Advances in Scalable Algorithms for Large-Scale Systems, DOI 10.1145/3148226.3148230.

G. Flegar, H. Anzt, Overcoming load imbalance for irregular sparse matrices, IA3'17 Proceedings of the Seventh Workshop on Irregular Applications: Architectures and Algorithms, DOI 10.1145/3149704.3149767.

H. Anzt, J. Dongarra, G. Flegar, E. S. Quintana-Ortí, A. E. Tomás, Variable-size batched Gauss-Huard for block-Jacobi preconditioning, Procedia Computer Science, DOI 10.1016/j.procs.2017.05.186.

H. Anzt, J. Dongarra, G. Flegar, E. S. Quintana-Ortí, Variable-size batched LU for small matrices and its integration into block-Jacobi preconditioning, 46th International Conference on Parallel Processing (ICPP), DOI 10.1109/ICPP.2017.18.

Simone Bernèche, University of Basel

F. T. Heer, D. J. Posson, W. Wojtas-Niziurski, C. M. Nimigean, S. Bernèche, Mechanism of activation at the selectivity filter of the KcsA channel, eLife, Biophysics and Structural Biology, DOI 10.7554/eLife.25844.

Y. Xu, A. Seelig, S. Bernèche, Unidirectional transport mechanism in an ATP dependent exporter, ACS Central Science, DOI 10.1021/acscentsci.7b00068.

George Biros, University of Texas at Austin

C. D. Yu, J. Levitt, S. Reiz, G. Biros, Geometry-oblivious FMM for compressing dense SPD matrices, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, SC' 17 Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, DOI 10.1145/3126908.3126921.

Filippo Broggini, ETH Zurich

D. Sollberger, S. A. Greenhalgh, C. Schmelzbach, C. Van Renterghem, J. O. A. Robertsson, 6-C polarisation analysis using point-measurements of translational and rotational ground-motion: Theory and applications, Geophysical Journal International, DOI 10.1093/gji/ggx542.

Dominik Brunner, EMPA

Y. Liu, N. Gruber, D. Brunner, Spatiotemporal patterns of the fossil-fuel CO_2 signal in central Europe: Results from a high-resolution atmospheric transport model, Atmospheric Chemistry and Physics, DOI 10.5194/acp-17-14145-2017.2017.

B. Oney, N. Gruber, S. Henne, M. Leuenberger, D. Brunner, A CO-based method to determine the regional biospheric signal in atmospheric CO_2, Tellus Series B-Chemical and Physical Meteorology, DOI 10.1080/16000889.2017.1353388.

Stephan Brunner, EPF Lausanne

J. Dominski, B. F. McMillan, S. Brunner, G. Merlo, T. M. Tran, L. Villard, An arbitrary wavelength solver for global gyrokinetic simulations, application to the study of fine radial structures on microinstabilities due to non-adiabatic passing electron dynamics, Physics of Plasmas, DOI 10.1063/1.4976120.

A. Mariani, S. Brunner, J. Dominski, A. Merle, G. Merlo, O. Sauter, T. Görler, F. Jenko, D. Told, Identifying microturbulence regimes in a TCV discharge making use of physical constraints on particle and heat fluxes, Physics of Plasmas, DOI 10.1063/1.5006408.

G. Merlo, S. Brunner, Z. Huang, S. Coda, T. Görler, L. Villard, N. A. Banon, J. Dominski, M. Fontana, F. Jenko, L. Porte, D. Told, Investigating the radial structure of axisymmetric fluctuations in the TCV tokamak with local and global gyrokinetic gene simulations, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/aaa2dc.

Amedeo Caflisch, University of Zurich

C. Langini, A. Caflisch, A. Vitalis, The ATAD2 bromodomain binds different acetylation marks on the histone H4 in similar fuzzy complexes, Journal of Biological Chemistry, DOI 10.1074/jbc.M117.786350.

M. Bacci, J. Vymetal, M. Mihajlovic, A. Caflisch, A. Vitalis, Amyloid b fibril elongation by monomers involves disorder at the Tip, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.7b00662.

M. Bacci, C. Langini, J. Vymetal, A. Caflisch, A. Vitalis, Focused conformational sampling in proteins, Journal of Chemical Physics, DOI 10.1063/1.4996879.

Michele Ceriotti, EPF Lausanne

C. Liang, G. Tocci, D. M. Wilkins, A. Grisafi, S. Roke, M. Ceriotti, Solvent fluctuations and nuclear quantum effects modulate the molecular hyperpolarizability of water, Physical Review B, DOI 10.1103/PhysRevB.96.041407.

Shyam S. Chikatamarla, ETH Zurich

B. Dorschner, S. S. Chikatamarla, I. V. Karlin, Transitional flows with the entropic lattice Boltzmann method, Journal of Fluid Mechanics, DOI 10.1017/jfm.2017.356.

A. M. Moqaddam, S. S. Chikatamarla, I. V. Karlin, Drops bouncing off macro-textured superhydrophobic surfaces, Journal of Fluid Mechanics, DOI 10.1017/jfm.2017.306.

B. Dorschner, S. S. Chikatamarla, I. V. Karlin, Entropic multirelaxation-time lattice Boltzmann method for moving and deforming geometries in three dimensions, Physical Review E, DOI 10.1103/PhysRevE.95.063306.

Mauro Chinappi, University of Rome Tor Vergata

E. L. Bonome, F. Cecconi, M. Chinappi, Electroosmotic flow through an a-hemolysin nanopore, Microfluidics and Nanofluidics, DOI 10.1007/s10404-017-1928-1.

Sergey Churakov, Paul Scherrer Institute

A. Kéri, R. Dähn, M. Krack, S. V. Churakov, Combined XAFS Spectroscopy and ab-initio study on the characterization of iron incorporation by montmorillonite, Environmental Science & Technology, DOI 10.1021/acs.est.7b01670.

S. V. Churakov, C. Labbez, Thermodynamics and molecular mechanism of Al incorporation in calcium silicate hydrates, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.6b12850.

G. Cametti, S. Churakov, T. Armbruster, Reinvestigation of the zemannite structure and its dehydration behavior: A single-crystal X-ray and atomistic simulation study, European Journal of Mineralogy, DOI 10.1127/ejm/2017/0029-2587.

G. Cametti, T. Armbruster, J. Hermann, S. Churakov, Crystal structure and phase transition in noelbensonite: A multimethodological study, Physics and Chemistry of Minerals, DOI 10.1007/s00269-017-0876-3.

William A. Curtin, EPF Lausanne

B. Yin, Z. Wu, W. A. Curtin, Comprehensive first-principles study of stable stacking fault energy in hpc metals, Acta Materialia, DOI 10.1016/j.actamat.2016.10.042.

Simone Deparis, EPF Lausanne

N. Dal Santo, S. Deparis, A. Manzoni, A numerical investigation of multi space reduced basis preconditioners for parametrized elliptic advection-diffusion equations, Communications in Applied and Industrial Mathematics, DOI 10.1515/caim-2017-0015.

D. Forti, M. Bukac, A. Quaini, S. Canic, S. Deparis, A monolithic approach to fluid–composite structure interaction, Journal of Scientific Computing, DOI 10.1007/s10915-017-0363-5.

Marco A. Deriu, SUPSI

M. A. Deriu, M. Cangiotti, G. Grasso, G. Licandro, A. Lavasanifar, J. A. Tuszynski, M. F. Ottaviani, A. Danani, Self-assembled ligands targeting TLR7: A molecular level investigation, Langmuir, DOI 10.1021/acs.langmuir.7b03168.

G. Grasso, J. A. Tuszynski, U. Morbiducci, G. Licandro, A. Danani, M. A. Deriu, Thermodynamic and kinetic stability of the Josephin Domain closed arrangement: Evidences from replica exchange molecular dynamics, Biology Direct, DOI 10.1186/s13062-016-0173-y.

G. Grasso, M. A. Deriu, V. Patrulea, G. Borchard, M. Möller, A. Danani, Free energy landscape of siRNA-polycation complexation: Elucidating the effect of molecular geometry, polymer flexibility, and charge neutralization, PLoS One, DOI 10.1371/journal.pone.0186816.

M. G. Lepre, S. Omar, G. Grasso, U. Morbiducci, M. Deriu, J. A. Tuszynski, Insights into the effect of the G245S single point mutation on the structure of p53 and the binding of the protein to DNA, Molecules, DOI 10.3390/molecules22081358.

Ritabrata Dutta, Università della Svizzera italiana

R. Dutta, M. Schöngens, J. P. Onnela, A. Mira, A user-friendly, extensible, and parallel library for approximate Bayesian computation, PASC' 17 Proceedings of the Platform for Advanced Scientific Computing Conference, DOI 10.1145/3093172.3093233.

Christian Ewerhart, University of Zurich

C. Ewerhart, A 'fractal' solution to the chopstick auction, Economic Theory, DOI 10.1007/s00199-017-1052-1.

Jiannong Fang, EPF Lausanne

S. Shamsoddin, F. Porté-Agel, A model for the effect of pressure gradient on turbulent axisymmetric wakes, Journal of Fluid Mechanics, DOI 10.1017/jfm.2017.864.

K. L. Wu, F. Porté-Agel, Flow adjustment inside and around large finite-size wind farms, Energies, DOI 10.3390/en10122164.

S. Shamsoddin, F. Porté-Agel, Large-Eddy simulation of atmospheric boundary-layer flow through a wind farm sited on topography, Boundary-Layer Meteorology, DOI 10.1007/s10546-016-0216-z.

Andreas Fichtner, ETH Zurich

P. Paitz, A. Gokhberg, A. Fichtner, A neural network for noise correlation classification, Geophysical Journal International, DOI 10.1093/gji/ggx495.

L. Ermert, K. Sager, M. Afanasiev, C. Boehm, A. Fichtner, Ambient seismic source inversion in a heterogeneous Earth: Theory and application to the Earth's hum, Journal of Geophysical Research Solid Earth, DOI 10.1002/2017JB014738.

Y. Cubuk-Sabuncu, T. Taymaz, A. Fichtner, 3-D crustal velocity structure of western Turkey: Constraints from full-waveform tomography, Physics of the Earth and Planetary Interiors, DOI 10.1016/j.pepi.2017.06.014.

A. Fichtner, L. Ermert, A. Gokhberg, Seismic noise correlation on heterogeneous supercomputers, Seismological Research Letters, DOI 10.1785/0220170043.

E. Delaney, L. Ermert, K. Sager, A. Kritski, S. Bussat, A. Fichtner, Passive seismic monitoring with nonstationary noise sources, Geophysics, DOI 10.1190/geo2016-0330.1.

N. Korta, C. Boehm, N. Vinard, I. Jovanovic Balic, A. Fichtner, Optimal experimental design to position transducers in ultrasound breast imaging, 2017 SPIE Conference Proceedings, DOI 10.1117/12.2252514.

A. Fichtner, L. Stehly, L. Ermert, C. Boehm, Generalized interferometry - I: Theory for interstation correlations, Geophysical Journal International, DOI 10.1093/gji/ggw420.

N. K. Martiartu, C. Boehm, N. Vinard, I. J. Balic, A. Fichtner, Optimal experimental design to position transducers in ultrasound breast imaging, Medical Imaging 2017: Ultrasonic Imaging and Tomography, DOI 10.1117/12.2252514.

José A. Flores-Livas, University of Basel

L. E. Ratcliff, A. Degomme, J. A. Flores-Livas, S. Goedecker, L. Genovese, Affordable and accurate large-scale hybrid-functional calculations on GPU-accelerated supercomputers, Journal of Physics: Condensed Matter, DOI 10.1088/1361-648X/aaa8c9.

J. A. Flores-Livas, A. Sanna, A. P. Drozdov, L. Boeri, G. Profeta, M. Eremets, S. Goedecker, Interplay between structure and superconductivity: Metastable phases of phosphorus under pressure, Physical Review Materials, DOI 10.1103/PhysRevMaterials.1.024802.

J. A. Flores-Livas, A. Sanna, M. Graužinytė, A. Davydov, S. Goedecker, M. A. L. Marques, Emergence of superconductivity in doped H_2O ice at high pressure, Scientific Reports, DOI 10.1038/s41598-017-07145-4.

J. A. Flores-Livas, A. Sanna, S. Goedecker, Accelerated materials design approaches based on structural classification: Application to low enthalpy high pressure phases of SH_3 and SeH_3, Novel Superconducting Materials, DOI 10.1515/nsm-2017-0002.

M. Graužinytė, S. Goedecker, J. A. Flores-Livas, Computational screening of useful hole electron dopants in SnO_2, Chemistry of Materials, DOI 10.1021/acs.chemmater.7b03862.

Y. Matsushita, G. Madjarova, J. A. Flores-Livas, J. K. Dewhurst, C. Felser, S. Sharma, E. K. U. Gross, L10 stacked binaries as candidates for hard-magnets: FePt, MnAl and MnGa, Annalen Der Physik, DOI 10.1002/andp.201600412.

Christos E. Frouzakis, ETH Zurich

B. O. Arani, C. E. Frouzakis, J. Mantzaras, F. Lucci, K. Boulouchos, Direct numerical simulation of turbulent channel-flow catalytic combustion: Effects of Reynolds number and catalytic reactivity, Combustion and Flame, DOI 10.1016/j.combustflame.2017.09.001.

M. Jafargholi, G. K. Giannakopoulos, C. E. Frouzakis, K. Boulouchos, Laminar syngas–air premixed flames in a closed rectangular domain: DNS of flame propagation and flame/wall interactions, Combustion and Flame, DOI 10.1016/j.combustflame.2017.09.029.

B. O. Arani, C. E. Frouzakis, J. Mantzaras, K. Boulouchos, Three-dimensional direct numerical simulations of turbulent fuel-lean H_2/air hetero-/homogeneous combustion over Pt with detailed chemistry, Proceedings of the Combustion Institute, DOI 10.1016/j.proci.2016.05.009.

Thomas Gehrmann, University of Zurich

R. Gauld, A. Gehrmann-De Ridder, T. Gehrmann, E. W. N. Glover, A. Huss, Precise predictions for the angular coefficients in Z-boson production at the LHC, Journal of High Energy Physics, DOI 10.1007/JHEP11(2017)003.

Antoine Georges, University of Geneva

W. Wu, M. Ferrero, A. Georges, E. Kozik, Controlling Feynman diagrammatic expansions: Physical nature of the pseudo gap in the two-dimensional Hubbard model, Physical Review B, DOI 10.1103/PhysRevB.96.041105.

A. Subedi, Midinfrared-light-induced ferroelectricity in oxide paraelectrics via nonlinear phononics, Physical Review B, DOI 10.1103/PhysRevB.95.134113.

A. Subedi, Modulated, three-directional, and polar structural instability in layered d^1 $NaTiO_2$, Physical Review B, DOI 10.1103/PhysRevB.95.195149.

A. Subedi, Mott-to-Goodenough insulator-insulator transition in $LiVO_2$, Physical Review B, DOI 10.1103/PhysRevB.95.214119.

P. Seth, O. E. Peil, L. Pourovskii, M. Betzinger, C. Friedrich, O. Parcollet, S. Biermann, F. Aryasetiawan, A. Georges, Renormalization of effective interactions in a negative charge transfer insulator, Physical Review B, DOI 10.1103/PhysRevB.96.205139.

Stefan Goedecker, University of Basel

M. Graužinytė, S. Goedecker, J. A. Flores-Livas, Computational screening of useful hole electron dopants in SnO_2, Chemistry of Materials, DOI 10.1021/acs.chemmater.7b03862.

H. A. Eivari, S. A. Ghasemi, H. Tahmasbi, S. Rostami, S. Faraji, R. Rasoulkhani, S. Goedecker, M. Amsler, Two-dimensional hexagonal sheet of TiO_2, Chemistry of Materials, DOI 10.1021/acs.chemmater.7b02031.

I. Piquero-Zulaica, J. Lobo-Checa, A. Sadeghi, Z. M. Abd El-Fattah, C. Mitsui, T. Okamoto, R. Pawlak, T. Meier, A. Arnau, J. E. Ortega, J. Takeya, S. Goedecker, E. Meyer, S. Kawai, Precise engineering of quantum dot array coupling through their barrier widths, Nature Communications, DOI 10.1038/s41467-017-00872-2.

G. Fisicaro, M. Sicher, M. Amsler, S. Saha, L. Genovese, S. Goedecker, Surface reconstruction of fluorites in vacuum and aqueous environment, Physical Review Materials, DOI 10.1103/PhysRevMaterials.1.033609.

S. Saha, L. Genovese, S. Goedecker, Metastable exohedrally decorated borospherene B_{40}, Scientific Reports, DOI 10.1038/s41598-017-06877-7.

G. Fisicaro, L. Genovese, O. Andreussi, S. Mandal, N. N. Nair, N. Marzari, S. Goedecker, Soft-sphere continuum solvation in electronic-structure calculations, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.7b00375.

J. A. Flores-Livas, A. Sanna, M. Graužinytė, A. Davydov, S. Goedecker, M. A. L. Marques, Emergence of superconductivity in doped H_2O ice at high pressure, Scientific Reports, DOI 10.1038/s41598-017-07145-4.

J. A. Flores-Livas, A. Sanna, A. P. Drozdov, L. Boeri, G. Profeta, M. Eremets, S. Goedecker, Interplay between structure and superconductivity: Metastable phases of phosphorus under pressure, Physical Review Materials, DOI 10.1103/PhysRevMaterials.1.024802.

S. R. Jensen, S. Saha, J. A. Flores-Livas, W. Huhn, V. Blum, S. Goedecker, L. Frediani, The elephant in the room of density functional theory calculations, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b00255.

R. Pawlak, A. Sadeghi, R. Jöhr, A. Hinaut, T. Meier, S. Kawai, L. Zajac, P. Olszowski, S. Godlewski, B. Such, T. Glatzel, S. Goedecker, M. Szymoński, E. Meyer, Hydroxyl-induced partial charge states of single porphyrins on titania rutile, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.6b11873.

Georgios Goumas, University of Athens

N. Papadopoulou, G. Goumas, N. Koziris, Predictive communication modeling for HPC applications, Cluster Computing, DOI 10.1007/s10586-017-0821-8.

Jonathan P. Graves, EPF Lausanne

S. Lanthaler, D. Pfefferlé, J. P. Graves, W. A. Cooper, Higher order Larmor radius corrections to guiding-centre equations and application to fast ion equilibrium distributions, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/aa5e70.

J. M. Faustin, J. P. Graves, W. A. Cooper, S. Lanthaler, L. Villard, D. Pfefferlé, J. Geiger, Ye. O. Kazakov, D. Van Eester, Modelling of advanced three-ion ICRF heating and fast ion generation scheme for tokamaks and stellarators, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/aa72a4.

M. Raghunathan, J. P. Graves, T. Nicolas, W. A. Cooper, X. Garbet, D. Pfefferlé, Heavy impurity confinement in hybrid operation scenario plasmas with a rotating 1/1 continuous mode, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/aa896f.

T. Nicolas, J. F. Luciani, H. Lütjens, X. Garbet, J. P. Graves, A novel approach to ion-ion Langevin self-collisions in particle-in-cell modules applied to hybrid MHD codes, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/aa5f71.

Sigve Haug, University of Bern

F. G. Sciacca, S. Haug on behalf of the ATLAS Collaboration, ATLAS and LHC computing on CRAY, Journal of Physics: Conference Series, DOI 10.1088/1742-6596/898/8/082004.

Jan Henneberger, ETH Zurich

O. Henneberg, J. Henneberger, U. Lohmann, Formation and development of orographic mixed-phase clouds, Journal of the Atmospheric Sciences, DOI 10.1175/Jas-D-16-0348.1.

Csaba Hetényi, Hungarian Academy of Science

M. Bálint, N. Jeszenöi, I. Horváth, D. Van Der Spoel, C. Hetényi, Systematic exploration of multiple drug binding sites, Journal of Cheminformatics, DOI 10.1186/s13321-017-0255-6.

M. Bálint, N. Jeszenöi, I. Horváth, I. M. Ábrahám, C. Hetényi, Dynamic changes in binding interaction networks of sex steroids establish their non-classical effects, Scientific Reports, DOI 10.1038/s41598-017-14840-9.

M. Poór, S. Kunsági-Máté, M. Bálint, C. Hetényi, Z. Gerner, B. Lemli, Interaction of mycotoxin zearalenone with human serum albumin, Journal of Photochemistry and Photobiology B-Biology, DOI 10.1016/j.jphotobiol.2017.03.016.

M. Poór, M. Bálint, C. Hetényi, B. Gődér, S. Kunsági-Máté, T. Kőszegi, B. Lemli, Investigation of non-covalent interactions of aflatoxins (B1, B2, G1, G2, and M1) with serum albumin, Toxins, DOI 10.3390/toxins9110339.

Torsten Hoefler, ETH Zurich

E. Solomonik, M. Besta, F. Vella, T. Hoefler, Scaling betweenness centrality using communication-efficient sparse matrix multiplication, SC'17 Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, DOI 10.1145/3126908.3126971.

T. Hoefler, S. Di Girolamo, K. Taranov, R. E. Grant, R. Brightwell, sPIN: High-performance streaming processing in the network, SC17 Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, DOI 10.1145/3126908.3126970.

C. Barthels, I. Müller, T. Schneider, G. Alonso, T. Hoefler, Distributed join algorithms on thousands of cores, Proceedings of the VLDB Endowment, DOI 10.14778/3055540.3055545.

M. Besta, M. Podstawski, L. Groner, E. Solomonik, T. Hoefler, To push or to pull: On reducing communication and synchronization in graph computations, HPDC '17 Proceedings of the 26th International Symposium on High-Performance Parallel and Distributed Computing, DOI 10.1145/3078597.3078616.

M. Besta, F. Marending, E. Solomonik, T. Hoefler, SlimSell: A vectorizable graph representation for breadth-first search, 2017 IEEE International Parallel and Distributed Processing Symposium, DOI 10.1109/IPDPS.2017.93.

T. Wicky, E. Solomonik, T. Hoefler, Communication-avoiding parallel algorithms for solving triangular systems of linear equations, 2017 IEEE International Parallel and Distributed Processing Symposium, DOI 10.1109/IPDPS.2017.104.

S. Ramos, T. Hoefler, Capability models for manycore memory systems: A case-study with Xeon Phi KNL, 2017 IEEE International Parallel and Distributed Processing Symposium, DOI 10.1109/IPDPS.2017.30.

S. Di Grirolamo, F. Vella, T. Hoefler, Transparent caching for RMA systems, 2017 IEEE International Parallel and Distributed Processing Symposium, DOI 10.1109/IPDPS.2017.92.

A. Arteaga, O. Fuhrer, T. Hoefler, T. Schulthess, Model-driven choice of numerical methods for the solution of the linear advection equation, Procedia Computer Science, DOI 10.1016/j.procs.2017.05.208.

Jürg Hutter, University of Zurich

M. Graf, G. Mette, D. Leuenberger, Y. Gurdal, M. Iannuzzi, W. D. Zabka, S. Schnidrig, B. Probst, J. Hutter, R. Alberto, J. Osterwalder, The impact of metalation on adsorption geometry, electronic level alignment and UV-stability of organic macrocycles on TiO_2(110), Nanoscale, DOI 10.1039/c7nr02317k.

A. Lazzaro, J. VandeVondele, J. Hutter, O. Schütt, Increasing the efficiency of sparse matrix-matrix multiplication with a 2.5D algorithm and one-sided MPI, PASC '17 Proceedings of the Platform for Advanced Scientific Computing Conference, DOI 10.1145/3093172.3093228.

J. Wilhelm, J. Hutter, Periodic GW calculations in the Gaussian and plane-waves scheme, Physical Review B, DOI 10.1103/PhysRevB.95.235123.

Y. Gurdal, J. Hutter, M. Iannuzzi, Insight into (Co)pyrphyrin adsorption on Au(111): Effects of herringbone reconstruction and dynamics of metalation, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.7b02069.

S. Barman, A. Remhof, R. Koitz, M. Iannuzzi, O. Blacque, Y. G. Yan, T. Fox, J. Hutter, A. Zuttel, H. Berke, Post-synthesis amine borane functionalization of a metal-organic framework and its unusual chemical hydrogen release phenomenon, Chemistry-a European Journal, DOI 10.1002/chem.201702013.

D. Golze, M. Iannuzzi, J. Hutter, Local fitting of the Kohn-Sham density in a Gaussian and plane waves scheme for large-scale density functional theory simulations, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.7b00148.

D. Golze, N. Benedikter, M. Iannuzzi, J. Wilhelm, J. Hutter, Fast evaluation of solid harmonic Gaussian integrals for local resolution-of-the-identity methods and range-separated hybrid functionals, Journal of Chemical Physics, DOI 10.1063/1.4973510.

Fortunat Joos, University of Bern

K. M. Keller, S. Lienert, A. Bozbiyik, T. F. Stocker, O. V. Churakova, D. C. Frank, S. Klesse, C. D. Koven, M. Leuenberger, W. J. Riley, M. Saurer, R. Siegwolf, R. B. Weigt, F. Joos, 20th century changes in carbon isotopes and water-use efficiency: Tree-ring-based evaluation of the CLM4.5 and LPX-Bern models, Biogeosciences, DOI 10.5194/bg-14-2641-2017.

Petros Koumoutsakos, ETH Zurich

E. R. Cruz-Chú, E. Papadopoulou, J. H. Walther, A. Popadić, G. Li, M. Praprotnik, P. Koumoutsakos, On phonons and water flow enhancement in carbon nanotubes, Nature Nanotechnology, DOI 10.1038/nnano.2017.234.

N. Karathanasopoulos, P. Angelikopoulos, C. Papadimitriou, P. Koumoutsakos, Bayesian identification of the tendon fascicle's structural composition using finite element models for helical geometries, Computer Methods in Applied Mechanics and Engineering, DOI 10.1016/j.cma.2016.10.024.

L. Kulakova, G. Arampatzis, P. Angelikopoulos, P. Hadjidoukas, C. Papadimitriou, P. Koumoutsakos, Data driven inference for the repulsive exponent of the Lennard-Jones potential in molecular dynamics simulations, Scientific Reports, DOI 10.1038/s41598-017-16314-4.

G. Novati, S. Verma, D. Alexeev, D. Rossinelli, W. M. van Rees, P. Koumoutsakos, Synchronisation through learning for two self-propelled swimmers, Bioinspiration & Biomimetics, DOI 10.1088/1748-3190/aa6311.

S. Verma, G. Abbati, G. Novati, P. Koumoutsakos, Computing the force distribution on the surface of complex, deforming geometries using vortex methods and Brinkman penalization, International Journal for Numerical Methods in Fluids, DOI 10.1002/fld.4392.

S. Wu, P. Angelikopoulos, C. Papadimitriou, P. Koumoutsakos, Bayesian annealed sequential importance sampling (BASIS): An unbiased version of transitional Markov chain Monte Carlo, ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering, DOI 10.1115/1.4037450.

A. Economides, L. Amoudruz, S. Litvinov, D. Alexeev, S. Nizzero, P. E. Hadjidoukas, D. Rossinelli, P. Koumoutsakos, Towards the virtual rheometer, PASC' 17 Proceedings of the Platform for Advanced Scientific Computing, DOI 10.1145/3093172.3093226.

U. Rasthofer, F. Wermelinger, P. Hadjidoukas, P. Koumoutsakos, Large scale simulation of cloud cavitation collapse, Procedia Computer Science, DOI 10.1016/j.procs.2017.05.158.

S. Verma, P. Hadjidoukas, P. Wirth, P. Koumoutsakos, Multi-objective optimization of artificial swimmers, 2017 IEEE Congress on Evolutionary Computation (CEC), DOI 10.1109/cec.2017.7969422.

S. Verma, P. Hadjidoukas, P. Wirth, D. Rossinelli, P. Koumoutsakos, Pareto optimal swimmers, PASC' 17 Proceedings of the Platform for Advanced Scientific Computing, DOI 10.1145/3093172.3093232.

S. Verma, G. Novati, F. Noca, P. Koumoutsakos, Fast motion of heaving airfoils, Procedia Computer Science, DOI 10.1016/j.procs.2017.05.166.

Matthias Krack, Paul Scherrer Institute

D. Bocharov, M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, A. Kuzmin, J. Purans, E. Kotomin, Analysis of the U L3-edge X-ray absorption spectra in UO_2 using molecular dynamics simulations, Progress in Nuclear Energy, DOI 10.1016/j.pnucene.2016.07.017.

Z. Guo, R. Ngayam-Happy, M. Krack, A. Pautz, Atomic-scale effects of chromium-doping on defect behaviour in uranium dioxide fuel, Journal of Nuclear Materials, DOI 10.1016/j.jnucmat.2017.02.043.

A. Kéri, R. Dähn, M. Krack, S. V. Churakov, Combined XAFS spectroscopy and ab-initio study on the characterization of iron incorporation by montmorillonite, Environmental Science & Technology, DOI 10.1021/acs.est.7b01670.

Rolf Krause, Università della Svizzera italiana

S. Pezzuto, P. Kaľavsky, M. Potse, F. W. Prinzen, A. Auricchio, R. Krause, Evaluation of a rapid anisotropic model for ECG simulation, Frontiers in Physiology, DOI 10.3389/fphys.2017.00265.

Martin Kunz, University of Geneva

M. Hindmarsh, J. Lizarraga, J. Urrestilla, D. Daverio, M. Kunz, Scaling from gauge and scalar radiation in Abelian-Higgs string networks, Physical Review D, DOI 10.1103/PhysRevD.96.023525.

J. Adamek, R. Durrer, M. Kunz, Relativistic N-body simulations with massive neutrinos, Journal of Cosmology and Astroparticle Physics, DOI 10.1088/1475-7516/2017/11/004.

M. Gosenca, J. Adamek, C. T. Byrnes, S. Hotchkiss, 3D simulations with boosted primordial power spectra and ultracompact minihalos, Physical Review D, DOI 10.1103/PhysRevD.96.123519.

J. Adamek, J. Brandbyge, C. Fidler, S. Hannestad, C. Rampf, T. Tram, The effect of early radiation in N-body simulations of cosmic structure formation, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stx1157.

Alexey Kuvshinov, ETH Zurich

A. V. Grayver, F. D. Munch, A. V. Kuvshinov, A. Khan, T. J. Sabaka, L. Tøffner-Clausen, Joint inversion of satellite-detected tidal and magnetospheric signals constrains electrical conductivity and water content of the upper mantle and transition zone, Geophysical Research Letters, DOI 10.1002/2017gl073446.

M. Kruglyakov, L. Bloshanskaya, High-performance parallel solver for integral equations of electromagnetics based on Galerkin method, Mathematical Geosciences, DOI 10.1007/s11004-017-9677-y.

F. D. Munch, A. V. Grayver, A. Kuvshinov, A. Khan, Stochastic inversion of geomagnetic observatory data including rigorous treatment of the ocean induction effect with implications for transition zone water content and thermal structure, Journal of Geophysical Research, DOI 10.1002/2017JB014691.

Matthias Liebendörfer, University of Basel

K. C. Pan, M. Liebendörfer, M. Hempel, F. K. Thielemann, Multi-dimensional core-collapse supernova simulations with neutrino transport, JPS Conference Proceedings, Proceedings of the 14th International Symposium on Nuclei in the Cosmos (NIC2016), DOI 10.7566/JPSCP.14.020703.

Michael Lehning, WSL

F. Gerber, M. Lehning, S. W. Hoch, R. Mott, A close-ridge small-scale atmospheric flow field and its influence on snow accumulation, Journal of Geophysical Research Atmosheres, DOI 10.1002/2016JD026258.

Vittorio Limongelli, Università della Svizzera italiana

S. De Marino, A. Carino, D. Masullo, C. Finamore, S. Marchiano, S. Cipriani, F. S. Di Leva, B. Catalanotti, E. Novellino, V. Limongelli, S. Fiorucci, A. Zampella, Hyodeoxycholic acid derivatives as liver X receptor alpha and G-protein-coupled bile acid receptor agonists, Scientific Reports, DOI 10.1038/srep43290.

F. Moraca, J. Amato, F. Ortuso, A. Artese, B. Pagano, E. Novellino, S. Alcaro, M. Parrinello, V. Limongelli, Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1612627114.

R. Casasnovas, V. Limongelli, P. Tiwary, P. Carloni, M. Parrinello, Unbinding Kinetics of a p38 MAP kinase Type II inhibitor from metadynamics simulations, Journal of the American Chemical Society, DOI 10.1021/jacs.6b12950.

C. Festa, S. De Marino, A. Carino, V. Sepe, S. Marchianò, S. Cipriani, F. S. Di Leva, V. Limongelli, M.C. Monti, A. Capolupo, E. Distrutti, S. Fiorucci, A. Zampella. Targeting bile acid receptors: Discovery of a potent and selective Farnesoid X receptor agonist as a new lead in the pharmacological approach to liver diseases, Frontiers in Pharmacology, DOI 10.3389/fphar.2017.00162.

Ulrike Lohmann, ETH Zurich

B. Gasparini, S. Münch, L. Poncet, M. Feldmann, U. Lohmann, Is increasing ice crystal sedimentation velocity in geoengineering simulations a good proxy for cirrus cloud seeding?, Atmospheric Chemistry and Physics, DOI 10.5194/acp-17-4871-2017.

A. Possner, A. M. L. Ekman, U. Lohmann, Cloud response and feedback processes in stratiform mixed-phase clouds perturbed by ship exhaust, Geophysical Research Letters, DOI 10.1002/2016gl071358.

Sandra Luber, ETH Zurich

M. Schilling, F. H. Hodel, S. Luber, Discovery of open cubane core structures for biomimetic $LnCo_3(OR)_4$ water oxidation catalysts, ChemSusChem, DOI 10.1002/cssc.201701527.

M. Gil-Sepulcre, M. Bohler, M. Schilling, F. Bozoglian, C. Bachmann, D. Scherrer, T. Fox, B. Spingler, C. Gimbert-Surinach, R. Alberto, R. Bofill, X. Sala, S. Luber, C. J. Richmond, A. Llobet, Ruthenium water oxidation catalysts based on pentapyridyl ligands, ChemSusChem, DOI 10.1002/cssc.201701747.

F. Y. Song, R. Moré, M. Schilling, G. Smolentsev, N. Azzaroli, T. Fox, S. Luber, G. R. Patzke, $\{Co_4O_4\}$ and $\{CoxNi_{4-x},O_4\}$ cubane water oxidation catalysts as surface cut-outs of cobalt oxides, Journal of the American Chemical Society, DOI 10.1021/jacs.7b07361.

F. H. Hodel, S. Luber, Dehydrogenation free energy of $Co^{2+}(aq)$ from density functional theory-based molecular dynamics, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b01077.

F. H. Hodel, P. Deglmann, S. Luber, Exploring solvation effects in ligand-exchange reactions via static and dynamic methods, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.7b00214.

S. Luber, Raman optical activity spectra from density functional perturbation theory and density-functional-theory-based molecular dynamics, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00820.

Mathieu Luisier, ETH Zurich

S. Brück, M. Calderara, M. H. Bani-Hashemian, J. VandeVondele, M. Luisier, Efficient algorithms for large-scale quantum transport calculations, Journal of Chemical Physics, DOI 10.1063/1.4998421.

C. Stieger, A. Szabo, T. Bunjaku, M. Luisier, Ab-initio quantum transport simulation of self-heating in single-layer 2-D materials, Journal of Applied Physics, DOI 10.1063/1.4990384.

A. Pedersen, M. Bieri, M. Luisier, L. Pizzagalli, Lithiation of silicon nanoclusters, Physical Review Applied, DOI 10.1103/PhysRevApplied.7.054012.

R. Rhyner, M. Luisier, Influence of thermal losses at the gate contact of Si nanowire transistors: A phenomenological treatment in quantum transport theory, Applied Physics Letters, DOI 10.1063/1.4978516.

J. Gooth, M. Borg, H. Schmid, V. Schaller, S. Wirths, K. E. Moselund, M. Luisier, S. Karg, H. Riel, Ballistic one-dimensional InAs nanowire cross-junction interconnects, Nano Letters, DOI 10.1021/acs.nanolett.7b00400.

S. N. Raja, R. Rhyner, K. Vuttivorakulchai, M. Luisier, D. Poulikakos, Length scale of diffusive phonon transport in suspended thin silicon nanowires, Nano Letters, DOI 10.1021/acs.nanolett.6b04050.

S. Andermatt, M. H. Bani-Hashemian, S. Brück, J. VandeVondele, M. Luisier, Transport simulations with density-matrix-based real-time time-dependant density functional theory, Proceedings of the 2017 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), DOI 10.23919/SISPAD.2017.8085293.

A. Ziegler, M. Luisier, Phonon confinement effects in diffusive quantum transport simulations with the effective mass approximation and k·p method, Proceedings of the 2017 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), DOI 10.23919/SISPAD.2017.8085255.

Ioannis Mantzaras, Paul Scherrer Institute

M. A. Safi, N. I. Prasianakis, J. Mantzaras, A. Lamibrac, F. N. Büchi, Experimental and pore-level numerical investigation of water evaporation in gas diffusion layers of polymer electrolyte fuel cells, International Journal of Heat and Mass Transfer, DOI 10.1016/j.ijheatmasstransfer.2017.07.050.

R. Sui, Et. Essebbar, J. Mantzaras, R. Bombach, Homogeneous ignition during fuel-rich $H_2/O_2/N_2$ combustion in platinum-coated channels at elevated pressures, Combustion and Flame, DOI 10.1016/j.combustflame.2017.02.033.

R. Sui, J. Mantzaras, Et. Essebbar, M.A. Safi, R. Bombach, Impact of gaseous chemistry in $H_2/O_2/N_2$ combustion over platinum at fuel-lean stoichiometries and pressures of 1.0 to 3.5 bar, Energy & Fuels, DOI 10.1021/acs.energyfuels.7b02011.

Nicola Marzari, EPF Lausanne

G. Fisicaro, L. Genovese, O. Andreussi, S. Mandal, N. N. Nair, N. Marzari, S. Goedecker, Soft-sphere continuum solvation in electronic-structure calculations, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.7b00375.

A. Bussy, G. Pizzi, M. Gibertini, Strain-induced polar discontinuities in two-dimensional materials from combined first-principles and Schrödinger-Poisson simulations, Physical Review B, DOI 10.1103/PhysRevB.96.165438.

A. Cepellotti, N. Marzari, Transport waves as crystal excitations, Physical Review Materials, DOI 10.1103/PhysRevMaterials.1.045406.

A. Cepellotti, N. Marzari, Boltzmann transport in nanostructures as a friction effect, Nano Letters, DOI 10.1021/acs.nanolett.7b01202.

Lucio Mayer, University of Zurich

J. Szulágyi, L. Mayer, T. Quinn, Circumplanetary discs around young giant planets: A comparison between core-accretion and disc instability, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw2617.

J. Szulágyi, C. Mordasini, Thermodynamics of giant planet formation: Shocking hot surfaces on circumplanetary discs, Monthly Notices of the Royal Astronomical Society Letters, DOI 10.1093/mnrasl/slw212.

J. Szulágyi, Effects of the planetary temperature on the circumplanetary disk and on the gap, Astrophysical Journal, DOI 10.3847/1538-4357/aa7515.

D. Fiacconi, L. Mayer, P. Madau, A. Lupi, M. Dotti, F. Haardt, Young and turbulent: The early life of massive galaxy progenitors, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stx335.

J. Szulágyi, G. van der Plas, M. R. Meyer, A. Pohl, S. P. Quanz, L. Mayer, S. Daemgen, V. Tamburello, Observability of forming planets and their circumplanetary discs – I. Parameter study for ALMA, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stx2602.

Siddhartha Mishra, ETH Zurich

U. S. Fjordholm, R. Käppeli, S. Mishra, E. Tadmor, Construction of approximate entropy measure valued solutions for hyperbolic systems of conservation laws, Foundations of Computational Mathematics, DOI 10.1007/s10208-015-9299-z.

J. Dick, R. N. Gantner, Q. T. Le Gia, C. Schwab, Multilevel higher-order quasi-Monte Carlo Bayesian estimation, Mathematical Models and Methods in Applied Sciences, DOI 10.1007/s10208-015-9299-z.

MeteoSwiss

D. Leutwyler, D. Lüthi, N. Ban, O. Fuhrer, C. Schär, Evaluation of the convection-resolving climate modeling approach on continental scales, Journal of Geophysical Research Atmospheres, DOI 10.1002/2016JD026013.

A. Voudouri, P. Khain, I. Carmona, O. Bellprat, F. Grazzini, E. Avgoustoglou, J. M. Bettems, P. Kaufmann, Objective calibration of numerical weather prediction models, Atmospheric Research, DOI 10.1016/j.atmosres.2017.02.007.

S. Robert, D. Leuenberger, H. Künsch, A local ensemble transform Kalman particle filter for convective scale data assimilation, Quarterly Journal of the Royal Meteorological Society, DOI 10.1002/qj.3116.

A. Arteaga, O. Fuhrer, T. Hoefler, T. Schulthess, Model-driven choice of numerical methods for the solution of the linear advection equation, Procedia Computer Science, DOI 10.1016/j.procs.2017.05.208.

D. Nerini, N. Besic, I. V. Sideris, U. Germann, L. Foresti, A non-stationary stochastic ensemble generator for radar rainfall fields based on the short-space Fourier transform, Hydrology and Earth System Sciences, DOI 10.5194/hess-21-2777-2017.

R. Stöckli, A. Duguay–Tetzlaff, J. Bojanowski, R. Hollmann, P. Fuchs, M. Werscheck, CM SAF ClOud Fractional Cover dataset from METeosat First and Second Generation - Edition 1, Satellite Application Facility on Climate Monitoring, DOI 10.5676/EUM_SAF_CM/CFC_METEOSAT/V001.

A. Duguay–Tetzlaff, R. Stöckli, J. Bojanowski, R. Hollmann, P. Fuchs, M. Werscheck, CM SAF Land SUrface Temperature dataset from METeosat First and Second Generation - Edition 1, Satellite Application Facility on Climate Monitoring, DOI 10.5676/EUM_SAF_CM/LST_METEOSAT/V001.

Dennis Palagin, Paul Scherrer Institute

X. Wang, J. A. Van Bokhoven, D. Palagin, Ostwald ripening versus single atom trapping: Towards understanding platinum particle sintering, Physical Chemistry Chemical Physics, DOI 10.1039/c7cp05887j.

S. Saedy, D. Palagin, O. Safonova, J. A. Van Bokhoven, A. A. Khodadadi, Y. Mortazavi, Understanding the mechanism of synthesis of Pt3Co intermetallic nanoparticles via preferential chemical vapor deposition, Journal of Materials Chemistry A, DOI 10.1039/C7TA06737B.

V. L. Sushkevich, D. Palagin, M. Ranocchiari, J. A. Van Bokhoven, Selective anaerobic oxidation of methane enables direct synthesis of methanol, Science, DOI 10.1126/science.aam9035.

D. Palagin, A. J. Knorpp, A. B. Pinar, M. Ranocchiari, J. A. Van Bokhoven, Assessing the relative stability of copper oxide clusters as active sites of a CuMOR zeolite for methane to methanol conversion: Size matters?, Nanoscale, DOI 10.1039/c6nr07723d.

Michele Parrinello, Università della Svizzera italiana

M. Nava, F. Palazzesi, C. Perego, M. Parrinello, Dimer metadynamics, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00691.

F. Moraca, J. Amato, F. Ortuso, A. Artese, B. Pagano, E. Novellino, S. Alcaro, M. Parrinello, V. Limongelli, Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1612627114.

P. M. Piaggi, O. Valsson, M. Parrinello, Enhancing entropy and enthalpy Fluctuations to drive crystallization in atomistic simulations, Physical Review Letters, DOI 10.1103/PhysRevLett.119.015701.

J. McCarty, M. Parrinello, A variational conformational dynamics approach to the selection of collective variables in metadynamics, Journal of Chemical Physics, DOI 10.1063/1.4998598.

F. Palazzesi, O. Valsson, M. Parrinello, Conformational entropy as collective variable for proteins, The Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b01770.

M. Invernizzi, O. Valsson, M. Parrinello, Coarse graining from variationally enhanced sampling applied to the Ginzburg-Landau model, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1618455114.

R. Casasnovas, V. Limongelli, P. Tiwary, P. Carloni, M. Parrinello, Unbinding kinetics of a p38 MAP kinase Type II inhibitor from metadynamics simulations, Journal of the American Chemical Society, DOI 10.1021/jacs.6b12950.

G. Piccini, J. J. McCarty, O. Valsson, M. Parrinello, Variational flooding study of a S_N2 reaction, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.6b02852.

E. Caldarulo, A. Barducci, K. Wüthrich, M. Parrinello, Prion protein $\beta 2$-$\alpha 2$ loop conformational landscape, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1712155114.

G. Piccini, D. Polino, M. Parrinello, Identifying slow molecular motions in complex chemical reactions, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b01889.

P. M. Piaggi, M. Parrinello, Entropy based fingerprint for local crystalline order, Journal of Chemical Physics, DOI 10.1063/1.4998408.

J. Bartl, F. Palazzesi, M. Parrinello, L. Hommers, P. Riederer, S. Walitza, E. Grünblatt, The impact of methylphenidate and its enantiomers on dopamine synthesis and metabolism in vitro, Progress in Neuro-Psychopharmacology & Biological Psychiatry, DOI 10.1016/j.pnpbp.2017.07.002.

Alfredo Pasquarello, EPF Lausanne

F. Evangelisti, M. Stiefel, O. Guseva, R. P. Nia, R. Hauert, E. Hack, L. P. H. Jeurgens, F. Ambrosio, A. Pasquarello, P. Schmutz, C. Cancellieri, Electronic and structural characterization of barrier-type amorphous aluminium oxide, Electrochimica Acta, DOI 10.1016/j.electacta.2016.12.090.

R. Meli, G. Miceli, A. Pasquarello, Oxygen DX center in In0.17Al0.83N: Nonradiative recombination and persistent photoconductivity, Applied Physics Letters, DOI 10.1063/1.4975934.

D. Colleoni, G. Pourtois, A. Pasquarello, Nature of electron trap states under inversion at $In_{0.53}Ga_{0.47}As/Al_2O_3$ interfaces, Applied Physics Letters, DOI 10.1063/1.4977980.

A. Bouzid, A. Pasquarello, Redox levels through constant Fermi-level ab-initio molecular dynamics, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b01232.

F. Ambrosio, G. Miceli, A. Pasquarello, Electronic levels of excess electrons in liquid water, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b00699.

W. Chen, A. Pasquarello, Accuracy of GW for calculating defect energy levels in solids, Physical Review B, DOI 10.1103/PhysRevB.96.020101.

J. Wiktor, I. Reshetnyak, F. Ambrosio, A. Pasquarello, Comprehensive modeling of the band gap and absorption spectrum of $BiVO_4$, Physical Review Materials, DOI 10.1103/PhysRevMaterials.1.022401.

A. Bouzid, A. Pasquarello, Identification of semiconductor defects through constant-fermi-level ab-initio molecular dynamics: Application to GaAs, Physical Review Applied, DOI 10.1103/PhysRevApplied.8.014010.

G. Miceli, A. Pasquarello, Migration of Mg and other interstitial metal dopants in GaN, Physica Status Solidi-Rapid Research Letters, DOI 10.1002/pssr.201700081.

J. Wiktor, F. Bruneval, A. Pasquarello, Partial molar volumes of aqua ions from first principles, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.7b00474.

J. Wiktor, U. Röthlisberger, A. Pasquarello, Predictive determination of band gaps of inorganic halide perovskites, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b02648.

J. Wiktor, F. Ambrosio, A. Pasquarello, Note: Assessment of the SCAN+rVV10 functional for the structure of liquid water, Journal of Chemical Physics, DOI 10.1063/1.5006146.

A. Bouzid, A. Pasquarello, Electron trap states at InGaAs/oxide interfaces under inversion through constant Fermi-level ab-initio molecular dynamics, Journal of Physics: Condensed Matter, DOI 10.1088/1361-648X/aa9a00.

Albino Perego, Technical University Darmstadt

A. Murguia-Berthier, E. Ramirez-Ruiz, G. Montes, F. De Colle, L. Rezzolla, S. Rosswog, K. Takami, A. Perego, W. H. Lee, The properties of short gamma-ray burst jets triggered by neutron star mergers, Astrophysical Journal Letters, DOI 10.3847/2041-8213/aa5b9e.

A. Perego, D. Radice, S. Bernuzzi, AT 2017gfo: An anisotropic and three-component Kilonova counterpart of GW170817, Astrophysical Journal Letters, DOI 10.3847/2041-8213/aa9ab9.

A. Perego, H. Yasin, A. Arcones, Neutrino pair annihilation above merger remnants: Implications of a long-lived massive neutron star, Journal of Physics G: Nuclear and Particle Physics, DOI 10.1088/1361-6471/aa7bdc.

Carlo A. Pignedoli, EMPA

J. I. Urgel, H. Hayashi, M. Di Giovannantonio, C. A. Pignedoli, S. Mishra, O. Deniz, M. Yamashita, T. Dienel, P. Ruffieux, H. Yamada, R. Fasel, On-surface synthesis of heptacene organometallic complexes, Journal of the American Chemical Society, DOI 10.1021/jacs.7b05192.

P. P. Shinde, O. Groning, S. Y. Wang, P. Ruffieux, C. A. Pignedoli, R. Fasel, D. Passerone, Stability of edge magnetism in functionalized zigzag graphene nanoribbons, Carbon, DOI 10.1016/j.carbon.2017.08.018.

L. Talirz, H. Sode, T. Dumslaff, S. Y. Wang, J. R. Sanchez-Valencia, J. Liu, P. Shinde, C. A. Pignedoli, L. Liang, V. Meunier, N. C. Plumb, M. Shi, X. Feng, A. Narita, K. Müllen, R. Fasel, P. Ruffieux, On-surface synthesis and characterization of 9-atom wide armchair graphene nanoribbons, ACS Nano, DOI 10.1021/acsnano.6b06405.

Igor Pivkin, Università della Svizzera italiana

K. Lykov, Y. Nematbakhsh, M. L. Shang, C. T. Lim, I. V. Pivkin, Probing eukaryotic cell mechanics via mesoscopic simulations, Plos Computational Biology, DOI 10.1371/journal.pcbi.1005726.

S. Christel, M. Herold, S. Bellenberg, M. El Hajjami, A. Buetti-Dinh, I. V. Pivkin, W. Sand, P. Wilmes, A. Poetsch, M. Dopson, Multi-omics reveal the lifestyle of the acidophilic, mineral-oxidizing model species *Leptospirillum ferriphilumT*, Applied and Environmental Microbiology, DOI 10.1128/AEM.02091-17.

Yury Podladchikov, EPF Lausanne

S. Omlin, B. Malvoisin, Y. Y. Podladchikov, Pore fluid extraction by reactive solitary waves in 3-D, Geophysical Research Letters, DOI 10.1002/2017GL074293.

S. Omlin, L. Räss, Y. Y. Podladchikov, Simulation of three-dimensional viscoelastic deformation coupled to porous fluid flow, Tectonophysics, DOI 10.1016/j.tecto.2017.08.012.

Christoph C. Raible, University of Bern

C. Kilic, C. C. Raible, T. F. Stocker, Multiple climate states of habitable exoplanets: The role of obliquity and irradiance, Astrophysical Journal, DOI 10.3847/1538-4357/aa7a03.

M. Messmer, J. J. Gomez-Navarro, C. C. Raible, Sensitivity experiments on the response of Vb cyclones to sea surface temperature and soil moisture changes, Earth System Dynamics, DOI 10.5194/esd-8-477-2017.

C. Kilic, C. C. Raible, T. F. Stocker, E. Kirk, Impact of variations of gravitational acceleration on the general circulation of the planetary atmosphere, Planetary and Space Science, DOI 10.10164/j.pss.2016.11.001.

Paolo Ricci, EPF Lausanne

F. Riva, E. Lanti, S. Jolliet, P. Ricci, Plasma shaping effects on tokamak scrape-off layer turbulence, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/aa5322.

C. Wersal, P. Ricci, J. Loizu, A comparison between a refined two-point model for the limited tokamak SOL and selfconsistent plasma turbulence simulations, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/aa5cf9.

F. Riva, C. F. Beadle, P. Ricci, A methodology for the rigorous verification of Particle-in-Cell simulations, Physics of Plasmas, DOI 10.1063/1.4977917.

F. Nespoli, I. Furno, B. Labit, P. Ricci, F. Avino, F. D. Halpern, F. Musil, F. Riva, Blob properties in full-turbulence simulations of the TCV scrape-off layer, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/aa6276.

C. Wersal, P. Ricci, Impact of neutral density fluctuations on gas puff imaging diagnostics, Nuclear Fusion, DOI 10.1088/1741-4326/aa7db0.

F. Riva, L. Milanese, P. Ricci, Uncertainty propagation by using spectral methods: A practical application to a two-dimensional turbulence fluid model, Physics of Plasmas, DOI 10.1063/1.4996445.

J. Loizu, J. A. Morales, F. D. Halpern, P. Ricci, P. Paruta, Scrape-off-layer current loops and floating potential in limited tokamak plasmas, Journal of Plasma Physics, DOI 10.1017/S0022377817000927.

Marcello Righi, Zurich University of Applied Science

M. Righi, A. Da Ronch, F. Mazzacchi, Analysis of resolved turbulent scales of motion in aeroelastic problems, 58th AIAA/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference, AIAA SciTech Forum, (AIAA 2017-0189), DOI 10.2514/6.2017-0189.

E. Molina, C. Spode, R. G. Annes da Silva, D. E. Manosalvas-Kjono, S. Nimmagadda, T. D. Economon, J. J. Alonso, M. Righi, Hybrid RANS/LES Calculations in SU2, 23rd AIAA Computational Fluid Dynamics Conference, AIAA AVIATION Forum, (AIAA 2017-4284), DOI 10.2514/6.2017-4284.

A. Da Ronch, M. Righi, M. Berci, Revised Indicial Aerodynamics for Parametric Search and Design Analysis, AIAA Atmospheric Flight Mechanics Conference, AIAA SciTech Forum, (AIAA 2017-1866), DOI 10.2514/6.2017-1866.

M. Righi, Turbulence modelling techniques for aeroelastic problems: Results and comments from the Second AIAA Aeroelastic Prediction Workshop, Aircraft Engineering and Aerospace Technology, DOI 10.1108/AEAT-01-2017-0051.

M. Berci, M. Righi, An enhanced analytical method for the subsonic indicial lift of two-dimensional aerofoils – with numerical cross-validation, Aerospace Science and Technology, DOI 10.1016/j.ast.2017.03.004.

Ursula Röthlisberger, EPF Lausanne

S. C. van Keulen, U. Röthlisberger, Effect of N-terminal myristoylation on the active conformation of $G\alpha_{i1}$ - GTP, Biochemistry, DOI 10.1021/acs.biochem.6b00388.

L. Casalino, G. Palermo, N. Abdurakhmonova, U. Röthlisberger, A. Magistrato, Development of site-specific Mg^{2+}-RNA force field parameters: A dream or reality? Guidelines from combined molecular dynamics and quantum mechanics simulations, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00905.

O. A. Syzgantseva, M. Saliba, M. Grätzel, U. Röthlisberger, Stabilization of the perovskite phase of formamidinium lead triiodide by methylammonium, Cs, and/or Rb Doping, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.6b03014.

Z. Adhireksan, G. Palermo, T. Riedel, Z. J. Ma, R. Muhammad, U. Röthlisberger, P. J. Dyson, C. A. Davey, Allosteric cross-talk in chromatin can mediate drug-drug synergy, Nature Communications, DOI 10.1038/ncomms14860.

N. J. Browning, R. Ramakrishnan, O. A. von Lilienfeld, U. Röthlisberger, Genetic optimization of training sets for improved machine learning models of molecular properties, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b00038.

S. C. Van Keulen, E. Gianti, V. Carnevale, M. L. Klein, U. Röthlisberger, L. Delemotte, Does proton conduction in the voltage-gated H+ channel hHv1 involve Grotthuss-like hopping via acidic residues?, Journal of Physical Chemistry B, DOI 10.1021/acs.jpcb.6b08339.

M. Micciarelli, B. F. E. Curchod, S. Bonella, C. Altucci, M. Valadan, U. Röthlisberger, I. Tavernelli, Characterization of the photochemical properties of 5-benzyluracil via time-dependent density functional theory, The Journal of Physical Chemistry A, DOI 10.1021/acs.jpca.6b12799.

S. C. Van Keulen, A. Solano, U. Röthlisberger, How rhodopsin tunes the equilibrium between protonated and deprotonated forms of the retinal chromophore, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.7b00229.

J. Wiktor, U. Röthlisberger, A. Pasquarello, Predictive determination of band gaps of inorganic halide perovskites, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b02648.

N. Ashari-Astani, S. Meloni, A. H. Salavati, G. Palermo, M. Grätzel, U. Röthlisberger, Computational characterization of the dependence of halide perovskite effective masses on chemical composition and structure, The Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.7b04898.

E. Bozkurt, T. A. Soares, U. Röthlisberger, Can biomimetic zinc compounds assist a (3+2) cycloaddition reaction? A theoretical perspective, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.7b00819.

Richard Sandberg, The University of Melbourne

R. Pichler, R. D. Sandberg, G. Laskowski, V. Michelassi, High-fidelity simulations of a linear HPT vane cascade subject to varying inlet turbulence, ASME Turbo Expo 2017: Turbomachinery Technical Conference and Exposition, DOI 10.1115/GT2017-63079.

Yohei Sato, Paul Scherrer Institute

Y. Sato, B. Niceno, Large eddy simulation of upward co-current annular boiling flow using an interface tracking method, Nuclear Engineering and Design, DOI 10.1016/j.nucengdes.2017.03.003.

Y. Sato, B. Niceno, Nucleate pool boiling simulations using the interface tracking method: Boiling regime from discrete bubble to vapor mushroom region, International Journal of Heat and Mass Transfer, DOI 10.1016/j.ijheatmasstransfer.2016.10.018.

Christoph Schär, ETH Zurich

A. Imamovic, L. Schlemmer, C. Schär, Collective impacts of orography and soil moisture on the soil moisture-precipitation feedback, Geophysical Research Letters, DOI 10.1002/2017gl075657.

N. Kröner, S. Kotlarski, E. Fischer, D. Lüthi, E. Zubler, C. Schär, Separating climate change signals into thermodynamic, lapse-rate and circulation effects: Theory and application to the European summer climate, Climate Dynamics, DOI 10.1007/s00382-016-3276-3.

D. Leutwyler, D. Lüthi, N. Ban, O. Fuhrer, C. Schär, Evaluation of the convection-resolving climate modeling approach on continental scales, Journal of Geophysical Research Atmospheres, DOI 10.1002/2016jd026013.

J. Rajczak, C. Schär, Projections of future precipitation extremes over Europe: A multimodel assessment of climate simulations, Journal of Geophysical Research Atmospheres, DOI 10.1002/2017jd027176.

C. Schär, N. Kröner, Sequential factor separation for the analysis of numerical model simulations, Journal of the Atmospheric Sciences, DOI 10.1175/Jas-D-16-0284.1.

Olaf Schenk, Università della Svizzera italiana

D. Kourounis, A. Fuchs, O. Schenk, Towards the next generation of multi-period optimal power flow solvers, IEEE Transactions on Power Systems, DOI 10.1109/TPWRS.2017.2789187.

F. Verbosio, A. De Coninck, D. Kourounis, O. Schenk, Enhancing the scalability of selectd inversion factorization algorithms in genomic prediction, Journal of Computational Science, DOI 10.1016/j.jocs.2017.08.013.

M. Rietmann, M. Grote, D. Peter, O. Schenk, Newmark local time stepping on high performance computing architectures, Journal of Computational Physics, DOI 10.1016/j.jcp.2016.11.012.

A. Eftekhari, O. Schenk, S. Scheidegger, Parallelized dimensional decomposition for dynamic stochastic economic models, PASC' 17 Proceedings of the ACM Platform for Advanced Scientific Computing Conference, DOI 3093172.3093234.

Ari P. Seitsonen, École Normale Supérieure

J. Li, B. Zhang, G. Médard, A. P. Seitsonen, F. Haag, F. Allegretti, J. Reichert, B. Kuster, J. V. Barth, A. C. Papageorgiou, N-heterocyclic carbenes on the close packed coinage metal surfaces: Bis-carbene metal adatom bonding scheme of monolayer films on Au, Ag and Cu, Chemical Science, DOI 10.1039/C7SC03777E.

M. Schwarz, A. Riss, M. Garnica, J. Ducke, P. S. Deimel, D. A. Duncan, P. K. Thakur, T.-L. Lee, A. P. Seitsonen, J. V. Barth, F. Allegretti, W. Auwärter, Corrugation in the weakly interacting hexagonal-BN/Cu(111) system: Structure determination by combining noncontact atomic force microscopy and X-ray standing waves, ACS Nano, DOI 10.1021/acsnano.7b04022.

James J. Shepherd, MIT

T. Dornheim, S. Groth, F. D. Malone, T. Schoof, T. Sjostrom, W. M. C. Foulkes, M. Bonitz, Ab-initio quantum Monte Carlo simulation of the warm dense electron gas, Physics of Plasmas, DOI 10.1063/1.4977920.

S. Groth, T. Dornheim, T. Sjostrom, F. D. Malone,W. M. C. Foulkes, M. Bonitz, Ab-initio exchange-correlation free energy of the uniform electron gas at warm dense matter conditions, Physical Review Letters, DOI 10.1103/PhysRevLett.119.135001.

Berend Smit, EPF Lausanne

G. Bauer, D. Ongari, X. Y. Xu, D. Tiana, B. Smit, M. Ranocchiari, Metal-organic frameworks invert molecular reactivity: Lewis acidic phosphonium zwitterions catalyze the Aldol-Tishchenko reaction, Journal of the American Chemical Society, DOI 10.1021/jacs.7b10928.

D. Ongari, D. Tiana, S. J. Stoneburner, L. Gagliardi, B. Smit, Origin of the strong interaction between polar molecules and copper(II) paddle-wheels in metal organic frameworks, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.7b02302.

M. Taddei, D. Tiana, N. Casati, J. van Bokhoven, B. Smit, M. Ranocchiari, Mixed-linker UiO-66: Structure-properties relations revealed by a combination of high-resolution powder x-ray diffraction and density functional theory calculations, Physical Chemistry Chemical Physics, DOI 10.1039/C6CP07801J.

S. L. Anderson, A. Gladysiak, P. G. Boyd, C. P. Ireland, P. Mieville, D. Tiana, B. Vlaisavljevich, P. Schouwink, W. van Beek, K. J. Gagnon, B. Smit, K. C. Stylianou, Formation pathways of metal-organic frameworks proceeding through partial dissolution of the metastable phase, CrystEngComm, DOI 10.1039/c7ce00589j.

Nicola A. Spaldin, ETH Zurich

S. M. Griffin, M. Reidulff, S. M. Selbach, N. A. Spaldin, Defect chemistry as a crystal structure design parameter: Intrinsic point defects and Ga substitution in $InMnO_3$, Chemistry of Materials, DOI 10.1021/acs.chemmater.6b04207.

D. M. Juraschek, M. Fechner, N. A. Spaldin, Ultrafast structure switching through nonlinear phononics, Physical Review Letters, DOI 10.1103/PhysRevLett.118.054101.

R. U. Chandrasena, W. B. Yang, Q. Y. Lei, M. U. Delgado-Jaime, K. D. Wijesekara, M. Golalikhani, B. A. Davidson, E. Arenholz, K. Kobayashi, M. Kobata, F. M. F. de Groot, U. Aschauer, N. A. Spaldin, X. X. Xi, A. X. Gray, Strain-engineered oxygen vacancies in $CaMnO_3$ thin films, Nano Letters, DOI 10.1021/acs.nanolett.6b03986.

S. M. Griffin, N. A. Spaldin, A density functional theory study of the influence of exchange-correlation functionals on the properties of FeAs, Journal of Physics: Condensed Matter, DOI 10.1088/1361-648X/aa6b9a.

D. M. Juraschek, M. Fechner, A. V. Balatsky, N. A. Spaldin, Dynamical multiferroicity, Physical Review Materials, DOI 10.1103/PhysRevMaterials.1.014401.

Q. N. Meier, M. Lilienblum, S. M. Griffin, K. Conder, E. Pomjakushina, Z. Yan, E. Bourret, D. Meier, F. Lichtenberg, E. K. H. Salje, N. A. Spaldin, M. Fiebig, A. Cano, Global formation of topological defects in the multiferroic hexagonal manganites, Physical Review X, DOI 10.1103/PhysRevX.7.041014.

A. Hampel, C. Ederer, Interplay between breathing mode distortion and magnetic order in rare-earth nickelates $RNiO_3$ within DFT+U, Physical Review B, DOI 10.1103/PhysRevB.96.165130.

Oskar Steiner, IRSOL

O. Steiner, F. Calvo, R. Salhab, G. Vigeesh, CO5BOLD for MHD: Progresses and deficiencies, Memorie della Società Astronomica Italiana, DOI 2017MmSAI..88...37S.

G. Vigeesh, O. Steiner, F. Calvo, M. Roth, On the effect of vorticity on the propagation of internal gravity waves, Memorie della Società Astronomica Italiana, DOI 2017MmSAI..88…54V.

Romain Teyssier, University of Zurich

M. Rieder, R. Teyssier, A small-scale dynamo in feedback-dominated galaxies - III. Cosmological Simulations, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stx2276.

M. Rieder, R. Teyssier, A small-scale dynamo in feedback-dominated galaxies - II. The saturation phase and the final magnetic configuration, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stx1670.

P. Biernacki, R. Teyssier, A. Bleuler, On the dynamics of supermassive black holes in gas-rich, star-forming galaxies: The case for nuclear star cluster co-evolution, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stx845.

D. Potter, J. Stadel, R. Teyssier, PKDGRAV3: Beyond trillion particle cosmological simulations for the next Era of galaxy surveys, DOI 10.1186/s40668-017-0021-1.

Joost VandeVondele, ETH Zurich

C. S. Praveen, A. Comas-Vives, C. Copéret, J. VandeVondele, Role of water, CO_2, and non-innocent ligands in the CO_2 hydrogenation to formate by an Ir(III) PNP pincer catalyst evaluated by static-DFT and ab-initio molecular dynamics under reaction conditions, Organometallics, DOI 10.1021/acs.organomet.7b00761.

S. Andermatt, M. H. Bani-Hashemian, S. Brück, J. VandeVondele, M. Luisier, Transport simulations with density-matrix-based real-time time-dependant density functional theory, 2017 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), DOI 10.23919/SISPAD.2017.8085293.

S. Brück, M. Calderara, M. H. Bani-Hashemian, J. VandeVondele, M. Luisier, Efficient algorithms for large-scale quantum transport calculations, Journal of Chemical Physics, DOI 10.1063/1.4998421.

C. Spreafico, W. Karim, Y. Ekinci, J. A. Van Bokhoven, J. VandeVondele, Hydrogen adsorption on nanosized platinum and dynamics of spillover onto alumina and titania, The Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.7b03733.

V. V. Rybkin, J. VandeVondele, Nuclear quantum effects on aqueous electron attachment and redox properties, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.7b00386.

W. Karim, C. Spreafico, A. Kleibert, J. Gobrecht, J. VandeVondele, Y. Ekinci, J. A. van Bokhoven, Catalyst support effects on hydrogen spillover, Nature, DOI 10.1038/nature20782.

A. Lazzaro, J. VandeVondele, J. Hutter, O. Schütt, Increasing the efficiency of sparse matrix-matrix multiplication with a 2.5D algorithm and one-sided MPI, PASC '17 Proceedings of the Platform for Advanced Scientific Computing Conference, DOI 10.1145/3093172.3093228.

Martin van Driel, ETH Zurich

E. Bozdag, Y. Ruan, N. Metthez, A. Khan, K. Leng, M. van Driel, M. Wieczorek, A. Rivoldini, C. Larmat, D. Giardini, J. Tromp, P. Lognonne, B. Banerdt, Simulations of seismic wave propagation on Mars, Space Science Reviews, DOI 10.1007/s11214-017-0350-z.

J. F. Clinton, D. Giardini, P. Lognonne, B. Banerdt, M. Van Driel, M. Drilleau, N. Murdoch, M. Panning, R. Garcia, D. Mimoun, M. Golombek, J. Tromp, R. Weber, M. Bose, M. Ceylan, I. Daubar, B. Kenda, A. Khan, L. Perrin, A. Spiga, Preparing for InSight: An invitation to participate in a blind test for martian seismicity, Seismological Research Letters, DOI 10.1785/0220170094.

L. Krischer, A. R. Hutko, M. Van Driel, S. Stahler, M. Bahavar, C. Trabant, T. Nissen-Meyer, On-demand custom broadband synthetic seismograms, Seismological Research Letters, DOI 10.1785/0220160210.

M. Böse, J. F. Clinton, S. Ceylan, F. Euchner, M. Van Driel, P. Lognonné, W. B. Banerdt, A probabilistic framework for single-station location of seismicity on Earth and Mars, Physics of the Earth and Planetary Interiors, DOI 10.1016/j.pepi.2016.11.003.

S. Ceylan, M. Van Driel, F. Euchner, A. Khan, J. Clinton, L. Krischer, M. Böse, S. Stahler, D. Giardini, From initial models of seismicity, structure and noise to synthetic seismograms for Mars, Space Science Reviews, DOI 10.1007/s11214-017-0380-6.

Harry van Lenthe, ETH Zurich

S. D. Badilatti, P. Christen, S. J. Ferguson, R. Müller, Computational modeling of long-term effects of prophylactic vertebroplasty on bone adaptation, Proceedings of the Institution of Mechanical Engineers Part H-Journal of Engineering in Medicine, DOI 10.1177/0954411916683222.

J. A. Steiner, P. Christen, R. Affentranger, S. J. Ferguson, G. H. van Lenthe, A novel in silico method to quantify primary stability of screws in trabecular bone, Journal of Orthopaedic Research, DOI 10.1002/jor.2355.

Franco Vazza, Hamburg Observatory

D. Wittor, F. Vazza, M. Brüggen, Testing cosmic ray acceleration with radio relics: A high-resolution study using MHD and tracers, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw2631.

F. Vazza, On the complexity and the information content of cosmic structures, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw3089.

D. Montanino, F. Vazza, A. Mirizzi, M. Viel, Enhancing the spectral hardening of cosmic TeV photons by mixing with axionlike particles in the magnetized cosmic web, Physical Review Letters, DOI 10.1103/PhysRevLett.119.101101.

F. Vazza, M. Brüggen, C. Gheller, S. Hackstein, D. Wittor, P. M. Hinz, Simulations of extragalactic magnetic fields and of their observables, Classical and Quantum Gravity, DOI 10.1088/1361-6382/aa8e60.

Laurent Villard, EPF Lausanne

J. Dominski, B. F. McMillan, S. Brunner, G. Merlo, T. M. Tran, L. Villard An arbitrary wavelength solver for global gyrokinetic simulations. Application to the study of fine radial structures on microturbulence due to non-adiabatic passing electron dynamics, Physics of Plasmas, DOI 10.1063/1.4976120.

N. Tronko, A. Bottino, T. Görler, E. Sonnendrücker, D. Told, L. Villard, Verification of gyrokinetic codes: Theoretical background and applications, Physics of Plasmas, DOI 10.1063/1.4982689.

Peter E. Vincent, Imperial College London

J. S. Park, F. D. Witherden, P. E. Vincent, High-order implicit Large-Eddy simulations of flow over a NACA0021 aerofoil, AIAA Journal, DOI 10.2514/1.J055304.

Viola Vogel, ETH Zurich

S. Arnoldini, A. Moscaroli, M. Chabria,M. Hilbert, S. Hertig, R. Schibli, M. Béhé, V. Vogel, Novel peptide probes to assess the tensional state of fibronectin fibers in cancer, Nature Communications, DOI 10.1038/s41467-017-01846-0.

F. A. Herzog, L. Braun, Ingmar Schoen, V. Vogel, Structural insights how PIP2 imposes preferred binding orientations of FAK at lipid membranes, The Journal of Physical Chemistry B, DOI 10.1021/acs.jpcb.6b09349.

Antigoni Voudouri, Hellenic National Meteorological Service

A. Voudouri, E. Avgoustoglou, P. Kaufmann, Impacts of observational data assimilation on operational forecasts, Perspectives on Atmospheric Sciences, DOI 10.1007/978-3-319-35095-0_21.

E. Avgoustoglou, A. Voudouri, P. Khain, F. Grazzini, J. M. Bettems, Design and evaluation of sensitivity tests of COSMO model over the Mediterranean area, Perspectives on Atmospheric Sciences, DOI 10.1007/978-3-319-35095-0.

Oleg V. Yazyev, EPF Lausanne

A. Crepaldi, G. Autès, G. Gatti, S. Roth, A. Sterzi, G. Manzoni, M. Zacchigna, C. Cacho, R. T. Chapman, E. Springate, E. A. Seddon, Ph. Bugnon, A. Magrez, H. Berger, I. Vobornik, M. Kalläne, A. Quer, K. Rossnagel, F. Parmigiani, O. V. Yazyev, M. Grioni, Enhanced ultrafast relaxation rate in the Weyl semimetal phase of MoTe2 measured by time- and angle-resolved photoelectron spectroscopy, Physical Review B, DOI 10.1103/PhysRevB.96.241408.

M. Pizzochero, O. V. Yazyev, Point defects in the 1*T*′ and 2*H* phases of single-layer MoS_2: A comparative first-principles study, Physical Review B, DOI 10.1103/PhysRevB.96.245402.

S. Borroni, E. Baldini, V. M. Katukuri, A. Mann, K. Parlinski, D. Legut, C. Arrell, F. van Mourik, J. Teyssier, A. Kozlowski, P. Piekarz, O. V. Yazyev, A. M. Oleś, J. Lorenzana, F. Carbone, Coherent generation of symmetry-forbidden phonons by light-induced electron-phonon interactions in magnetite, Physical Review B, DOI 10.1103/PhysRevB.96.104308.

A. Pulkin, O. V. Yazyev, Robustness of the quantum spin Hall insulator phase in monolayer 1*T*′ transition metal dichalcogenides, Journal of Electron Spectroscopy and Related Phenomena, DOI 10.1016/j.elspec.2016.11.005.

G. Manzoni, A. Crepaldi, G. Autès, A. Sterzi, F. Cilento, A. Akrap, I. Vobornik, L. Gragnaniello, P. Bugnon, M. Fonin, H. Berger, M. Zacchigna, O. V. Yazyev, F. Parmigiani, Temperature dependent non-monotonic bands shift in ZrTe5, Journal of Electron Spectroscopy and Related Phenomena, DOI 10.1016/j.elspec.2016.09.006.

L. Yang, M. Jeong, P. Babkevich, V. M. Katukuri, B. Náfrádi, N. E. Shaik, A. Magrez, H. Berger, J. Schefer, E. Ressouche, M. Kriener, I. Živković, O. V. Yazyev, L. Forró, H. M. Rønnow, J_1-J_2 square lattice antiferromagnetism in the orbitally quenched insulator $MoOPO_4$, Physical Review B, DOI 10.1103/PhysRevB.96.024445.

M.-W. Chen, D. Ovchinnikov, S. Lazar, M. Pizzochero, M. B. Whitwick, A. Surrente, M. Baranowski, O. L. Sanchez, P. Gillet, P. Plochocka, O. V. Yazyev, A. Kis, Highly oriented atomically thin ambipolar $MoSe_2$ grown by molecular beam epitaxy, ACS Nano, DOI 10.1021/acsnano.7b02726.

N. Xu, G. Autès, C. E. Matt, B. Q. Lv, M. Y. Yao, F. Bisti, V. N. Strocov, D. Gawryluk, E. Pomjakushina, K. Conder, N. C. Plumb, M. Radovic, T. Qian, O. V. Yazyev, J. Mesot, H. Ding, M. Shi, Distinct evolutions of Weyl fermion auasiparticles and Fermi arcs with bulk band topology in Weyl semimetals, Physical Review Letters, DOI 10.1103/PhysRevLett.118.106406.

G. E. Pacchioni, M. Pivetta, L. Gragnaniello, F. Donati, G. Autès, O. V. Yazyev, S. Rusponi, H. Brune, Two-orbital kondo screening in a self-assembled metal–organic complex, ACS Nano, DOI 10.1021/acsnano.6b07431.

D. Gresch, G. Autès, O. V. Yazyev, M. Troyer, D. Vanderbilt, B. A. Bernevig, A. A. Soluyanov, Z2Pack: Numerical implementation of hybrid Wannier centers for identifying topological materials, Physical Review B, DOI 10.1103/PhysRevB.95.075146.

H. Lee, O. V. Yazyev, Lattice-matched heterojunctions between topological and normal insulators: A first-principles study, Physical Review B, DOI 10.1103/PhysRevB.95.085304.

A. Crepaldi, G. Autès, A. Sterzi, G. Manzoni, M. Zacchigna, F. Cilento, I. Vobornik, J. Fujii, P. Bugnon, A. Magrez, H. Berger, F. Parmigiani, O. V. Yazyev, M. Grioni, Persistence of a surface state arc in the topologically trivial phase of $MoTe_2$, Physical Review B, DOI 10.1103/PhysRevB.95.041408.

I. Crassee, F. Borondics, M. K. Tran, G. Autès, A. Magrez, P. Bugnon, H. Berger, J. Teyssier, O. V. Yazyev, M. Orlita, A. Akrap, BiTeCl and BiTeBr: A comparative high-pressure optical study, Physical Review B, DOI 10.1103/PhysRevB.95.045201.

Lailai Zhu, EPF Lausanne

S. Y. Reigh, L. Zhu, F. Gallaire, E. Lauga, Swimming with a cage: Low-Reynolds-number locomotion inside a droplet, Soft Matter, DOI 10.1039/C6SM01636G.

“High-performance computing facilities such as ‘Piz Daint’ allow us to push the boundaries in terms of scale and accuracy when simulating complex turbulent flow problems. This leads to enhanced insight and understanding, which we hope will ultimately result in a new generation of ‘greener’ more environmentally friendly aircraft that are quieter and more fuel efficient.”

Peter Vincent, Imperial College London

Name
Peter Vincent

Position
Reader in Aeronautics

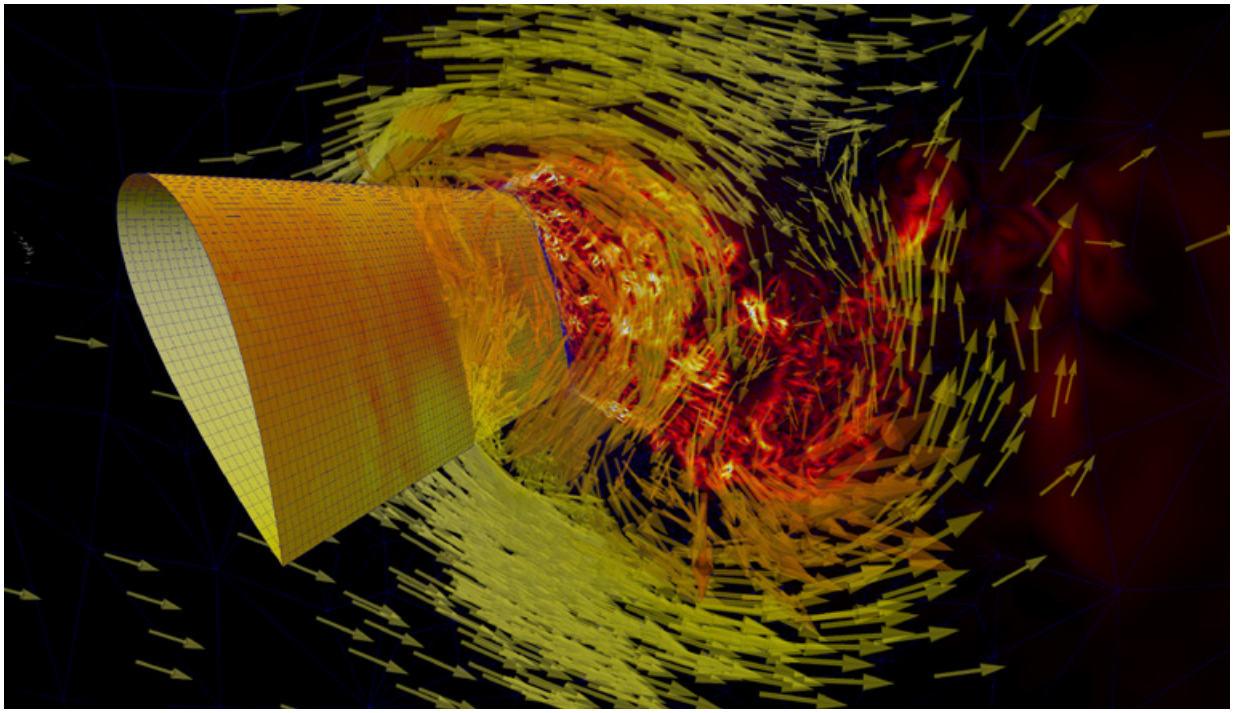
Institution
Imperial College London, UK

Background
2001-2005 MSc Student in Physics, Imperial College London, UK
2006-2009 PhD Student in Aeronautics, Imperial College London, UK
2009-2011 Post-doctoral Scholar in Aeronautics and Astronautics, Stanford University, USA

Area of research
Computational fluid dynamics.

Specialised in
High-order numerical methods, GPU acceleration, compressible flows and biological fluid mechanics.

HPC means for me
I remain amazed by the culmination of human endeavour that running a large-scale fluid flow simulation represents. The mathematical models, consistent and stable discretisations, compiler technology, hardware design and fabrication processes, semiconductor physics, cooling, power, logistics, and indeed politics, all working in unison to simulate the physics of our world.



Simulating Extreme Aerodynamics

Peter Vincent and his team have used "Piz Daint" to simulate flow over aerofoils in deep stall with unprecedented accuracy. Specifically, they employed so-called "high-order" numerical methods to resolve turbulent flow features all the way down to the surface of the aerofoils.

Their results correlate very well with wind tunnel test data - far closer than previous simulations. Simulations like these can help design 'greener' aircraft with reduced noise and CO_2 emissions.
(Image: Peter Vincent)

"The Swiss Institute of Particle Physics and CSCS are paving the way for the upcoming computational challenges"

For more than ten years, CSCS has been operating the cluster "Phoenix" for the Swiss Institute of Particle Physics (CHIPP). "Phoenix" is used to analyse data collected by the three detectors ATLAS, CMS and LHCb at the Large Hadron Collider (LHC) at CERN. The data from ATLAS and CMS were instrumental for the discovery of the Higgs boson, for instance. The cluster is part of the World Wide LHC Computing Grid (WLCG), which is available for LHC experiments to analyse and store data. This year, a pilot project was launched with the goal of enabling the supercomputer "Piz Daint" to perform the same tasks as "Phoenix". In an interview, particle physicist and ETH Zurich professor Christoph Grab, who as chairman of the Swiss physicists computing board coordinates everything to do with "Phoenix" in Switzerland, explains why a changeover is being considered.

Professor Grab, with the Phoenix cluster, CSCS has been operating what's known as a Tier-2 system to analyse data from the LHC experiments for more than ten years. The supercomputer "Piz Daint", a Cray XC40/XC50, is now analysing the data instead of "Phoenix" in a pilot project that is currently underway. What induced you to do that?

Christoph Grab: Our job is to provide the tools such as computational power, storage and services for Swiss particle researchers to evaluate LHC data. Until now, we've bought the hardware that's run at CSCS ourselves with the centre's support. In around eight years, the upgraded High Luminosity LHC (HiLumi-LHC) will go online, giving us 10 to 20 times more particle collisions in the LHC. This means much more data in the multi-exabyte range, and we estimate that the overall global computing resources for the LHC will have to be increased at least 50-fold. And all this with the same annual budget. Investing more money in the existing cluster and expanding it won't upscale sufficiently. Therefore, together with CSCS, we came up with the idea of using highly scalable resources such as "Piz Daint" for all our workflows. Other physicists in the USA are already using HPC resources for certain parts of the workflow.

The LHC-Tier-network has been based on clusters that are connected via a grid. You say that others in the USA are already partially using supercomputers like "Piz Daint". Is it difficult to incorporate these HPC computers into the grid architecture?

It isn't an insurmountable problem. Someone who sits in America and conducts analyses sends the job to the computer network, which itself looks for available resources, and subsequently the job is usually sent there. The actual kind of computer is secondary, provided it is outwardly transparent, in other words, the same compatible software interfaces and services are offered. Imagine a power plug that you stick into the plug socket to draw resources. Provided the plug fits and the same voltage is used, there aren't any major problems.

ETH Zurich professor Christoph Grab is chairman of the Swiss physicists computing board. (Image: ETH Zurich)

How heavily are you using "Piz Daint" for your analysis during the current pilot phase?

On average, 25 percent of our analyses have been conducted on it since the beginning of the year. We have two different kinds of needs when using the supercomputer: on the one hand, pure computing for the simulations and, on the other hand, crunching data. The latter involves moving data back and forth; this data transfer has other demands than pure computing and is necessary to analyse the data measured in the experiment. We are now in the fortunate situation at CSCS where we can use an uncomplicated technical solution on "Piz Daint" that rules out an additional bottleneck. As mentioned above, others have also deployed HPCs before, but only for the simulation part.

How satisfied are you with the first test results on "Piz Daint"?
The data transfer and access for the analyses works extremely well, and we've managed to iron out all the major problems. In other words, we've honed the software in collaboration with the CSCS specialists in the course of the year. This already makes the Cray system more or less as efficient as the "Phoenix" cluster, both in terms of cost and computer efficiency. Understandably, it isn't quite as stable to operate yet as the "Phoenix" cluster, which has been running for years.
In addition, in close collaboration with CSCS and the University of Bern, LHC researchers successfully scaled ATLAS simulations on "Piz Daint" up to 25 000 cores. The main objectives were to test whether the infrastructure can scale up with this specific workload and whether "Piz Daint" could sustain this sort of experiment on a large scale. This is the largest run conducted at CSCS by an LHC experiment so far and one of the first large-scale tests on Cray HPC platforms using standard World Wide LHC Computing Grid workflows.

"Piz Daint" is used by many research groups, who sometimes have to wait in a queue for their computing jobs. For you, however, it's important to be able to access the computer resources around the clock.
That's a model we have to agree on with CSCS. If we stop using "Phoenix" completely and switch to "Piz Daint", I imagine we'll agree to a guaranteed resource quota with the service in question.

The dedicated cluster named "Phoenix" (in the picture) analysed for 10 years the data from the LHC experiment. The supercomputer "Piz Daint", a Cray XC40/XC50, is now taking over this role. (Image: CSCS)

What do you hope will result from the switch overall?
First and foremost, scalability for the next five to ten years and a simplified system, both cost-wise and operationally. Currently, we have to maintain two completely separate systems with CPUs and disk space, parallel to the other infrastructures at CSCS. In case of switching, only a single shared system in regards to hardware needs to be operated, which should be sufficient for all our needs. In this case, being part of a larger entity not only has operational advantages, but also financial ones for purchasing components.

Due to its architecture, "Piz Daint" is particularly suitable for structuring large data quantities. Is this also the case for the Data of the LHC experiments?
Probably not in the immediate future. But the advantages for us also lie in the combination of CPUs and GPUs. That's something we can exploit extremely effectively in physics in the long term. Presently, we already apply certain machine learning techniques in the analyses; it's just that we've been referring to it as multivariate analyses in the last years. GPUs are particularly well suited to some of these tasks, and we want to benefit from this, of course. We've already run initial analyses of special physics problems successfully on the GPUs and are currently expanding and enlarging these applications to study the potential of these architectures.

Can you give an example?
Neuronal networks for analyses of particular event topologies. These networks have to be trained extensively usually on simulated data sets to obtain reliable results afterwards when applied to data, and that works very efficiently on "Piz Daint's" GPUs. That's just one potential application. When simulating materials, for instance, you also have recurring processes that can be shown to be calculated very effectively on GPUs.

Several special pilot projects to be conducted on "Piz Daint" are now scheduled. Can you say a bit more about them?
They involve running scalings of LHC software and workflows, without all the red tape, transparently via the network on the supercomputer and trying out new ideas. We've got ideal conditions for this, as there is a very reliable network between CERN and CSCS without any artificial barriers. The idea came during a discussion with CSCS Director Thomas Schulthess during a visit to CSCS by CERN Director Fabiola Gianotti last summer and will now be implemented directly. That kind of thing is only possible in Switzerland. One of these pilot projects is the one I mentioned earlier regarding GPUs with a view to exploiting

the computer architecture more effectively. Our institute and the CMS experiment are primarily involved in this.

Are there any other plans?
In the near future, we're due to test the concept of "data lakes". These involve holding large quantities of raw data in a cloud-like space. Researchers from CERN and the Swiss ATLAS experiment are interested in these tests as CSCS also provides ideal conditions for them with "Piz Daint". The goal is to conduct the major data processing near the lakes and run smaller jobs directly via the network. Currently, the grid consists of over 180 different-sized systems worldwide. That will no longer be the case in five to ten years, as it simply isn't efficient. One day, we might have ten large installations worldwide with a likely power consumption of 2 to 5 megawatts each. The idea is to consolidate the small systems and make the technologies available for widespread use. HPC is one of them.

So ultimately, in regards to the data lakes on "Piz Daint", it's about incorporating the further development of the HPC into CERN research?
Yes. The Swiss Institute of Particle Physics and CSCS are paving the way for the upcoming computational challenges. The idea for this was born at the Directors' Meeting in August. As chairman of CHIPP, I have now taken on a kind of mediator role to realise such projects. My main duty, however, is to make the computer service available to Switzerland for the three different experiments at CERN and make sure our particle physicists are able to analyse their data and conduct physics.

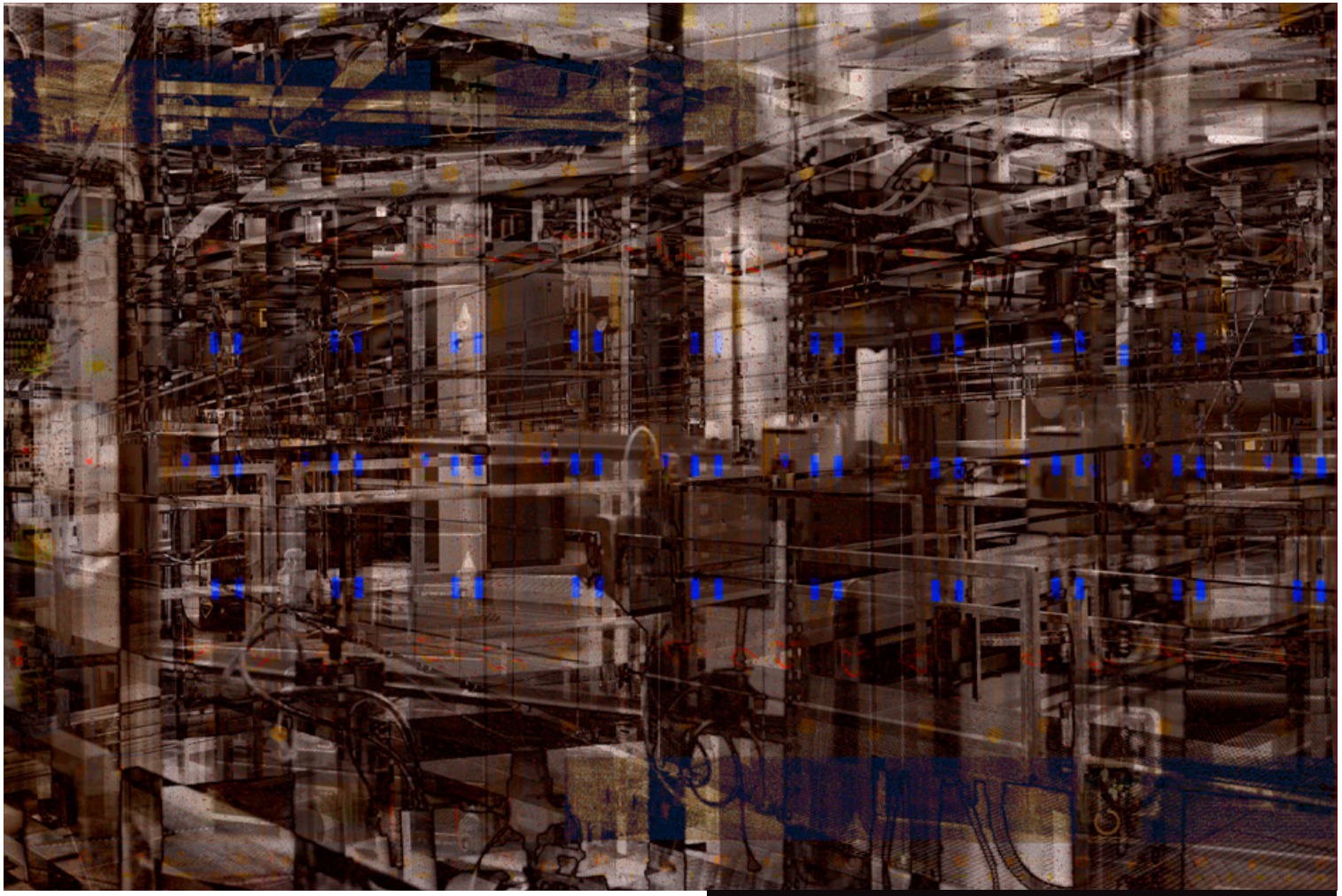
Are you planning to perform the calculation solely on "Piz Daint" in the future?
That's the goal if it is more economical. Within the community, we're clarifying the individual needs, testing them on "Piz Daint" and comparing the efficiency and costs. We should have the comparisons by the end of November. On this basis, the PIs from the individual Swiss institutions will then decide on what to do next.

What role does CHIPP play in an international context?
Needless to say, we're a small beacon on the grand scale of things; but our cluster has always worked well, and we're assuming a particular pioneering role with the current pilot projects and gaining more visibility. We were the first to analyse data reasonably on a supercomputer–apart from anything else, because we're able to access the data in the memory and every single hub externally. This means that every hub we use can communicate directly with the data in the memory. That currently isn't possible anywhere else due to security regulations. What it will look like in five years is uncertain, but I'm confident that both we and CSCS will learn a great deal via these pilot projects and develop a lot of expertise.

Will anything change fundamentally in the global particle physics data network, and will other Tier systems such as the Tier-0 system at CERN also switch to classic high-performance computers?
I think our model will change as our parameters have to evolve, too. Yesterday, we only spoke about grids; today, the cloud is on everyone's lips. But these are actually very similar concepts. The networks will grow and become even faster and more reliable. But for now, what the architecture and our computing models of the future will look like in ten years and whether this will be HPC systems in the current sense is anybody's guess, of course.

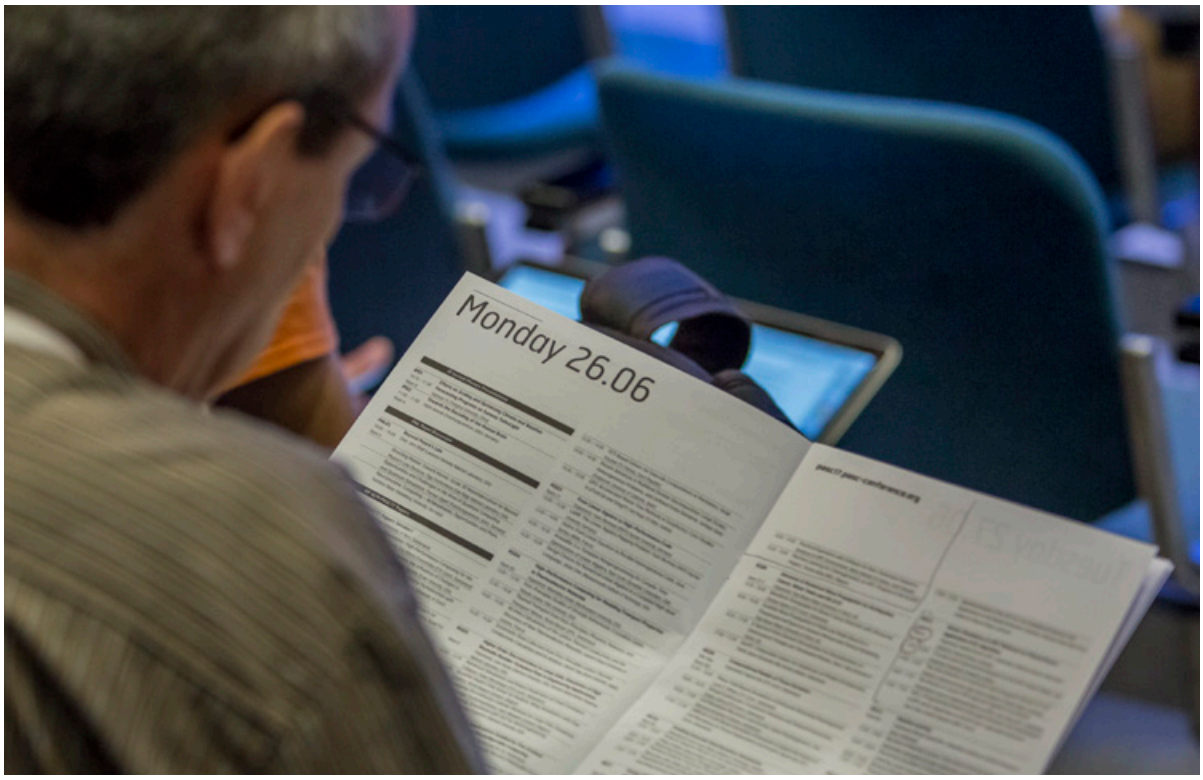
Where is there room for improvement?
We need more manpower. We currently employ people for the operations and new projects whose total employment level at CSCS for our LHC needs corresponds to between three and four full-time equivalents. That's not very much, but we need experts if new technologies are to be promoted. In particular, there is still a lot of room for improvement on the software side of things, both at system level and on the experimental software side. However, it is extremely difficult to find truly suitable people and then only hire them temporarily for two or three years.

Transcriptions – *The Medium Is the Message*
William Gibson, Count Zero (1986)



Transcriptions – *The Medium Is the Message*
Aldous Huxley, Brave New World (1931)

PASC17 Conference



From 26 to 28 June 2017, close to 400 scientists and researchers from 23 countries convened at the Palazzo dei Congressi in Lugano, Switzerland, for PASC17, the fourth edition of the PASC Conference series. The annual conference focuses on advancing the quality of scientific communication between the various disciplines of computational science and engineering in the context of high performance computing, placing particular emphasis on methods, tools, algorithms and novel techniques.

CSCS has led the organization of the PASC Conference since its inauguration in 2014, and is proud to be a co-sponsor alongside the Association for Machine Computing (ACM). The conference has its origins in the Swiss Platform for Advanced Scientific Computing, a structuring project initiated in 2013 by the ETH Board. The overarching goal of the platform is to position Swiss computational sciences in the emerging Exascale era: its focus on software development complementing the hardware-focused elements of the Swiss High-Performance Computing and Networking (HPCN) strategy, launched in 2009.

Focused on interdisciplinarity

As in previous years, the PASC17 technical program was organized around eight scientific domains: chemistry and materials, life sciences, physics, climate and weather, solid earth dynamics, engineering, computer science, and applied mathematics, and emerging application domains (social sciences and finance). Such an interdisciplinary audience makes for a rather unique platform, with domain scientists, computer scientists and applied mathematicians all under the same roof, working together to enable and improve the art of large-scale computational science. The three-day program included more than 40 topically-focused "minisymposia", four sessions of peer-reviewed papers (published in the Proceedings of the PASC Conference, accessible via the ACM's Digital Library), poster sessions, and five invited plenary talks – one of which being a public lecture by EPF Lausanne professor and materials scientist Nicola Marzari.

Marzari opened his keynote on the history and development of modern-day materials research with a photograph of the quantum physicist Erwin Schrödinger flying through the air on a skiing vacation in Arosa at the end of 1925.

Materials Scientist Nicola Marzari from EPF Lausanne.
(Image: CSCS)

Neuroscientist Katrin Amunts of the Jülich Research Centre.
(Image: CSCS)

It was during this New Year's stay that the physicist succeeded in formulating the equation named after him, something which would earn him a Nobel Prize and become a milestone for modern materials research. The Schrödinger equation described for the first time the quantum mechanical states of atoms and molecules, which among other things determine a material's properties. A further breakthrough came with the development of density functional theory by physicist Walter Kohn. His work made it possible to solve the Schrödinger equation efficiently on a computer, and for this, Kohn was likewise honoured with a Nobel.

"Edisonian" materials development

In spite of the ever-increasing computing power at our disposal, the simulation and development of new materials – in the search for alternative energy sources, for example – remains a major challenge. As Marzari remarked in his plenary, materials development is still "Edisonian": Thomas Edison, inventor of the incandescent light bulb, is said to have tested 3 000 different materials until he found one suitable as a filament. Today, that testing is done by supercomputers: they are the virtual laboratories of theoretical material scientists, and computational science is an indispensable element of modern materials research.

Alongside the public lecture by Marzari, four other invited plenary speakers from various scientific disciplines stimulated lively interdisciplinary discussions amongst the conference participants. Haohuan Fu, Deputy Director of the National Supercomputing Centre in Wuxi, China, presented the Sunway TaihuLight supercomputer and his group's efforts on scaling and optimising climate and weather forecasting programs for the world's most powerful supercomputer. Katrin Amunts from the Jülich Research Centre is one of the world's foremost neuroscientists in the field of brain mapping. In her plenary, Amunts presented her research aimed at decoding the human brain as part of the Human Brain Project. Cosmologist Katrin Heitmann from the University of Chicago then gave an introduction to dark matter and dark energy and described the cosmology code she develops to better simulate the mysteries of our Universe. On the last day of the conference, Matthias Troyer, a Principal Researcher in the Quantum Architectures and Computation Group at Microsoft Research, discussed cutting-edge progress in quantum computing. Quantum computers are devices with computational power far beyond anything we can imagine in classical computing – and the first such systems are becoming available today. Troyer focused on the need to educate a new generation of quantum software engineers with knowledge in quantum computing and HPC in order to be able to exploit such exotic machines.

New additions to the program

The inclusion of two panel discussions was a new addition to the technical program at PASC17. The first of the panels addressed the question of what lies beyond Moore's law. Chaired by John Shalf from Lawrence Berkeley National Laboratory, it began with short talks from the panel members: Olga Ovchinnikova from Oak Ridge National Laboratory, Thomas Lippert from the Jülich Research Centre and Karlheinz Meier from Heidelberg University. The panellists discussed the future of conventional digital computers alongside more disruptive architectures such as neuromorphic and quantum computers. The unanimous conclusion was that no single architecture is likely to dominate – rather, each will be best suited to its own certain set of applications.

The second panel tackled the topic of publication practices in the computational sciences. The panellists, comprising editors from three computationally-focused scientific journals, touched on aspects of traceability and reproducibility of scientific results, as well as the lack of recognition that code development and publication tends to receive in our community.

Planning is already well underway for the next edition of the conference, which will be held in Basel from July 2 to 4, 2018. The theme of PASC18 is *Fast and Big Data, Fast and Big Computation,* emphasizing the ever-tighter coupling of data and computation in modern high-performance computing. The meeting will be chaired by Florina Ciorba from the University of Basel and Erik Lindahl from the University of Stockholm.

Panel discussion at PASC17. From left to right: Walter Dehnen, Robert Pincus, Jack Wells, Michael Heroux and Thomas Schulthess. (Image: CSCS)

Thomas Schulthess, Director of CSCS. (Image: CSCS)

“For me and my group, supercomputers like ‘Piz Daint’ are essential for computing observables needed for discovering new physics. Today, with the help of large-scale simulations, we gain insights into the complex dynamics of the strong force that binds the matter of our world, that we could not imagine possible a decade before.”
Constantia Alexandrou, University of Cyprus and the Cyprus Institute

Name
Constantia Alexandrou

Position
Professor

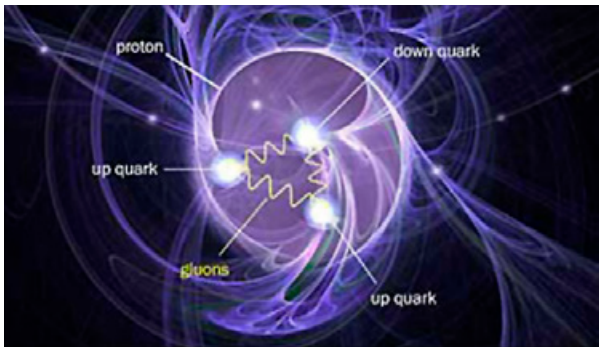
Institution
University of Cyprus and the Cyprus Institute, Cyprus

Background
1970-1980 BA degree in Physics, Oxford University, UK
1980-1985 PhD in Theoretical Nuclear Physics, Massachusetts Institute of Technology, USA
1985-1992 Post-doctoral researcher at the Swiss Institute of Nuclear Physics, Erlangen University, Germany and Paul Scherrer Institute
Since 1993 Faculty at the University of Cyprus, Cyprus
Since 2010 Institute professor at the Cyprus Institute, Cyprus

Area of research
Fundamental particles and fields.

Specialised in
Lattice quantum chromodynamics.

HPC means for me
Advanced infrastructure and algorithms that enable researchers to investigate and understand complex phenomena opening new horizons that would have been unthinkable without HPC.



With help of “Piz Daint” supercomputer towards solving the proton spin puzzle

Scientists in a research group led by Constantia Alexandrou, made a crucial step towards solving a three-decades-old puzzle: they have successfully deciphered the total angular momentum (spin) of the nucleon determining how its shared among its constituents. CSCS supercomputer “Piz Daint” provided computational resources needed for accomplishing this.
(Image: Courtesy Brookhaven National Laboratory)

Finances

User Lab Expenditures & Income

	Expenses CHF
Investments	**4 218 972.81**
Equipment and Furniture	**35 413.60**
Personnel	**9 478 259.90**
Payroll	7 427 612.67
Employer's Contributions	1 268 307.35
Further Education, Travel, Recruitment	782 339.88
Other Material Expenses	**6 791 323.37**
Maintenance Building & Technical Infrastructure	488 833.55
Energy	1 886 060.52
Administrative Expenses	8 681.70
Hardware, Software, Services	3 895 805.75
Remunerations, Marketing Workshops, Services	506 046.48
Other	5 895.37
Extraordinary Expenditures	**50 724.19**
Membership Fees	50 724.19
Total Expenses	**20 574 693.87**

	Income CHF
Basic Budget Income	**19 201 164.50**
ETH Zurich Operations	16 111 603.00
ETH-Rat - HPCN Investments	2 000 000.00
.+. Rollover from 2017	29 561.50
ETH-Rat - PASC Initiative Software Development	1 060 000.00
Other Income	**185 346.23**
Services / Courses	80 826.97
Reimbursements	14 880.10
Other	89 639.16
Total Income	**19 386 510.73**

Balance	**- 1 188 183.14**
./. Balance ETH-Rat - HPCN Investments	-2 228 014.08
./. Balance ETH-Rat - PASC Initiative Software Development	428 083.64
Balance ETH Zurich Operations Transferred Back	**611 747.30**

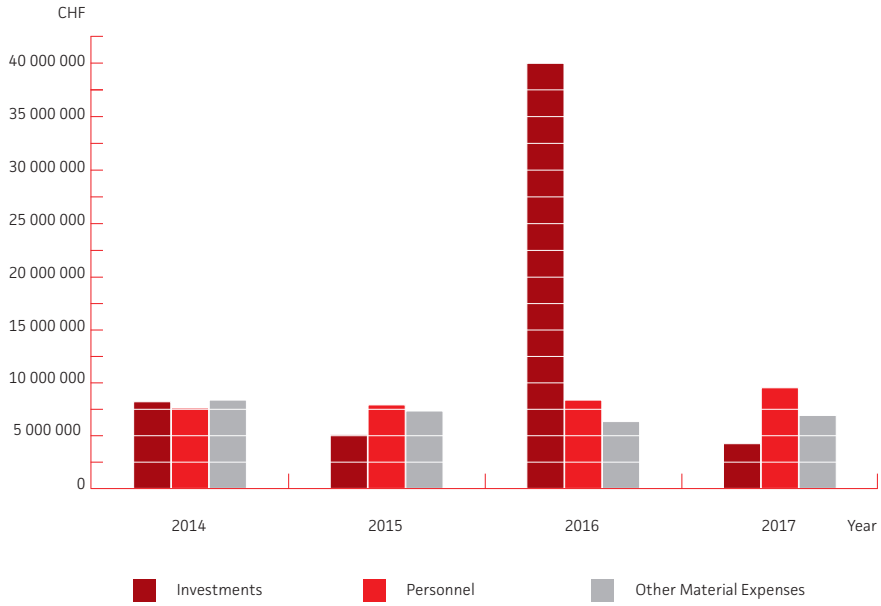
CSCS acts as leading house for the PASC Initiative with contribution of "External Projects" that amounts to 1.64 Mio CHF.

Third-Party Contributions

	CHF
Third-Party Contributions	**7 608 374.57**
MeteoSwiss	2 186 400.00
EU Projects (excl. 2/3 overhead ETH Zurich)	1 426 359.57
Blue Brain Project	874 472.00
PRACE High-Level Support Team	772 780.00
University of Zurich	718 136.00
Monch Cluster	325 000.00
Paul Scherrer Institute	279 440.00
Università della Svizzera italiana	240 000.00
MARVEL	205 000.00
University of Geneva	200 000.00
CHIPP	203 000.00
Hilti	164 287.00
Partner Re	13 500.00

User Lab Expenses Development (CHF)

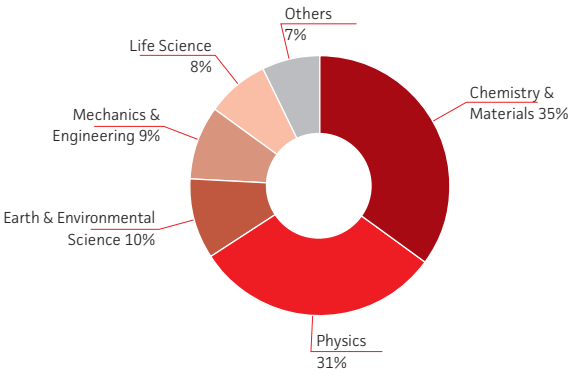
	2014	2015	2016	2017
Investments	8 118 445	5 042 501	40 023 533	4 218 973
Personnel	7 538 405	7 842 930	8 313 178	9 478 260
Other Material Expenses	8 268 005	7 271 103	6 293 094	6 877 461

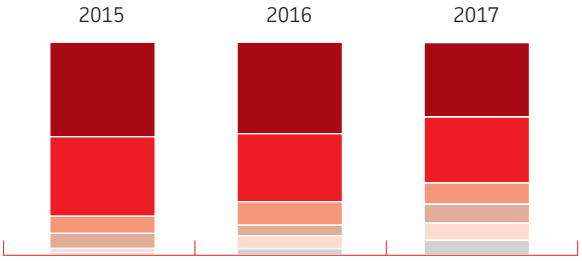


Usage Statistics

User Lab Usage by Research Field

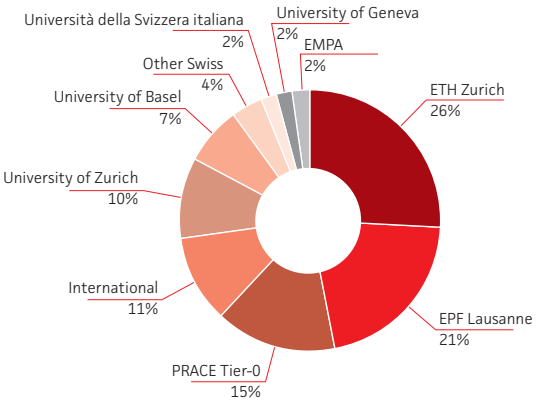
Research Field	Node h	%
Chemistry & Materials	13 393 066	35
Physics	11 628 941	31
Earth & Environmental Science	3 801 317	10
Mechanics & Engineering	3 274 333	9
Life Science	2 878 274	8
Others	2 595 250	7
Total Usage	**37 571 181**	**100**

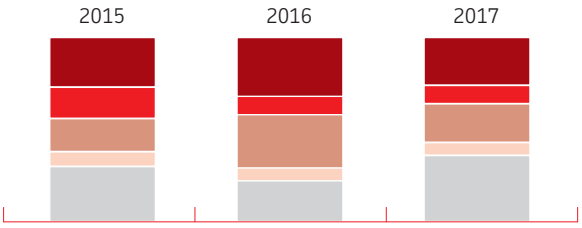




User Lab Usage by Institution

Institution	Node h	%
ETH Zurich	9 968 002	26
EPF Lausanne	7 965 382	21
PRACE Tier-0	5 826 711	15
International	3 959 901	11
University of Zurich	3 697 728	10
University of Basel	2 573 825	7
Other Swizerland	1 402 172	4
Università della Svizzera italiana	879 374	2
University of Geneva	721 526	2
EMPA	576 560	2
Total Usage	**37 571 181**	**100**





Compute Infrastructure

Computing Systems Overview

Name	Model	Installation/Upgrades	Owner	TFlops
Piz Daint	Cray XC50/Cray XC40	2012 / 13 / 16	User Lab, UZH, NCCR Marvel	25 326 + 2 193
Blue Brain BG/Q	IBM BG/Q	2013	EPF Lausanne	839
Blue Brain Viz	IBM Cluster	2013	EPF Lausanne	13
Monch	NEC Cluster	2013 / 14	ETH Zurich	132
Phoenix	x86 Cluster	2007 / 12 / 14 / 15 / 16	CHIPP (LHC Grid)	86
Piz Kesch	Cray CS-Storm	2015	MeteoSwiss	196
Piz Escha	Cray CS-Storm	2015	MeteoSwiss	196
Monte Leone	HP Cluster	2015	User Lab	7 + 15
Grand Tavé	Cray X40	2017	Research & Development	437

Computing Systems Specifications

Name	Interconnect Type	CPU Type	No. Cores	No. Sockets per Node	No. Nodes
Piz Daint	Cray Aries	Intel Xeon E5-2690 v3 + Nvidia P100 Intel Xeon E5-2695 v4	12 18	1 + 1 2	5 320 1 813
Blue Brain BG/Q	IBM BGQ 3D Torus	PowerPC A2	16	1	4 096
Blue Brain Viz	Infiniband FDR	Intel Xeon E5-2670	8	2	40
Monch	Infiniband FDR	Intel Xeon E5-2660 v2	10	2	376
Phoenix	Infiniband FDR	Intel Xeon E5-2670 Intel Xeon E5-2690 Intel Xeon E5-2680 v2 Intel Xeon E5-2680 v4	8 8 10 14	2 2 2 2	64 1 48 40
Piz Kesch	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2 + 8	12
Piz Escha	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2 + 8	12
Monte Leone	10 Gb Ethernet	Intel Xeon E5-2667 v3 Intel Xeon E5-2667 v3 Intel Xeon E5-2690 v3 + Nvidia K40C	8 8 12	2 2 2 + 1	6 7 4
Grand Tavé	Cray Aries	Intel Xeon Phi CPU 7230	64	1	164

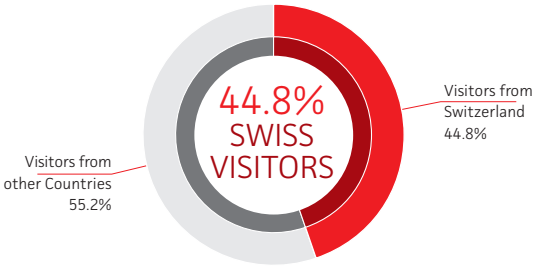
Communications Statistics

Website cscs.ch

	2016	2017
Total Website Visitors	69 833	87 678
Average Website Visits (Minutes)	2:84	2:49

New Visitors

Visitors Origin



Top 5 Most Visited Website Pages

1. CSCS Homepage www.cscs.ch
2. Piz Daint www.cscs.ch/computers/piz-daint/
3. Staff www.cscs.ch/about/staff
4. Open Positions www.cscs.ch/about/open-positions/
5. Working at CSCS www.cscs.ch/about/working-at-cscs/

Twitter

	2016	2017
Followers	592	866

LinkedIn

	2016	2017
Followers	5 831	6 164

YouTube

	2016	2017
Watch Time (Minutes)	424 011	568 872
Average View Duration (Minutes)	4:00	4:41
Number of Views	105 797	121 234

Facebook

Find us on

	2016	2017
Followers	89	139

CSCS in the News

	2016	2017
News Websites	406	334
Print	186	159
Radio & TV	15	12

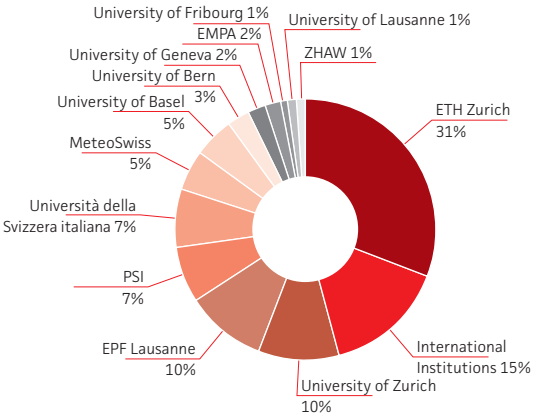
Word Cloud of News Related to CSCS

User Satisfaction

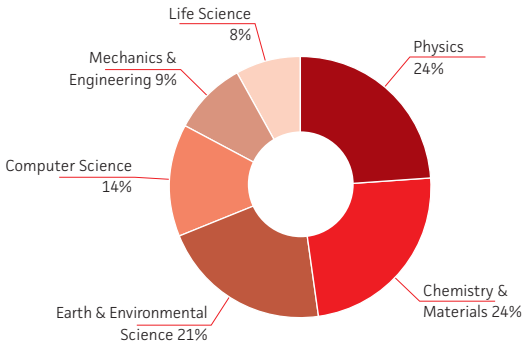
A user satisfaction survey was submitted to 1313 users in January 2018. The response rate was of 17.7% (232 answers).

User Profile

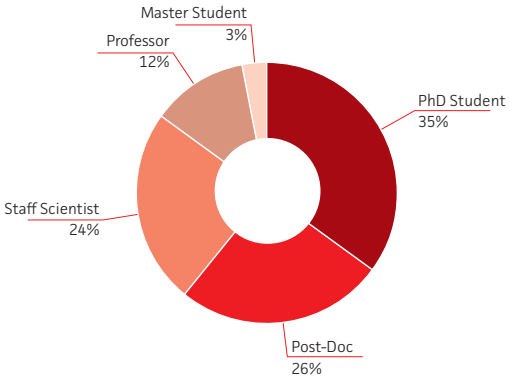
Your institution



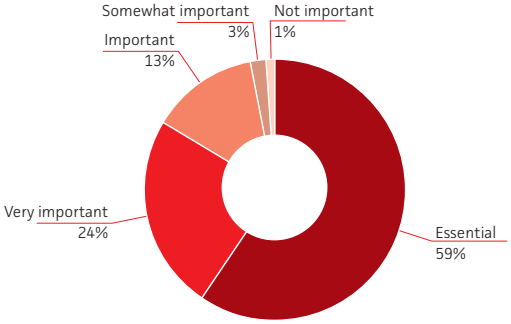
Your scientific field



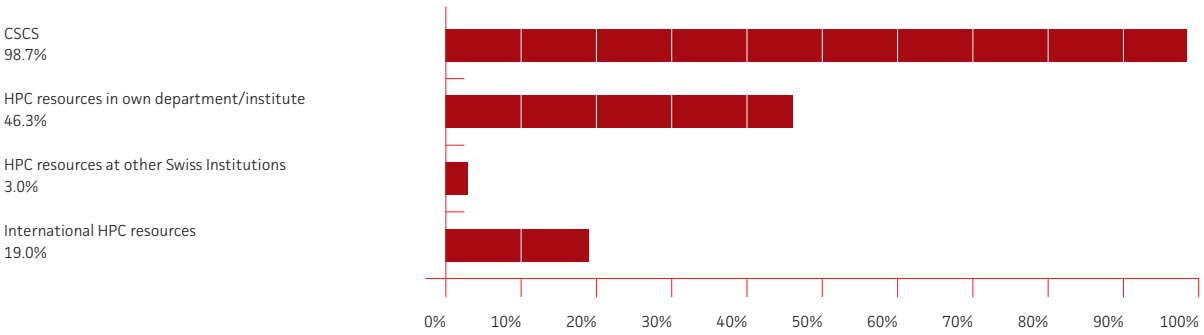
Your position



For my research, CSCS resources are:

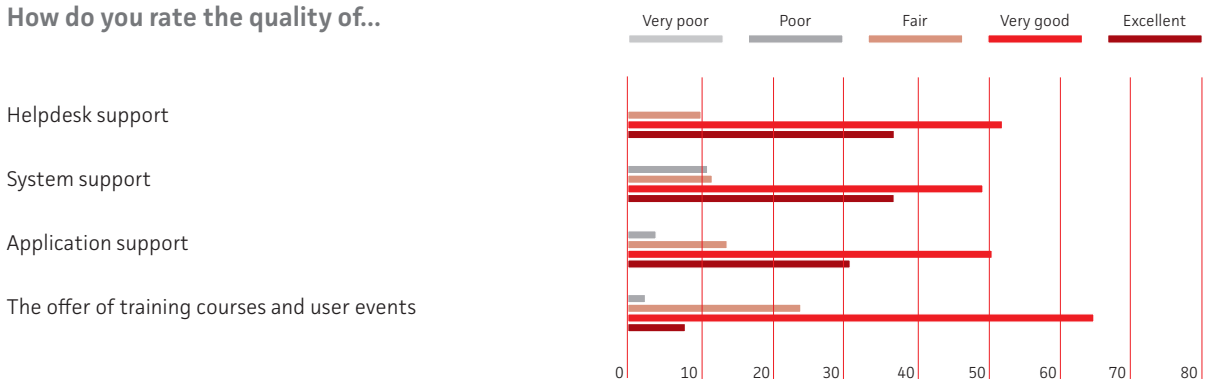


Which HPC resources are you using?

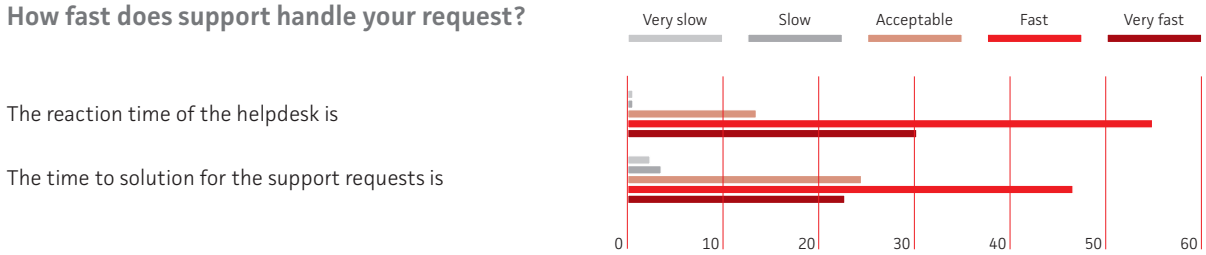


User Support

How do you rate the quality of...

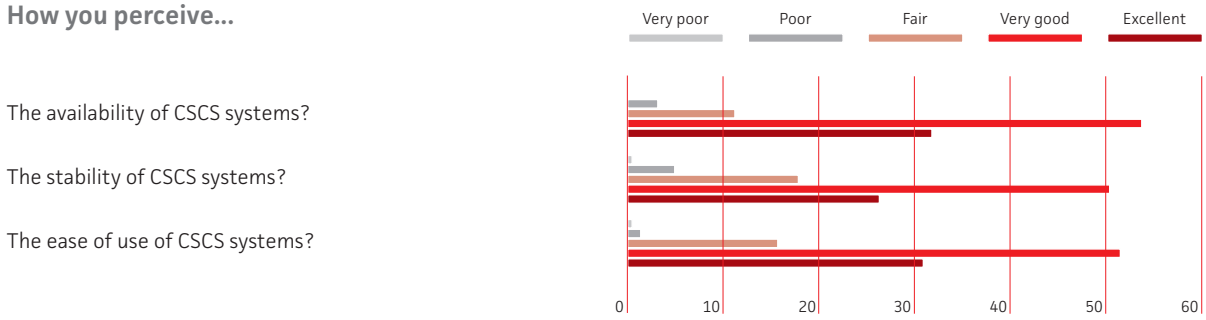


How fast does support handle your request?

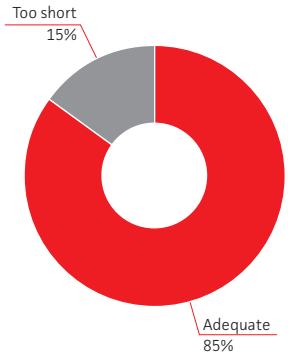


System Availability, Stability and Usability

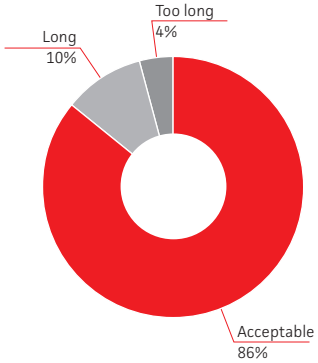
How you perceive...



The run time limits for batch jobs are:

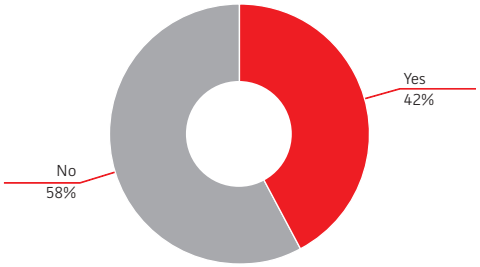


The job waiting time in the queue is:

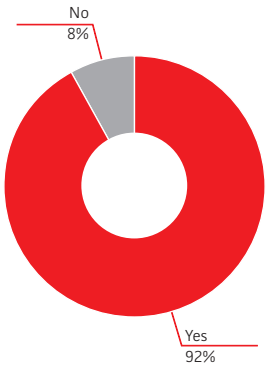


Project Proposal Process

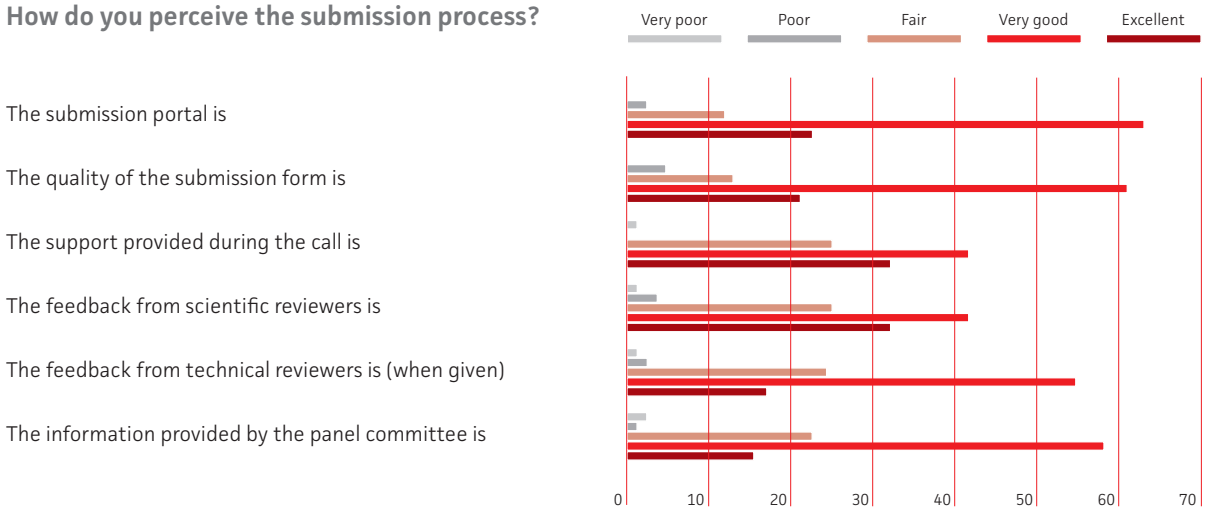
Have you been submitting project proposals to CSCS (as PI or supporting the PI?)



Is the reviewing process transparent?

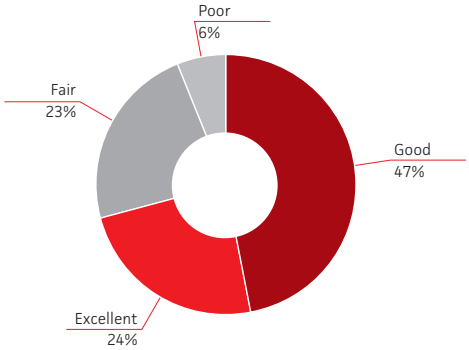


How do you perceive the submission process?

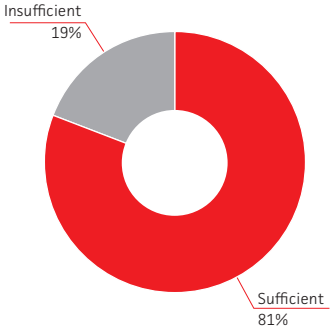


Adequacy of Allocated Resources

The resources assigned to my project are:

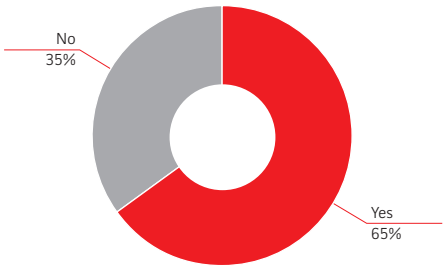


My storage allocation on "project" is:

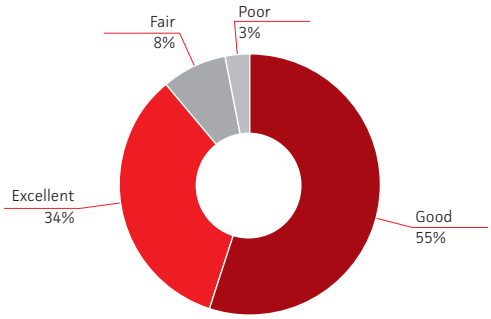


Application Development

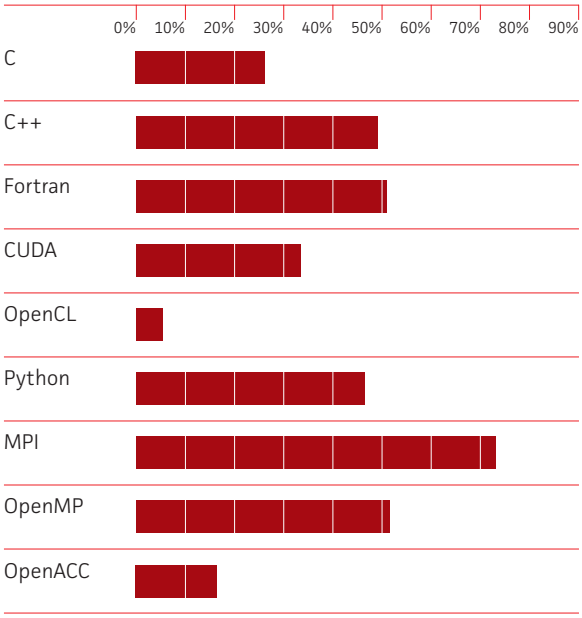
Do you develop and maintain application codes?



How do you rate the offered range of programming tools (compilers, libraries, editors, etc.)?



Which programming languages and parallelization paradigms are you using primarily?



Information & Communication

How do you feel informed about...

Status of the systems

Software and applications

Hardware configuration

Available computing resources

Own allocations

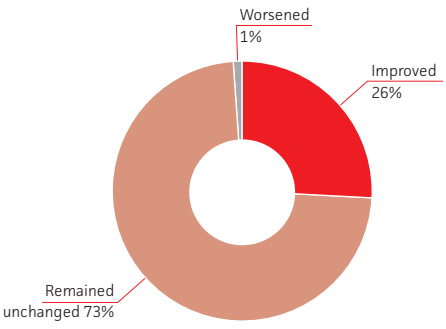
Your consumption of your allocation

Upcoming events and courses

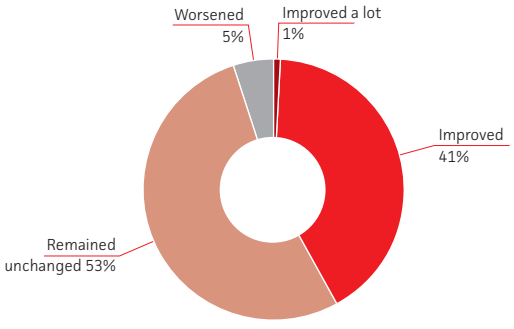
Future developments at CSCS

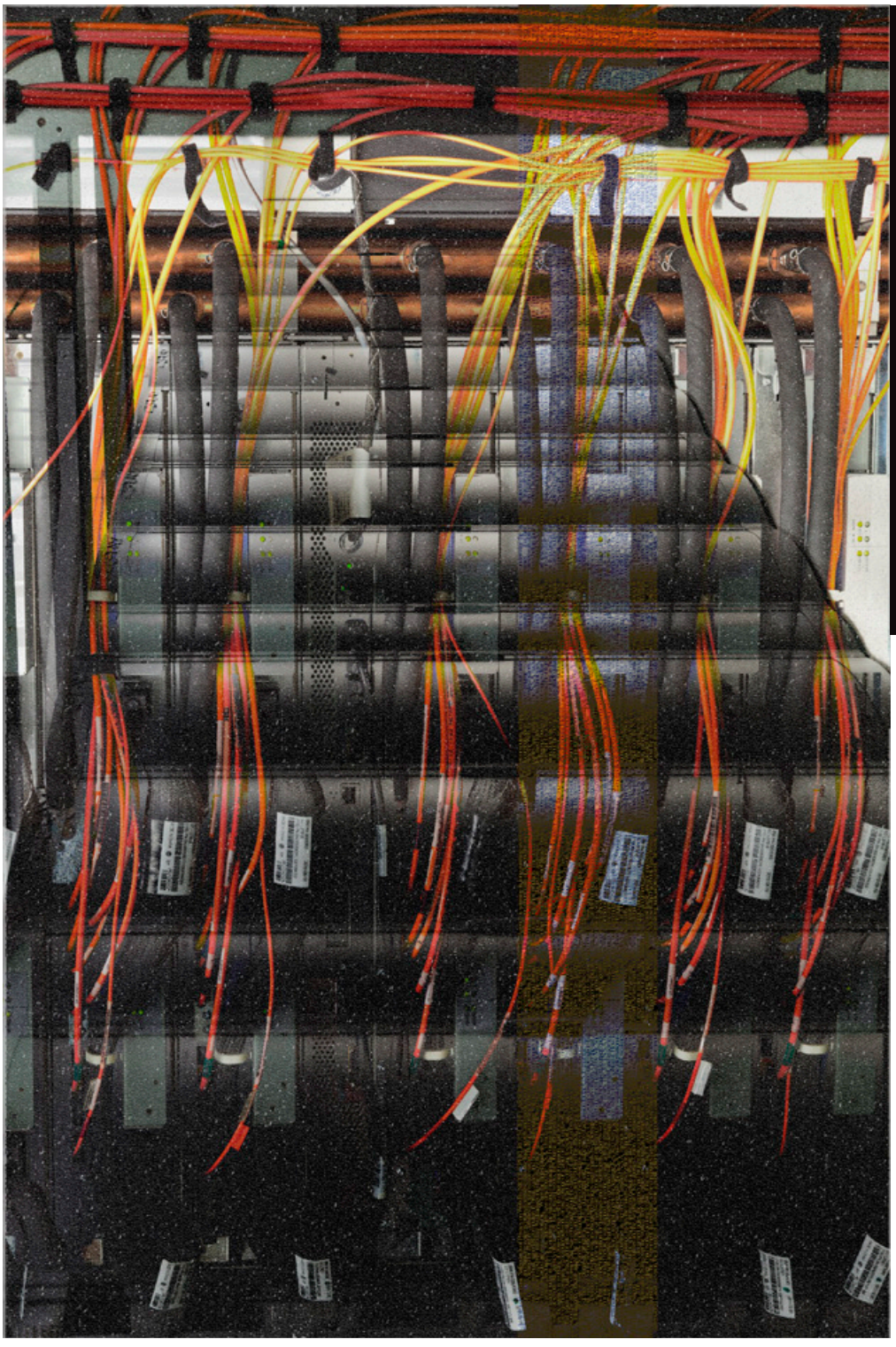
Perception of CSCS

How has the communication between CSCS and the user community developed during last year?



My general view in the last year is that CSCS (systems, services, support) has:





Transcriptions – *The Medium Is the Message*
Marshall McLuhan, Understanding Media – The Extensions of Man (1964)

Impressum

CSCS Swiss National Supercomputing Centre
Via Trevano 131
6900 Lugano
Switzerland

Phone +41 91 610 82 11
Fax +41 91 610 82 09
www.cscs.ch

Design & Layout
Humus Brand Culture

Editorial Board
Michele De Lorenzi
Maria Grazia Giuffreda
Timothy Robinson
Angela Schneebeli
Simone Ulmer

Photos
CSCS, Marco Abram, Matteo Aroldi
Scientists portraits: Alessandro Della Bella, Thomas Angus, Panayiotis Kyriacou
Transcriptions: Stefano Spinelli

Printing
Lepori & Storni

Print-run
300