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CSCS

Annual Report
2016

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

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The photographer Alessandro Della Bella has portrayed five scientists of different scientific fields who use CSCS supercomputers for their research work: Andreas Fichtner (ETH Zurich), Martin Kunz (University of Geneva), Mathieu Luisier (ETH Zurich), Matthias Krack (Paul Scherrer Institute), Petros Koumoutsakos (ETH Zurich). The photos in this Annual Report presents the scientists and their research.

Welcome from the Director

Thomas Schulthess, Director of CSCS.

The Swiss National Supercomputing Centre (CSCS) can again look back on a successful and eventful year, with 2016 marking a jubilee that will blaze new trails for us going forward. I welcome you to this retrospective and outlook.

A significant upgrade of our flagship supercomputer "Piz Daint" in the final quarter of 2016 means we now have a machine that sets yet another historic milestone for CSCS, both in terms of performance and technological versatility of use.

The upgrade secures the position of CSCS among the global leaders in high-performance computing (HPC), while "Piz Daint" still counts among the most energy-efficient supercomputers anywhere in the world. Equipped with conventional processors and graphics processors too, this hybrid system is set to meet user needs not only in the area of complex simulations, but also with highly topical themes of the moment: big data, data analytics and deep learning. CSCS with its long term, ongoing and fruitful cooperation involving users from a multiplicity of research disciplines, mathematicians and computer scientists, as well as industry, was paving the way for a universally applicable "Piz Daint".

Along with our efforts on the hardware front, our work on software to boost the efficiency of our supercomputer did not go unnoticed. Take weather modelling, for example: MeteoSwiss switched to using graphics processors last year and developed new code for that purpose. These innovations gained CSCS and MeteoSwiss the Swiss ICT award in Lucerne this November. In the jury's view, this novel method of calculating vast amounts of weather data on a supercomputer marked the beginning of a trend.

For me, this is all evidence that CSCS with its hybrid system is on a good track in HPC. Furthermore, this Autumn ETH Zurich signed a memorandum of understanding to establish an international institute together with two other leading high-performance computing centres in the USA and Japan that have likewise opted for hybrid systems. The institute will dedicate itself to focusing on common goals, sharing experience in HPC and keeping an anticipatory eye on possible future computer architectures.

Credit for all these achievements I have mentioned is due not least to the Swiss High-Performance Computing and Networking Initiative launched by the ETH Board in 2009, and implemented under the leadership of CSCS and the Università della Svizzera italiana. It is a very special pleasure for me to report these success stories in what is a highly historical year for CSCS: 2016 marks a quarter-century since the opening of the computing centre in Ticino. For this we held a festive celebration in October, attended by then-founders of the computing centre and its early users, as well as further guests from the political, research and business worlds.

Now I would very much like to thank all those who have contributed to the success of CSCS. My special thanks go to my staff and to ETH Zurich for their confidence, support and tireless effort towards the success of our plans and projects.

I cordially invite you to find out more in the following literature.

Prof. Thomas Schulthess
Director of CSCS

Content

“High-performance computing is an essential pillar of modern seismology that drives progress in the field. It allows us to simulate the propagation of waves excited by earthquakes and explosions with unprecedented accuracy, to process and assimilate massive amounts of data, and to produce sharper images of the Earth’s internal structure”.
Andreas Fichtner, ETH Zurich

Name
Andreas Fichtner

Position
Assistant professor

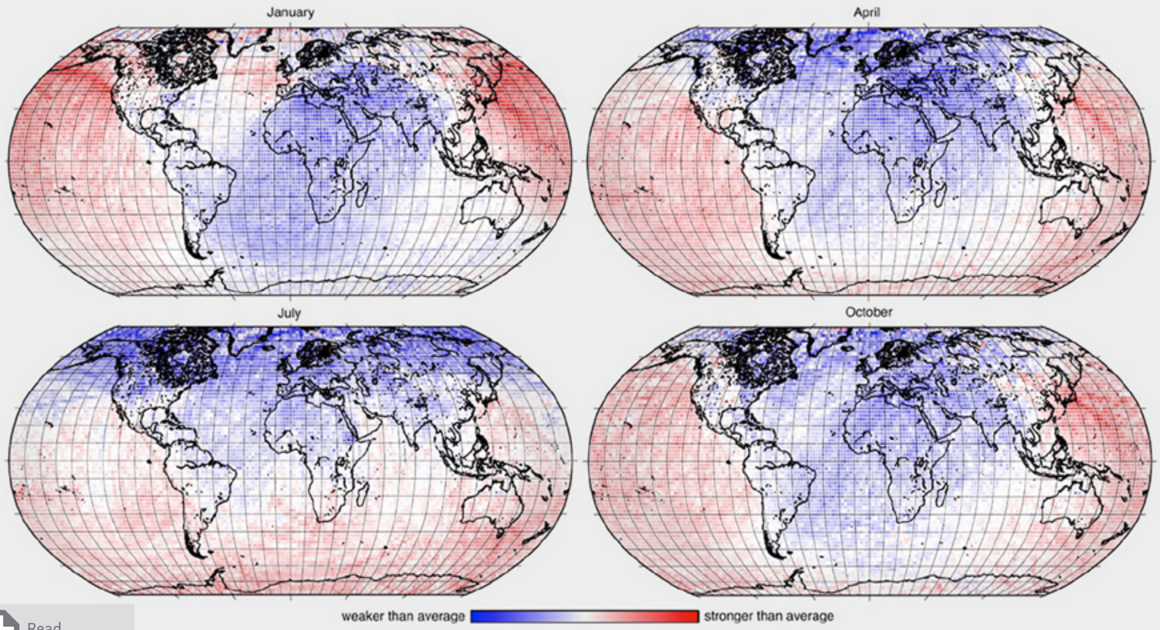
Institution
ETH Zurich

Background
1999-2002 Studies in geophysics, University of Freiberg, Germany
2002-2003 Fulbright exchange student, University of Washington, USA
2003-2005 MSc in geophysics, LMU Munich, Germany
2005-2009 PhD in geophysics, LMU Munich, IPG Paris, Australian National University
2010-2012 Post-doctoral researcher, Utrecht University, Netherlands
Since 2013 Assistant professor, Institute of Geophysics, ETH Zurich

Area of research
Theoretical seismology, wave propagation phenomena, structure of the Earth's crust and mantle.

Specialised in
Developing methods to image the deep Earth's interior to understand its dynamics and evolution over geological times.

HPC means for me
Being able to model the propagation of seismic waves through the Earth with high accuracy, and being able to use these models to constrain the internal structure of the Earth with unprecedented detail.



Read
the article

Where the Earth is humming and whistling

Researchers at ETH developed a novel technique to image the sources of incessant, micrometer-scale vibrations of the whole Earth known as the ambient seismic field. With the help of "Piz Daint" they were able to process massive amounts of seismic data recorded world-wide every second over a period of 10 years. Their method can be used to reduce errors in tomographic imaging of the crust and is in the process of being expanded to a framework for the daily monitoring of hydro-carbon and geothermal reservoirs.

(Image: Andreas Fichtner, ETH Zurich)

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, 23.5 PFlops
Piz Daint, Cray XC40, 1.7 PFlops

Computing Time for User Lab
2016: 43 446 610 node h
2015: 1 201 734 615 CPU h

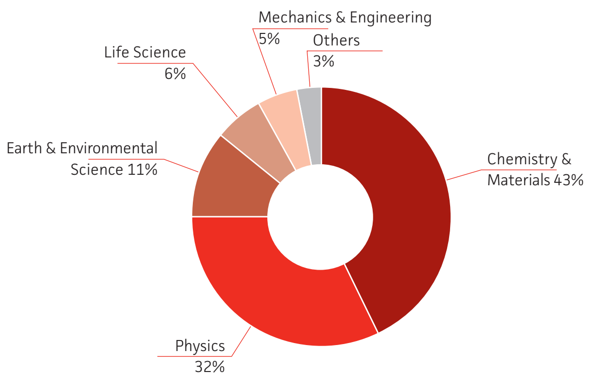
User Community
2016: 109 Projects, 754 Users
2015: 105 Projects, 568 Users

Employees
2016: 79
2015: 70

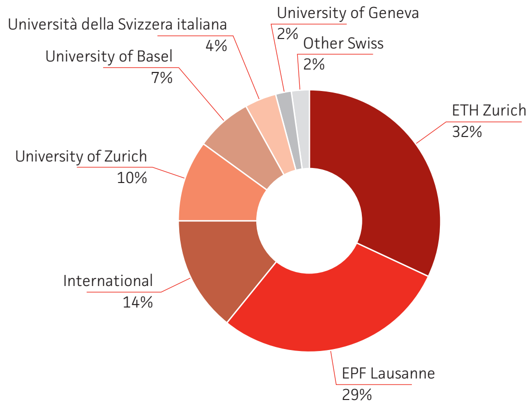
Investments
2016: 40 Mio CHF
2015: 5.1 Mio CHF

Operational Costs
2016: 14.6 Mio CHF
2015: 15.1 Mio CHF

Usage by Research Field



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	23 498 + 1 731
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	33
Pilatus	x86 Cluster	2012	User Lab	13

Computing Systems Specifications

Name	Interconnect Type	CPU Type	No. Cores	No. Cores	No. Nodes
Piz Daint	Cray Aries	Intel Xeon E5-2690 v3 + Nvidia P100	12	1	4 936
		Intel Xeon E5-2695 v4	18	2	1 431
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	8	2	64
Piz Kesch	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2	12
Piz Escha	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2	12
Monte Leone	10 Gb Ethernet	Intel Xeon E5-2667 v3	8	2	20
		Intel Xeon E5-2667 v3	8	2	7
		Intel Xeon E5-2690 v3 + Nvidia K40C	12	2	4
Pilatus	Infiniband FDR	Intel Xeon E5-2670	8	2	38

"Supercomputers like 'Piz Daint' are essential in modern cosmology to study the non-linear evolution of matter and fields in the Universe. Without supercomputers, current and future large astronomical surveys would not be able to realize their full potential. Thanks to the rapid increase in computing power we are, on the theory and data analysis side, able to keep up with the increase in data volume and quality, and the resulting progress in understanding our Universe has been breath-taking."

Martin Kunz, University of Geneva

Name
Martin Kunz

Position
Associate professor

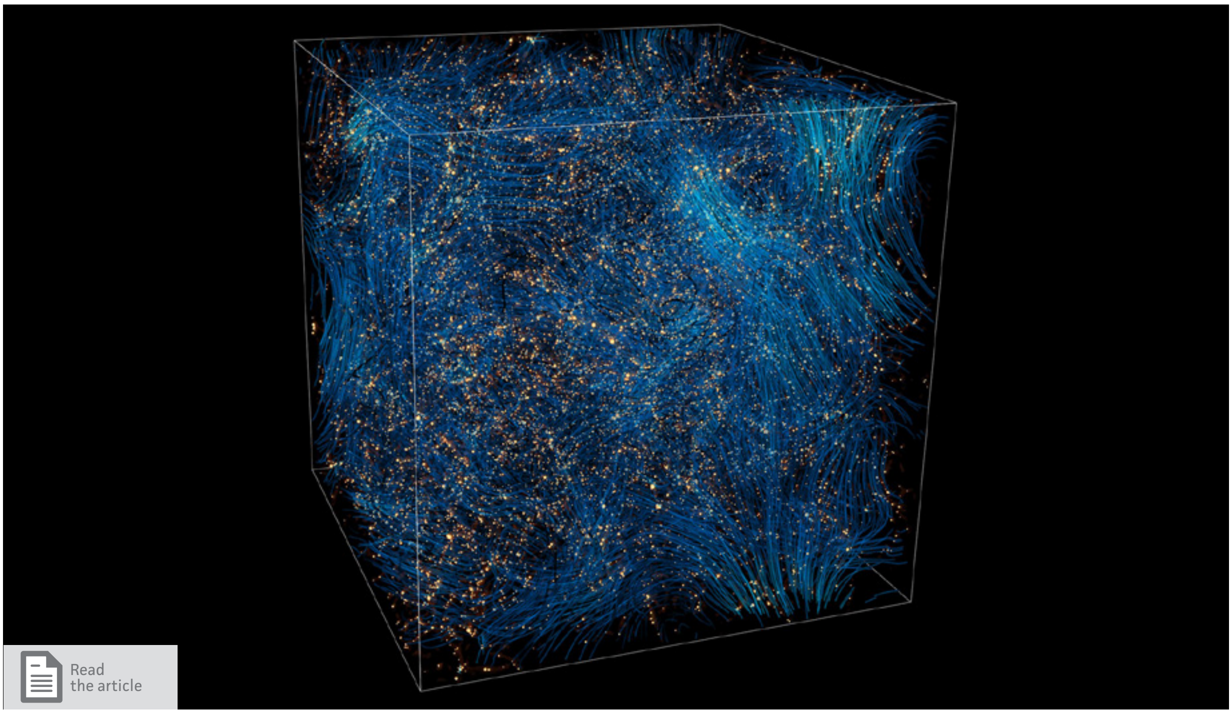
Institution
University of Geneva

Background
1990-1995 Diploma in physics, ETH Zurich
1995-1999 PhD in theoretical physics, University of Geneva
1999-2002 Postdoctoral researcher, University of Oxford, UK
2002-2004 Postdoctoral researcher, University of Sussex, UK
2004-2007 SNF professor, University of Geneva
2007-2009 Lecturer in theoretical cosmology, University of Sussex, UK
2009-2016 Senior researcher, University of Geneva
Since 2016 Associate professor in theoretical physics, University of Geneva

Area of research
Cosmology, origin and large scale structure of the universe, nature of dark energy and dark matter.

Specialised in
Calculation/simulation of predictions from theoretical models, comparison of theory and observations.

HPC means for me
Having (aspects of) the universe in a box where I can study it up close and from all angles.



More realistic simulation of the evolution of cosmic structures

Cosmologists at the University of Geneva are the first to simulate the structure of the universe in a way that consistently accounts for the general theory of relativity using “Piz Daint”. This was made possible with a new simulation code developed by the researchers.
(Image: Cosmology and Astroparticle Physics Group University of Geneva)

January

27 Watch the video

Webinar: Allinea DDT

In a webinar focused on debugging tools at CSCS, Patrick Wohlschlegel, Allinea Technical Services Manager, guided participants through using the Allinea DDT parallel debugger. This tool is used for debugging serial, multi-threaded (OpenMP), multi-process (MPI) and accelerator-based (Cuda, OpenACC) programs running on research and production systems.

February

03

5 000 followers on LinkedIn

CSCS attained more than 5 000 followers on its LinkedIn page and celebrated this milestone with a small internal event. LinkedIn has gained relevance at CSCS in recent years because it facilitates engagement with potential candidates for new positions at our centre.

22

Webinar: Deep-dive GPU debugging with Allinea DDT

Following the previous Allinea DDT webinar introducing the development toolkit available at CSCS and key points for getting started with debugging on “Piz Daint”, Allinea focused here on challenges coming from accelerators. This webinar helped participants speed up problem resolution on GPUs.

March

21/23

HPC Advisory Council Switzerland Conference 2016

More than 130 professionals attended the seventh Switzerland Conference of the HPC Advisory Council in Lugano. Co-sponsored by CSCS, the conference focused on HPC essentials, new developments and emerging technologies, best practices and hands-on training.

31 Read the article

MeteoSwiss and COSMO-1

The Federal Office of Meteorology and Climatology, MeteoSwiss, put into operation the new high-resolution forecasting model COSMO-1, which runs on the “Piz Escha” and “Piz Kesch” supercomputers.

April

06

Read the article

More computing power for Swiss research

CSCS announced the upgrade of “Piz Daint”, a move that is expected to at least double its computing power. ETH Zurich invested around CHF 40 million to allow researchers to perform simulations, data analyses and visualisations even more efficiently in the future. Read more on page 64.

29

User meeting at EPF Lausanne and ETH Zurich

In addition to the user meeting organised during the PASC16 Conference, CSCS invited its local user community both to EPF Lausanne on 29 April and ETH Zurich on 4 May. The meetings were occasions to focus on and discuss key issues related to proposal submission.

May

09

“Piz Dora”’s upgrade

As a first step in a major upgrade of CSCS computational resources, on May 9 “Piz Dora” went down for about 10 days while all its processors were upgraded from Haswell (12-core @2.5 GHz) to Broadwell (18-core @2.1 GHz), providing a significant performance improvement. With the new processors installed, application performance has been seen to increase by 1.2-1.5 times on average

10

Allocation of computer time, April 2016 to March 2017

32 new projects have been running on the CSCS supercomputer infrastructure since April. Together with ten smaller and twenty existing multi-year projects, they share 27 681 622 node hours to conduct simulations in scientific disciplines that employ high-performance computing – especially astrophysics, materials science, fluid dynamics and life sciences.

June

08/10

Watch the video

Read the article

PASC16 Conference

Scientists from a wide range of disciplines gathered at the SwissTech Convention Center in Lausanne for the third annual PASC Conference. The use of high-performance computing in their research was the common link that brought them together.

10

CSCS director meets the scientific community at EPF Lausanne

At the close of the PASC16 Conference, CSCS invited the user community to a short User Assembly. The main item on the agenda was a presentation by CSCS director Thomas Schulthess on the CSCS roadmap and the upgrade of “Piz Daint”.

12/14

ADAC workshop Switzerland

The Accelerated Data Analytics and Computing (ADAC) workshop, organised by CSCS, was hosted at Hotel de la Paix in Lugano. Leaders in hybrid accelerated HPC in the United States, Japan and Switzerland met to discuss performance portability and resource management to accommodate data science.

20/22

CSCS at ISC16

CSCS had a booth at ISC16 in Frankfurt, presenting the latest HPC developments in Switzerland.

Watch the video

ISC Best Visualization award

The visualization of ab-initio simulation of electron flow through a silicon nanowire on “Piz Daint” garnered the Best Visualization award at the ISC Visualization Showcase 2016. Two research groups from ETH Zurich led by the scientists Mathieu Luisier and Joost VandeVondele and supported by Jean Favre, visualization specialist at CSCS, showed in their visualization how electrons flow through a nanotransistor, a silicon nanowire composed of 50 000 atoms

July

04/08

Second EuroHack

The second edition of the GPU programming hackathon in Lugano allowed development teams to port their scalable applications to GPU accelerators, or optimize existing GPU-enabled applications on a state-of-the-art GPU system..

17/28

Summer School 2016

CSCS in collaboration with the Institute of Computational Science at the Università della Svizzera italiana organised a two-weeks summer school dedicated to HPC, attended by around 30 students.

September

13/15

Watch the video

Data science with [a] Spark

This two-and-a-half day workshop organised by CSCS and the InterDisciplinary Institute of Data Science (IDIDS) at the Università della Svizzera italiana addressed high-level parallelization for data analytics workloads using the Apache Spark framework.

26

Allocation of computer time, October 2016 to September 2017

Demand for computer time through the new computing period from October 2016 to September 2017 was more than three times the amount of compute resources actually available. In all, thirty-eight researchers applied for 39.5 million node hours.

26/28

Watch the video

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.

29/30

Watch the video

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.

October

03

Watch the video

"Albis" & "Monte Lema" shutdown

After more than 4.5 years of 24/7 tireless and reliable service for MeteoSwiss, the Cray XE6 "Albis" and "Monte Lema" computers were decommissioned. Together they comprised the first production system installed in the new CSCS building in early 2012. Through the closing six months of parallel operation, the new system comprised of "Piz Escha" and "Piz Kesch" gradually took over all operational tasks from the earlier system to provide even more accurate weather forecasts.

04

"Monte Leone": a new small high memory cluster

A new small cluster called "Monte Leone" went into production in early October. The cluster has 20 compute nodes with Haswell processors (8 cores per socket) and 768 GB memory capacity per node. The cluster aims to serve scientists with a demonstrated need for high memory per node. Those include for example researchers interested in very high-accuracy ab-inizio calculations on medium-sized and larger molecules, which require large memory for elements of the composite calculational scheme.

05

Shutdown of "Castor", "Tödi", "Matterhorn" and "Rothorn"

2016 saw the shutdown of several systems that were instrumental to the Centre's earlier development. These included "Castor", an IBM iDataPlex cluster; "Tödi", a Cray XK7 and the first highly scalable GPU/CPU hybrid supercomputing system at CSCS designed to run data-parallel and computationally intensive applications; "Matterhorn", a Cray XMT system featuring a massively multi-threaded platform with shared memory architecture that was used mainly for large-scale data analysis, mining and structuring; and "Rothorn", the SGI Altix UV 1000 general-purpose system featuring a large amount of addressable memory.

17

“Piz Daint”’s major upgrade

As the second step in the major upgrade started in May, “Piz Daint” went down on 17 October followed by the “Piz Dora” multicore system on 31 October. Total system downtime amounted to about 8 weeks while processors in the hybrid partition were upgraded from SandyBridge (8-core @2.6 GHz) to Haswell (12-core @2.6 GHz) and GPUs from NVIDIA Tesla K20X (Kepler) to the latest NVIDIA Tesla P100 (Pascal), and the multicore system was finally merged into the hybrid one.

19 Watch the video · Read the article

25 Years anniversary celebration

Around 60 representatives from politics, industry and science celebrated the 25th anniversary of CSCS in Lugano. Read more on page 60.

November

11 Read the article

World-leading HPC Centres partner to form accelerated computing institute

Leaders in hybrid accelerated high-performance computing (HPC) in the United States, Japan and Switzerland met in Lugano in June to discuss performance portability and resource management to accommodate data science. In November they signed a Memorandum Of Understanding (MOU) establishing an international institute dedicated to common goals, the sharing of HPC expertise, and forward-thinking evaluation of computing architecture: the Accelerated Data Analytics and Computing (ADAC) institute.

14/17

CSCS at Supercomputing 2016

CSCS and the Swiss HPC community hpc-ch had a brand-new booth at the world’s largest supercomputing conference, SC16 in Salt Lake City, Utah, where they presented the latest HPC developments in Switzerland.

15 Read the article

CSCS and MeteoSwiss winners of the SwissICT Award 2016

This year's award by the Swiss Information and Communication Technology Association (ICT) goes to MeteoSwiss and CSCS for the development of new software and hardware: the MeteoSwiss high-resolution weather forecast model COSMO-1 and the ensemble system COSMO-E running on the hybrid machine "Piz Kesch". (Photos: Jonas Weibel, SwissICT)

30

Webinar: "Piz Daint" upgrade – What's new?"

In the wake of the "Piz Daint" upgrade, the user support team organised a webinar focused on describing the new configuration and providing useful information on job submission, queue organisation and other relevant topics.

December

07 Read the article

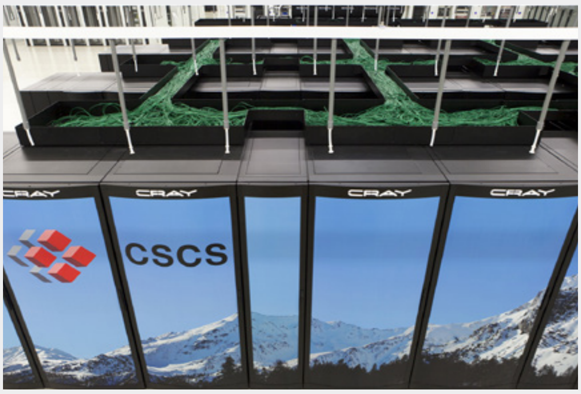
CSCS and Cray work with industry leaders to reach new performance milestone for deep learning at scale

The results of a deep learning collaboration between Cray, Microsoft and CSCS that will expand the horizons of running deep learning algorithms at scale using the power of Cray supercomputers was announced at the 2016 Neural Information Processing Systems (NIPS) Conference in Barcelona, Spain.

12

"Piz Daint" back in service

The major upgrade of "Piz Daint" and the merge with "Piz Dora" concluded successfully on 12 December. A much more performant system was put back into service and opened to the CSCS user community as expected, and without any delays to the announced schedule.



“The modelling of nanoscale devices heavily depends on the access to large computational resources to be able to investigate realistic structures within short simulation times. With ‘Piz Daint’ at CSCS we could not only reach this goal, but also significantly improve the quality of the underlying physical models, going from simple empirical to fully ab-initio methods”.
Mathieu Luisier, ETH Zurich

Name
Mathieu Luisier

Position
Associate professor

Institution
ETH Zurich

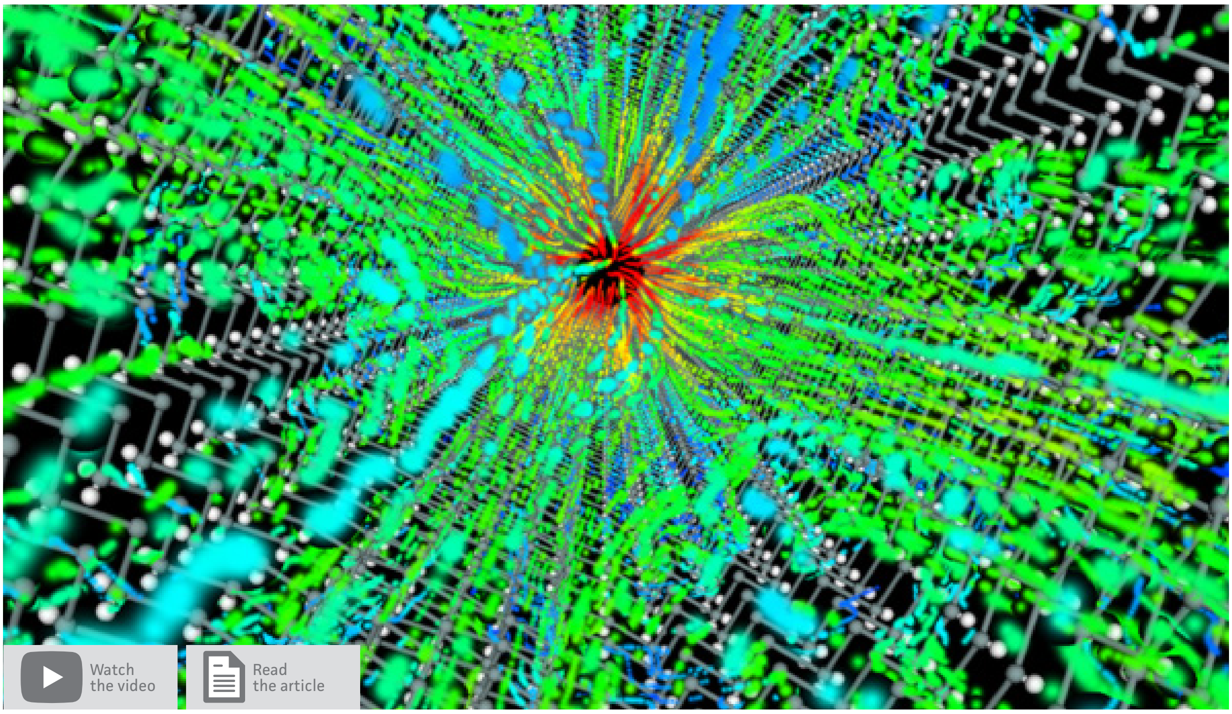
Background

1998-2003	Studies of electrical engineering, ETH Zurich
2003-2007	PhD at the Integrated Systems Laboratory, Department of Information Technology and Electrical Engineering, ETH Zurich
2007	Post-doc at the Integrated Systems Laboratory, ETH Zurich
2008-2011	Research assistant professor, Network for Computational Electronics, Purdue University, USA
2011-2016	SNF assistant professor, Integrated Systems Laboratory, ETH Zurich
Since 2016	Associate professor, Integrated Systems Laboratory, ETH Zurich

Area of research
Computational nanoelectronics, computer-aided design of nanoscale devices.

Specialised in
The development of advanced, physics-based, and massively parallel simulation methods to predict the electrical and thermal characteristics of not-yet-fabricated nanoelectronic components and to explain the behaviour of existing ones.

HPC means for me
Having the possibility to model always larger and more realistic systems, incorporating more relevant phenomena into our simulation approach, going beyond the state-of-the-art, and enjoying the first successful execution of a complex parallel algorithm.



Watch the video

Read the article

Ab-initio simulation of electron flow trough a nanowire

Two research teams from ETH Zurich combined two software programs and also developed a new algorithm to maximise the throughput rate for hybrid computer systems. This enabled them to reduce the time taken to simulate nanoscale devices by one fifty times and to increase the size of the nanocomponents to 100 000 atoms. (Image: Jean M. Favre, CSCS)

Yet another exciting year

Once again CSCS experienced a successful year full of exciting research. 343 high-quality publications appeared in 2016, resulting from the work of 85 groups using CSCS resources. Major system upgrades contributed to keeping CSCS a top-tier computing resource. In May, “Piz Dora” was upgraded from Haswell (12-core @2.5 GHz) to Broadwell (18-core @2.1 GHz) processors, increasing computational efficiency of tested applications by 20 to 50%. During the fall of 2016, CSCS upgraded its flagship computer “Piz Daint” by introducing the highly acclaimed new accelerator NVIDIA Tesla P100 (PASCAL) on each of its nodes. Cray team and CSCS staff made it possible to complete such a major upgrade in only 8 weeks, during which all processors were also upgraded from SandyBridge (8-core @2.6 GHz) to Haswell (12-core @2.6 GHz). The final step was the integration of the multicore (“Dora”) and hybrid systems (“Daint”) to create a single heterogeneous system now known as “Piz Daint”.

The upgraded “Piz Daint” keeps its position as one of the most energy efficient systems worldwide, and increases compute efficiency for tested applications by factors between 2 and 5.

In October CSCS further introduced a new small high-memory cluster for applications that depend more on large-memory resources than on either scalability or high-throughput. The new, relatively small cluster features 20 compute nodes, each equipped with two 8-core Haswell processors and 768 GB of memory. It has been named after “Monte Leone”, the highest mountain of the Lepontine Alps, which are located on the border between Switzerland and Italy.

Resources allocated in 2016

Analysis of usage statistics reveals that Chemistry & Materials still remains by far the most compute-intensive research field at CSCS, using 43% of the total allocation (virtually unchanged from 2015). Physics and Earth & Environmental Science also maintain a sizeable share of compute-intensive projects, the former decreasing from 37% in 2015 to 32% in 2016 and the latter increasing from 8% to 11%. Life Sciences, so far under-represented in terms of compute resources, appears to be gaining momentum, going from 3% to 6% of the total resource utilisation. Mechanics & Engineering (5% after 7% in 2015) loses a few percentage points to the remaining disciplines (3% after 1% in 2015).

Usage by institution statistics show some new trends: although ETH Zurich is still the largest user, gaining even a few percent (32%) compared to 2015 (27%), EPF Lausanne now finishes as a close runner-up (29% after 18% in 2015). The University of Zurich and International institutions, on the other hand, lose in shares, from 17% to 10% and 18 to 14%, respectively. The University of Basel keeps its share (7% in 2016 after 8% in 2015), whereas the Università della Svizzera italiana rises at the horizon, moving from a mere 1% in 2015 to 4% in 2016. The total utilization remains high at nearly 27 mio node hours, despite the almost 3 months of downtime due to the upgrades. This and the changes in usage patterns demonstrate that there is still a lot of room for new challenges both at the scientific and institutional levels, where CSCS continues to make a difference as provider of HPC resources.

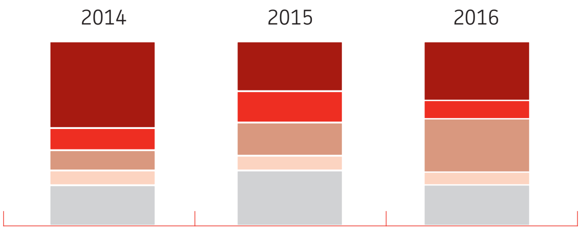
List of CHRONOS Projects

Principal Investigator	Organisation	Research Field	Project Title	Node h
Stephan Brunner	EPF Lausanne	Physics	Turbulent transport simulations with the gyrokinetic code GENE	1 800 000
Nicola Marzari	EPF Lausanne	Chemistry & Materials	Computational materials science in the cloud: an open-access database of materials' data and computational workflows	3 333 000
Andreas Fichtner	ETH Zurich	Earth & Environ. Science	Global waveform inversion across the scales	500 000
Petros Koumoutsakos	ETH Zurich	Others	Simulation of microfluidics for mechanical cell separation: building the in-silico lab-on-a-chip	2 000 000
Christoph Schär	ETH Zurich	Earth & Environ. Science	Continental-scale cloud-resolving climate simulations for Europe	1 333 000
Joost VandeVondele	ETH Zurich	Chemistry & Materials	Exploring frontiers in nanoscale simulation: new models and improved accuracy	3 333 000
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

Usage Statistics

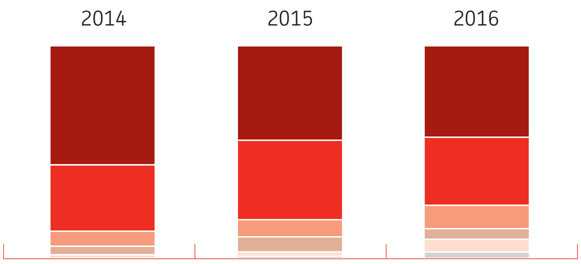
Usage by Institution (%)

Institution	2014	2015	2016
ETH Zurich	35	27	32
University of Zurich	20	17	10
EPF Lausanne	20	18	29
University of Basel	4	8	7
Others	21	30	22
Total Usage	**100**	**100**	**100**



Usage by Research Field (%)

Research Field	2014	2015	2016
Chemistry & Materials	56	44	43
Physics	31	37	32
Earth & Environ. Science	7	8	11
Mechanics & Engineering	4	7	5
Life Science	2	3	6
Others	0	1	3
Total Usage	**100**	**100**	**100**



17 Largest Projects

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
Alireza Rahmati	University of Zurich	Physics	Spatially adaptive radiation-hydrodynamical simulations of cosmic reionization in a representative volume	1 000 000
Franco Vazza	Hamburg Observatory	Physics	Galaxies in filaments: a high-resolution view from adaptive mesh refinement MHD simulations	822 530
Michael Francis	EPF Lausanne	Chemistry & Materials	Stress controlled surface chemistry: towards the rational design of core-shell nanoparticles catalysts	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	737 000
Francesco Miniati	ETH Zurich	Physics	Transonic MHD intracluster turbulence	700 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	First-principles simulation of van der Waals homo- and hetero-junctions for optoelectronic applications	600 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	Ab-initio simulations of conductive bridging memristors for application as plasmonic optical switches	600 000
Jürg Hutter	University of Zurich	Chemistry & Materials	Properties of liquids, solutions, and interfaces from density functional theory	600 000
Jan Burjánek	ETH Zurich	Earth & Environ. Science	Numerical modeling of seismic response unstable rock slopes	550 000
Maximilian Amsler	Northwestern University	Chemistry & Materials	Discovery of energy materials through large-scale lattice dynamics	550 000
Jonathan Graves	EPF Lausanne	Physics	Energetic particle physics in magnetically confined configuration	500 000
Paolo Ricci	EPF Lausanne	Physics	Simulation of plasma turbulence in the periphery of tokamak devices	500 000
Ursula Röthlisberger	EPF Lausanne	Chemistry & Materials	Multiscale simulations of biological systems and bioinspired devices	500 000
Nicolas Noiray	ETH Zurich	Mechanics & Engineering	Identification of thermoacoustic instability driving mechanism in a new generation gas turbine combustor	500 000
Martin Kunz	University of Geneva	Physics	Relativistic cosmological simulations with gevolution	500 000

List of Projects by Institution

CERN

Signature of compositeness at the LHC, Vincent Drach (Physics, 250 000 node h)

Leading isospin breaking effects of the hadronic vacuum polarisation, Marina Marinkovic (Physics, 450 000 node h)

New strategies in the determination of the QCD running coupling, Alberto Ramos (Physics, 200 000 node h)

EMPA

Screening of the electronic and optical properties of carbon based 1D heterostructures, Carlo Pignedoli (Chemistry & Materials, 300 000 node h)

EPF Lausanne

Application of large-eddy simulation to atmospheric boundary layer flows and transports of scalars above urban surfaces, Wai Chi Cheng (Mechanics & Engineering, 200 000 node h)

Unravelling the atomistic basis of Hsp70/client interactions by means of enhanced-sampling molecular dynamics simulations, Paolo De Los Rios (Life Science, 59 880 node h)

Stress controlled surface chemistry: towards the rational design of core-shell nanoparticles catalysts, Michael Francis (Chemistry & Materials, 800 000 node h)

Simulation of scrape-off-layer plasma turbulence in the TCV tokamak, Ivo Furno (Physics, 150 000 node h)

Energetic particle physics in magnetically confined configuration, Jonathan Graves (Physics, 500 000 node h)

Nuclear quantum effect on ion solvation, Chuweng Liang (Chemistry & Materials, 452 000 node h)

Simulation of plasma turbulence in the periphery of tokamak devices, Paolo Ricci (Physics, 500 000 node h)

Organic molecules on metallic surfaces: porphycene cis-trans transition including nuclear quantum effects, Mariana Rossi (Chemistry & Materials, 450 000 node h)

Multiscale simulations of biological systems and bioinspired devices, Ursula Röthlisberger (Chemistry & Materials, 500 000 node h)

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

Electronic structure and charge transfer properties of mixed perovskite materials, Olga Syzgantseva (Chemistry & Materials, 67 540 node h)

The materials genome in action, Davide Tiana (Chemistry & Materials, 56 160 node h)

Novel topological electronic phases of materials, Oleg Yazyev (Chemistry & Materials, 150 000 node h)

Numerical investigation of three-dimensional droplets in microfluidic circuits, Lailai Zhu (Mechanics & Engineering, 65 000 node h)

ETH Zurich

High fidelity CFD of a real, supersonic, multi-stage steam turbine using water droplet model, Reza Abhari (Mechanics & Engineering, 59 000 node h)

First principles computation of perovskite oxynitride surfaces, Ulrich Aschauer (Chemistry & Materials, 60 000 node h)

Implementation of immersive boundary conditions for modeling inversion, and imaging: applications to a wave propagation laboratory, Filippo Broggini (Earth & Environmental Science, 200 000 node h)

Numerical modelling of seismic response unstable rock slopes, Jan Burjánek (Earth & Environmental Science, 550 000 node h)

Quantum dynamics of strongly correlated systems from ultracold atoms to quantum computing, Giuseppe Carleo (Physics, 300 000 node h)

The mechanism of Fischer-Tropsch synthesis on ruthenium nanoparticles under reactive conditions, Aleix Comas-Vives (Chemistry & Materials, 65 000 node h)

Land-climate feedbacks in a changing climate, Edouard Davin (Earth & Environmental Science, 64 000 node h)

Investigating high frequency attenuation to reduce epistemic uncertainty in seismic hazard assessment, Walter Imperatori (Earth & Environmental Science, 65 000 node h)

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

Learning and optimization for collective swimming, Petros Koumoutsakos (Mechanics & Engineering, 250 000 node h)

Development of novel high-performance MT 3-D inverse solver, Alexey Kuvshinov (Earth & Environmental Science, 100 000 node h)

The impact of aerosols in the past, present, and future climate, Ulrike Lohmann (Earth & Environmental Science, 737 000 node h)

First-principles simulation of van der Waals homo- and hetero-junctions for optoelectronic applications, Mathieu Luisier (Chemistry & Materials, 600 000 node h)

Ab-initio simulations of conductive bridging memristors for application as plasmonic optical switches, Mathieu Luisier (Chemistry & Materials, 600 000 node h)

Transonic MHD intracluster turbulence, Francesco Miniati (Physics, 700 000 node h)

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

Identification of thermoacoustic instability driving mechanism in a new generation gas turbine combustor, Nicolas Noiray (Mechanics & Engineering, 500 000 node h)

Silicon, a promising anode material for Li-ion batteries; a computational study, Andreas Pedersen (Chemistry & Materials, 60 000 node h)

Structure of the hydrated electron from many-body perturbation theory, Vladimir Rybkin (Chemistry & Materials, 100 000 node h)

High resolution glacier modelling with PISM, Julien Seguinot (Earth & Environmental Science, 65 000 node h)

Topological quantum computation and the fractional quantum Hall effect, Matthias Troyer (Physics, 139 320 node h)

High-frequency Green's function databases for the Mars inSight mission, Martin van Driel (Earth & Environmental Science, 65 000 node h)

Assessing structure and dynamics of the nuclear pore's Y-complex, Viola Vogel (Life Science, 100 000 node h)

Computation investigation of the influence of surface treatments on the electronic and phononic structure of PbS nanocrystals, Vanessa Wood (Chemistry & Materials, 50 000 node h)

Hamburg Observatory

Galaxies in filaments: a high-resolution view from adaptive mesh refinement MHD simulations, Franco Vazza (Physics, 822 530 node h)

Hungarian Academy of Science

Development of a new blind docking method, Csaba Hetényi (Life Science, 65 000 node h)

IRB Bellinzona

Identification of potential molecular clips as new therapeutic tools against light-chain amyloidosis, Andrea Cavalli (Life Science, 63 900 node h)

IRSOL

Magnetohydrodynamic models of the Solar atmosphere, Oskar Steiner (Physics, 40 000 node h)

Italian Institute of Technology Rome

Assessing the protein sequencing capability of nanopore based devices, Mauro Chinappi (Chemistry & Materials, 100 000 node h)

Leiden University

The fine structure of the Milky Way, Simon Portegies Zwart (Physics, 200 000 node h)

Northwestern University

Discovery of energy materials through large-scale lattice dynamics, Maximilian Amsler (Chemistry & Materials, 550 000 node h)

Paul Scherrer Institute

First-principle molecular dynamics simulation of Cu_3N, Matthias Krack (Chemistry & Materials, 63 400 node h)

SUPSI

Protein-protein interactions characterizing AXH domain of Ataxin 1 by molecular dynamics, Marco Deriu (Life Science, 61 000 node h)

Swiss Institute of Bioinformatics

How does the T cell receptor function as a mechanosensor?, Michel Cuendet (Life Science, 92 930 node h)

Technische Universität Darmstadt

Neutrinos in the aftermath of neutron star mergers, Albino Perego (Physics, 250 000 node h)

Twente University

Rayleigh-Bénard convection: towards the ultimate regime, Detlef Lohse (Mechanics & Engineering, 450 000 node h)

Universidad Politécnicade de Madrid

Time resolved evolution of large scales in turbulent channel flow at Re = 5 000, Javier Jimenez (Mechanics & Engineering, 65 000 node h)

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Structural and energetic characterization of the binding mechanism of antagonists of GP-BAR1 through metadynamics simulations, Daniele Di Marino (Life Science, 61 000 node h)

Homo- and heterodimerization mechanism of chemokines receptors CCR5 and CXCR4 investigated by coarse-grained metadynamics simulations, Vittorio Limongelli (Life Science, 300 000 node h)

Transport processes across microvessel walls: parallel simulations, Igor Pivkin (Life Science, 153 000 node h)

Electron transfer processes for VO^{+}_2 at carbon-based electrodes, Daniela Polino (Chemistry & Materials, 300 000 node h)

Analysis of ventricular conduction abnormalities in heart-failure patients using tailored numerical heart models, Mark Potse (Life Science, 65 000 node h)

Development and validation of structurally complex models of the human atria for atrial fibrillation studies, Mark Potse (Life Science, 300 000 node h)

Efficient calculation of protein folding free energies using variationally-enhanced sampling, Patrick Shaffer (Life Science, 100 000 node h)

Accurate kinetic models for catalysed ammonia synthesis reaction through enhanced sampling metadynamics, Vincenzo Verdolino (Chemistry & Materials, 62 720 node h)

University of Basel

Molecular mechanisms of CFTR: relating chloride channel function with ATPase activity, Simon Bernèche (Life Science, 64 800 node h)

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

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)

University of Geneva

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

University of Zurich

First principles simulation of the drift phenomenon in phase change memory cell, Sebastiano Caravati (Chemistry & Materials, 200 000 node h)

Properties of liquids, solutions, and interfaces from density functional theory, Jürg Hutter (Chemistry & Materials, 600 000 node h)

Simulation of dissociation processes at the aqueous electrolyte-electrode interface, Marcella Iannuzzi (Chemistry & Materials, 400 000 node h)

Emulating the Euclid Universe: predictions for weak lensing and galaxy clustering, Aurel Schneider (Physics, 400 000 node h)

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

The properties of protoplanets formed by disk instability in massively parallel radiation hydrodynamics simulations, Lucio Mayer (Physics, 100 000 node h)

Spatially adaptive radiation-hydrodynamical simulations of cosmic reionization in a representative volume, Alireza Rahmati (Physics, 1 000 000 node h)

Solving large-scale overlapping generations models and medium-scale monetary policy models, Simon Scheidegger (Others, 350 000 node h)

Zurich University of Applied Science

GARTEUR AG-54: RaLESin: RANS-LES interfacing for hybrid RANS-LES and embedded LES approaches, Marcello Righi (Mechanics & Engineering, 100 000 node h)

Renewals

EPF Lausanne

Large scale atomic simulations of dislocation plasticity and fracture in magnesium and alloys, William Curtin (Mechanics & Engineering, 652 000 node h)

Large Eddy simulation of very-large-scale motions in atmospheric boundary layer flows: the influences of the Coriolis force and thermal stability, Jiannong Fang (Mechanics & Engineering, 195 000 node h)

Study of land-atmosphere interaction over Antarctic snow-ice formations by large eddy simulation, Michael Lehning (Earth & Environmental Science, 400 000 node h)

Study on snow precipitation and accumulation over complex alpine terrain, Michael Lehning (Earth & Environmental Science, 342 527 node h)

THEOS NANO: thermal, electrical, and optical properties of nanoscale materials, Nicola Marzari (Chemistry & Materials, 500 000 node h)

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

Cardiac and vascular numerical simulations, Alfio Quarteroni (Life Science, 500 000 node h)

ORB5-GENE turbulence, Laurent Villard (Physics, 522 000 node h)

ETH Zurich

Entropic lattice Boltzmann method for fluid dynamics, Shyam Chikatamarla (Mechanics & Engineering, 115 330 node h)

Entropic lattice Boltzmann method for compressible flows, Shyam Chikatamarla (Mechanics & Engineering, 295 799 node h)

Direct numerical simulation of formation and propagation of turbulent spherical premixed syngas/air flames, Christos Frouzakis (Mechanics & Engineering, 112 500 node h)

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

Cloud cavitation collapse, Petros Koumoutsakos (Mechanics & Engineering, 216 000 node h)

Evaluating aerosol cloud interactions at the regional scale, Ulrike Lohmann (Earth & Environmental Science, 108 230 node h)

European regional climate simulations of stable water isotopes in the atmospheric water cycle with COSMOiso (EURECIS), Stephan Pfahl (Earth & Environmental Science, 177 600 node h)

Coupled and competing instabilities in complex oxides, Nicola Spaldin (Chemistry & Materials, 905 000 node h)

The role of mechanics in fracture healing and bone turnover, Harry van Lenthe (Life Science, 452 000 node h)

MIT

High temperature electronic structure by a novel Monte Carlo method for the warm dense electron gas and plasmonic catalysis, James Shepherd (Chemistry & Materials, 208 330 node h)

Università della Svizzera italiana

Improving diagnosis of atrial fibrillation, Mark Potse (Life Science, 33 600 node h)

University of Bern

ISOTOPE (Modelling ISOTOPEs in the Earth system), Fortunat Joos (Earth & Environmental Science, 41 000 node h)

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

University of Geneva

Quantum systems with strong correlations: materials and novel computational approach, Antoine Georges (Chemistry & Materials, 433 330 node h)

University of Lausanne

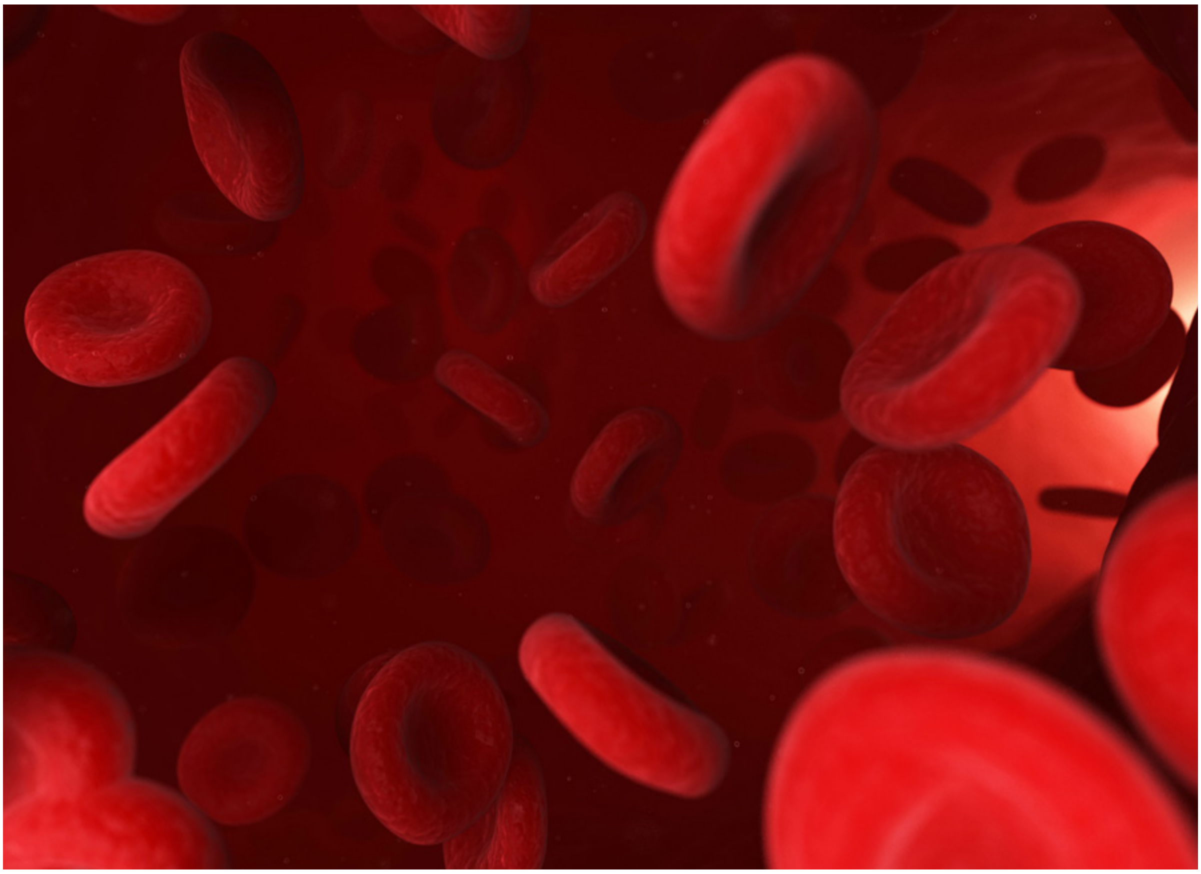
Mechanisms controlling acid-sensing ion channel (ASIC) activity, Stephan Kellenberger (Life Science, 112 000 node h)

University of Zurich

Investigation and design of Co(II)-based cubane water-oxidation catalysts, Sandra Luber (Chemistry & Materials, 470 080 node h)

Applications of a scalable algorithm to improve sampling efficiency in molecular dynamics simulations of biological systems, Andreas Vitalis (Life Science, 150 000 node h)

The spleen and its effect on red blood cells



Red blood cells flowing through an arteria. (Image: Eraxion / 123RF Licence free pictures)

The size and shape of red blood cells could be determined by the spleen, or so it would seem from simulations on "Piz Daint".

Based on a study done in the late 1960s, it was assumed that capillaries in the circulatory system determined the size of red blood cells. Red blood cells supply the tissues in the body with oxygen. If oxygen is to reach those tissues, red blood cells must be able to pass through capillaries finer than four microns in diameter. An international research collaboration led by Igor Pivkin, Professor of Computational Science at the Università della Svizzera italiana, has now concluded on the basis of simulations that not the capillaries, but rather the spleen could exert significant influence on the size and shape of red blood cells. The new findings were published in Proceedings of the National Academy of Sciences (PNAS).

Micro filter for red blood cells

The spleen is part of the lymphatic system that disposes of altered or aged blood cells. This takes place in structures called the interendothelial slits. About ten percent of the blood circulating through the spleen flows through this 'filter'. Red blood cells are squeezed through the slits, which are 1.2 microns wide (about one eightieth of the thickness of a human hair), 4 microns long and 1.9 microns deep. Rigid and misshapen blood cells might not be able to pass through these narrow passages.

There is no experimental technique currently available that allows us to observe this process in vivo. Therefore, Igor Pivkin and colleagues used "Piz Daint" to simulate the mechanical filter function of the interendothelial slit and how red blood cells are squeezed through the tiny openings.

The simulations are based on the red blood cell (RBC) model which Pivkin started to develop during his PhD studies at Brown University in the group of George Karniadakis. Based on the size of the slits and taking into account the prevailing pressure difference across them, the researchers determined possible sizes and mechanical characteristics of red blood cells that would allow them to pass through the slits. They combined their simulations with a theoretical analysis, by investigating how the geometry of the slits and the blood cells influenced the process.

Survival of the fittest

It emerged that only red blood cells with a certain surface area and volume are able to pass through the filter. Their shape and size were similar to those found circulating in the blood of healthy people, which usually have a surface area of 80 to 180 square microns and a volume of 60 to 160 cubic microns. Investigations with independent laboratory experiments and a mechanical model showed similar results, according to the researchers. The scientists call this passage of cells through the interendothelial slit in the spleen the ‘physical fitness test' for red blood cells.

Although the theory that the capillaries determine the size of red blood cells has been widely accepted since the late 1960s, it had been noticed that people without a spleen had larger red blood cells, Pivkin explains. For this reason scientists suspected that the spleen might play a role in the size and shape of red blood cells. “Our study, however, is to my knowledge the first to look into the matter and demonstrate that this indeed could be the case, indicating a new function for a well-known organ.”

Support for drug development

The findings improve the understanding of the functioning of the spleen, and how the ‘filter' may influence disease like sickle cell anaemia or malaria. They also can provide new insights in drug treatments, for example to explain why specific malaria drugs which stiffen healthy and malaria-infected red blood cells, could lead to severe anaemia. Co-author Subra Suresh, president of Carnegie Mellon University, emphasizes that the results offer better understanding of how the circulatory bottleneck for the red blood cell in the spleen could affect a variety of acute and chronic disease states arising from hereditary disorders, human cancers and infectious diseases, with implications for therapeutic interventions and drug efficacy assays.

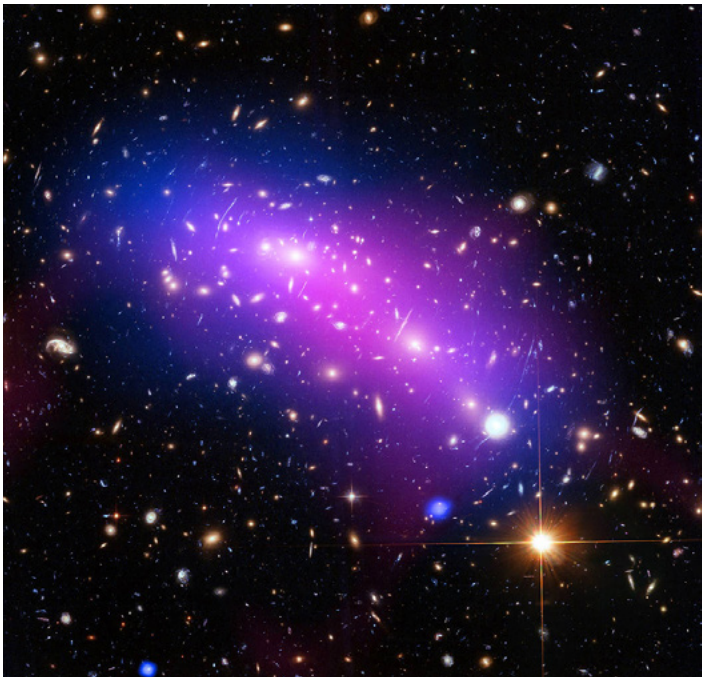
The work on modelling of the RBC passage through the endothelial slits in the spleen began when Pivkin joined Subra Suresh's group at MIT as a postdoctoral researcher. However, the first signficant results were obtained years later, after Pivkin moved to USI in Lugano. For experts the study shows that blood-cell and blood-flow modeling and simulation have reached a stage where they can contribute significantly to the understanding and treatment of blood-related disorders.

Reference: Pivkin IV, Peng Z, Karniadakis GE, Buffetf PA, Dao M & Suresh S: Biomechanics of red blood cells in human spleen and consequences for physiology and disease, PNAS (2016), 133, 7804-7809.

Supercomputers on the trail of dark matter

Particle physicists using "Piz Daint" have determined what is known as the scalar quark content of the proton. Now they hope, amongst other things, that this will make it easier to detect and research dark matter.

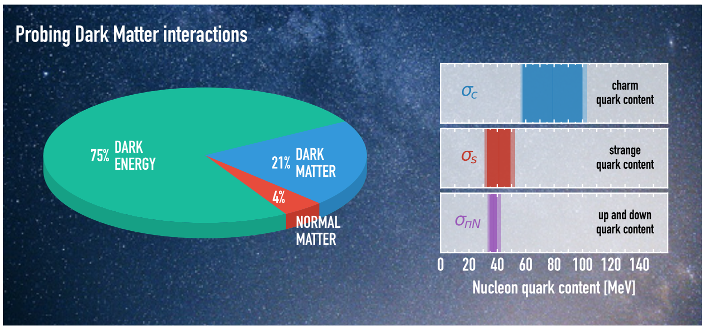
Almost all mass on Earth, humans included, derives from the atomic nuclei. These nuclei consist mainly of protons and neutrons, also called nucleons. Each nucleon in turn is made of three constituent quarks. However, the number of quark particles in the nucleon is actually much higher. This due to what are known as quantum fluctuations, where pairs of particles and anti-particles form spontaneously in a vacuum and immediately disintegrate again. A research team from Cyprus, Germany and Italy led by Constantia Alexandrou of the Computation-based Science and Technology Research Center of the Cyprus Institute and the Physics Department of the University of Cyprus in Nicosia, has now for the first time calculated the scalar quark content of the proton. For the elaborate simulations they made extensive use of the graphics processors (GPUs) of the CSCS supercomputer "Piz Daint". The researchers expect that their calculations will aid research into physical processes in particle physics and the as yet unknown dark matter that accounts for an estimated 21 percent of matter in the universe.



Galaxy clusters, which contain a significant amount of dark matter. In this image, the dark matter appears to align well with the blue-hued hot gas. (Image: NASA)

Quark condensates couple to the Higgs-boson

For every quark, there exists an anti-quark. A tightly coupled quark/anti-quark pair forms a condensate, similar to a water droplet on a pane of glass. This condensate is called the scalar quark content, and has a scalar quantum number. So the condensates can couple to the Higgs boson, which itself is a scalar particle. The Higgs boson – it is suspected – could interact with scalar particles of dark matter. "If we are to interpret experimental results as direct evidence for dark matter, then it is essential to know the numeric value we determined for the condensates and hence the exact proportion of scalar quark content in the nucleon, in particular what are known as strange quarks", says Alexandrou.



The visible matter that we know seems to form only about four percent of the total matter. Astronomical observations and Einstein's theory of general relativity call for the existence of the unknown "Dark Matter" and "Dark Energy" that make the rest of about 95%. The question is if it is possible to compute the quantities that can help to search for dark matter. The quark content of the proton (σc, σs, $\sigma \pi N$) is such a quantity and using computational resources on "Piz Daint" Constantia Alexandrou and her team were able to provide the best to date computation of all four quark flavour contents as shown on the right hand in this figure. (Image: Constantia Alexandrou)

Quarks interact mutually via gluon particles, and quarks with gluons via their respective colour charges, which may be red, green or blue. The strong force acting and being transmitted by the gluons – called the strong interaction – is one of the four fundamental forces of physics along with the weak interaction, the electromagnetic interaction and gravitation. The research field of Alexandrou and her team is quantum chromodynamics (QCD), which theoretically describes the strong interaction between quarks and gluons, and hence explains the origin of the nucleon large mass as well as what binds together neutrons and protons in atomic nuclei. For without the strong interaction, protons, for example, with their similar electrical charges, would repel each other rather than sticking together in the nucleus. And that would negate the existence of matter as we now understand it.

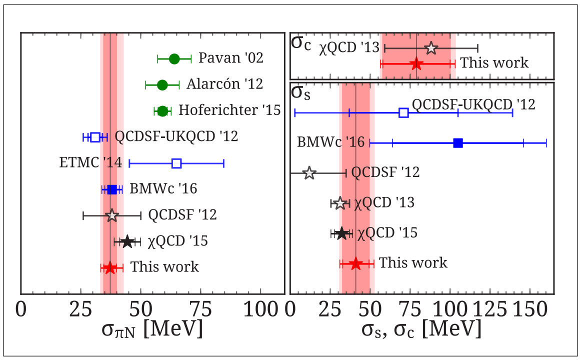
Heavy mass from binding energy

The strong interaction is indeed so strong that the mass-equivalent of the binding energy represents to a substantial degree the mass of a nucleon: "While a quark weighs around 10 mega electron volts (MeV), a proton due to its binding energy weighs 1 GeV (giga electron volts), or 100 times more", says physicist Karl Jansen of the John von Neumann Institute for Computing at DESY in Zeuthen, Germany, who was involved with the study published in Physical Review Letters. The force is so strong that quarks can never be extracted from protons experimentally. "That is a property that is characteristic for QCD and is termed 'confinement'", says Alexandrou. Attempts to isolate quarks using large quantities of energy result in their behaving like a spring or an elastic band, where increasing force must be exerted the further they are pulled apart. If the band is overstretched, it 'rips' and a quark-antiquark is formed that immediately binds via the strong interaction, and leads to a new hadron (a composite particle of quarks) being formed.

Strong force with extremely short radius of action

However, the strong force acts only on a very small space inside the atomic nucleus and defies approximate calculation, because the coupling between particles can grow very strong. Thus, it is not possible to identify a sufficiently small parameter that would be necessary for a perturbation theory calculation, explains Jansen. With the ground-breaking formulation of a theory of quarks and gluons in a four-dimensional space-time lattice, physicist and Nobel Prize winner Kenneth Wilson succeeded in 1974 with developing the lattice theory of quantum chromodynamics (lattice QCD) – a non-perturbative method. He thus laid the foundation for future numerical simulation.

In the lattice QCD theory, space-time is a four-dimensional lattice, a crystal with hyper-cubic symmetry. "By also moving from Minkowski to Euclidean time, we can consider the quantum field theory as a statistical physical system and carry out numerical simulations of that system", explains Jansen.



Key observables required for dark matter searches computed to unprecedented precision using allocation at CSCS supercomputer "Piz Daint". The red stars (this work) are showing the scalar quark content of the different quark flavours. Open symbols denote previous computations within lattice QCD which did not used simulations with physical parameters of the pion mass and may thus carry a systematic error.
The filled blue squares and filled black stars are calculations within lattice QCD using different discretization schemes. Green dots are the results of phenomenology using recent experimental input.
(Image: A. Abdel-Rehim et al.)

Nevertheless, it took over 30 years until the first researchers managed in 2008 to calculate the weight of nucleons and other particles directly from lattice QCD. This was made possible by a spectacular further development of the simulation algorithm in use, together with continually improving and more powerful supercomputers, says Jansen. "Now, by further refining the existing techniques and developing new and better algorithms, we successfully determined the scalar quark content in a proton – another non-trivial step."

The research results of Alexandrou and her team are already finding use in experiments that look for evidence of an interaction between the Higgs boson and the scalar condensate inside the nucleon. In the involved researchers' view, the most recent results from "Piz Daint" could thus push open a new window along the way to finally solving the mystery of dark matter.

Reference: Abdel-Rehim A, Alexandrou C, Constantinou C, Hadjiyiannakou K, Jansen K, Kallidonis Ch, Koutsou G & Vaquero Aviles-Casco A: Direct evaluation of the quark content of the nucleon from lattice QCD at the physical point, Phys. Rev. Lett. (2016), 116, 252001.

Papers with Highest Journal Impact Factor[1)]

Nature

Impact Factor: 42.35

D. Bozyigit, N. Yazdani, M. Yarema, O. Yarema, W. M. M. Lin, S. Volk, K. Vuttivorakulchai, M. Luisier, F. Juranyi, V. Wood, Soft surfaces of nanomaterials enable strong phonon interactions, Nature, DOI 10.1038/nature16977.

A. Parmigiani, S. Faroughi, C. Huber, O. Bachmann, Y. Su, Bubble accumulation and its role in the evolution of magma reservoirs in the upper crust, Nature, DOI 10.1038/nature17401.

P. Ruffieux, S. Y. Wang, B. Yang, C. Sanchez-Sanchez, J. Liu, et al., On-surface synthesis of graphene nanoribbons with zigzag edge topology, Nature, DOI 10.1038/nature17151.

A. Sheyko, C. C. Finlay, A. Jackson, Magnetic reversals from planetary dynamo waves, Nature, DOI 10.1038/nature.

Nature Materials

Impact Factor: 36.43

N. Marzari, The frontiers and the challenges, Nature Materials, DOI 10.1038/nmat4613.

Science

Impact Factor: 31.48

K. Lejaeghere, G. Bihlmayer, T. Bjorkman, P. Blaha, S. Blugel, et al., Reproducibility in density functional theory calculations of solids, Science, DOI 10.1126/science.aad3000.

Nature Physics

Impact Factor: 20.14

J. Adamek, D. Daverio, R. Durrer, M. Kunz, General relativity and cosmic structure formation, Nature Physics, DOI 10.1038/Nphys3673.

A. Fasoli, S. Brunner, W. A. Cooper, J. P. Graves, P. Ricci, O. Sauter, L. Villard, Computational challenges in magnetic-confinement fusion physics, Nature Physics, DOI 10.1038/Nphys3744.

Nature Cell Biology

Impact Factor: 19.68

M. Hilbert, A. Noga, D. Frey, V. Hamel, P. Guichard, S. H. W. Kraatz, M. Pfreundschuh, S. Hosner, I. Flückiger, R. Jaussi, M. M. Wieser, K. M. Thieltges, X. Deupi, D. J. Müller, R. A. Kammerer, P. Gönczy, M. Hirono, M. O. Steinmetz, SAS-6 engineering reveals interdependence between cartwheel and microtubules in determining centriole architecture, Nature Cell Biology, DOI 10.1038/ncb3362.

Nature Climate Change

Impact Factor: 14.55

A. K. Magnan, M. Colombier, R. Bille, F. Joos, O. Hoegh-Guldberg, H.-O. Pörtner, H. Waisman, T. Spencer, J.-P. Gattuso, Implications of the Paris agreement for the ocean, Nature Climate Change, DOI doi:10.1038/nclimate3038.

Nano Letters

Impact Factor: 13.59

A. Emboras, B. Cheng, P. Ma, C. Haffner, Y. Salamin, C. Hoessbacher, W. Heni, Y. Fedoryshyn, A. Pedersen, M. Luisier, J. Leuthold, Atomic scale plasmonic switch, Nano Letters, DOI 10.1021/acs.nanolett.5b04537.

R. Rhyner, M. Luisier, Minimizing self-heating and heat dissipation in ultrascaled nanowire transistors, Nano Letters, DOI 10.1021/acs.nanolett.5b04071.

T. Y. Kim, C. H. Park, N. Marzari, The electronic thermal conductivity of graphene, Nano Letters, DOI 10.1021/acs.nanolett.5b05288.

ACS Nano

Impact Factor: 12.88

A. Basagni, G. Vasseur, C. A. Pignedoli, M. Vilas-Varela, D. Pena, et al., Tunable band alignment with unperturbed carrier mobility of on-surface synthesized organic semiconducting wires, ACS Nano, DOI 10.1021/acsnano.5b07683.

Journal of the American Chemical Society

Impact Factor: 12.11

L. Foppa, C. Copéret, A. Comas-Vives, Increased back-bonding explains step-edge reactivity and particle size effect for CO activation on Ru nanoparticles, Journal of the American Chemical Society, DOI 10.1021/jacs.6b08697.

M. Lelimousin, V. Limongelli, M. S. P. Sansom, Conformational changes in the epidermal growth factor receptor: role of the transmembrane domain investigated by coarse-grained metadynamics free energy, Journal of the American Chemical Society, DOI 10.1021/jacs.6b05602.

[1)] 2015 JCR Science Edition, ISI Web of Knowledge[SM]

Bulletin of the American Meteorological Society

Impact Factor: 11.81

F. Hourdin, T. Mauritsen, A. Gettelmann, J.-C. Golaz, V. Balaji, Q. Duan, D. Folini, D. Ji, D. Klocke, Y. Qian, F. Rauser, C. Rio, L. Tomassini, M. Watanabe, D. Williamson, The art and sciences of climate model tuning, Bulletin of the American Meteorological Society: BAMS, DOI 10.1175/BAMS-D-15-00135.1.

Nature Geoscience

Impact Factor: 11.74

F. Giorgi, C. Torma, E. Coppola, N. Ban, C. Schär, S. Somot, Enhanced summer convective rainfall at alpine high elevations in response to climate warming, Nature Geoscience, DOI: 10.1038/Ngeo2761.

Angewandte Chemie-International Edition

Impact Factor: 11.26

S. M. Clarke, J. P. S. Walsh, M. Amsler, C. D. Malliakas, T. Yu, S. Goedecker, Y. B. Wang, C. Wolverton, D. E. Freedman, Discovery of a superconducting Cu-Bi intermetallic compound by high-pressure synthesis, Angewandte Chemie-International Edition, DOI 10.1002/anie.201605902.

P. Oulevey, S. Luber, B. Varnholt, T. Burgi, Symmetry breaking in chiral ionic liquids evidenced by vibrational optical activity, Angewandte Chemie-International Edition, DOI 10.1002/anie.201605792.

Z. J. Ma, G. Palermo, Z. Adhireksan, B. S. Murray, T. Von Erlach, P. J. Dyson, U. Röthlisberger, C. A. Davey, An organometallic compound which exhibits a DNA topology-dependent one-stranded intercalation mode, Angewandte Chemie-International Edition, DOI 10.1002/anie.201602145.

Astrophysical Journal Supplement Series

Impact Factor: 11.22

A. Perego, R. M. Cabezón, R. Käppeli, An advanced leakage scheme for neutrino treatment in astrophysical simulations, Astrophysical Journal Supplement Series, DOI 10.3847/0067-0049/223/2/22.

Nature Communications

Impact Factor: 10.74

Y. Li, S. Tang, M. Kröger, W. K. Liu, Molecular simulation guided constitutive modeling on finite strain viscoelasticity of elastomers, Journal of the Mechanics and Physics of Solids, DOI 10.1016/j.jmps.2015.12.007.

M. Schuppler, F. C. Keber, M. Kröger, A. R. Bausch, Boundaries steer the contraction of active gels, Nature Communications, DOI 10.1038/ncomms13120.

S. Meloni, T. Moehl, W. Tress, M. Franckevičius, M. Saliba, Y. H. Lee, P. Gao, M. K. Nazeeruddin, S. M. Zakeeruddin, U. Röthlisberger, M. Grätzel, Ionic polarization-induced current-voltage hysteresis in $CH_3NH_3PbX_3$ perovskite solar cells, Nature Communications, DOI 10.1038/ncomms10334.

B. Náfrádi, P. Szirmai, M. Spina, H. Lee, O. V. Yazyev, A. Arakcheeva, D. Chernyshov, M. Gibert, L. Forró and E. Horváth, Optically switched magnetism in photovoltaic perovskite $CH_3NH_3(Mn:Pb)I_3$, Nature Communications, DOI 10.1038/ncomms13406.

G. Pizzi, M. Gibertini, E. Dib, N. Marzari, G. Iannaccone, G. Fiori, Performance of arsenene and antimonene double-gate MOSFETs from first principles, Nature Communications, DOI 10.1038/ncomms12585.

W. Thiery, E. L. Davin, S. I. Seneviratne, K. Bedka, S. Lhermitte, N. P. M. van Lipzig, Hazardous thunderstorm intensification over Lake Victoria, Nature Communications, DOI 10.1038/ncomms12786.

K. Voïtchovsky, D. Giofrè, J. J. Segura, F. Stellacci, M. Ceriotti, Thermally-nucleated self-assembly of water and alcohol into stable structures at hydrophobic interfaces, Nature Communications, DOI 10.1038/ncomms13064.

S. Y. Wang, L. Talirz, C. A. Pignedoli, X. L. Feng, K. Müllen, R. Fasel, P. Ruffieux, Giant edge state splitting at atomically precise graphene zigzag edges, Nature Communications, DOI 10.1038/ncomms11507.

ACS Catalysis,

Impact Factor: 9.31

F. H. Hodel, S. Luber, Redox-inert cations enhancing water oxidation activity: the crucial role of flexibility, ACS Catalysis, DOI 10.1021/acscatal.6b01218.

F. H. Hodel, S. Luber, What influences the water oxidation activity of a bioinspired molecular (Co_4O_4)-O-II cubane? An in-depth exploration of catalytic pathways, ACS Catalysis, DOI 10.1021/acscatal.5b02507.

Chemical Science

Impact factor: 9.21

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

EMBO Reports

Impact factor: 9.06

A. Singhal, Y. Guo, M. Matkovic, G. Schertler, X. Deupi, E. C. Y. Yan, J. Standfuss, Structural role of the T94I rhodopsin mutation in congenital stationary night blindness, Embo Reports, DOI 10.15252/embr.201642671.

Physical Review X

Impact factor: 8.39

A. Cepellotti, N. Marzari, Thermal transport in crystals as a kinetic theory of relaxons, Physical Review X, DOI 10.1103/PhysRevX.6.041013.

S. Kawai, A. Sadeghi, T. Okamoto, C. Mitsui, R. Pawlak, T. Meier, J. Takeya, S. Goedecker, E. Meyer, Organometallic bonding in an Ullmann-type on-surface chemical reaction studied by high-resolution atomic force microscopy, Small, DOI 10.1002/smll.201601216.

Chemistry of Materials

Impact factor: 8.35

M. Amsler, S. Goedecker, W. G. Zeier, G. J. Snyder, C. Wolverton, L. Chaput, ZnSb polymorphs with improved thermoelectric properties, Chemistry of Materials, DOI 10.1021/acs.chemmater.5b03856.

Global Change Biology

Impact factor: 8.04

S. Mystakidis, E. L. Davin, N. Gruber, S. I. Seneviratne, Constraining future terrestrial carbon cycle projections using observation-based water and carbon flux estimates, Global Change Biology, DOI 10.1111/gcb.13217.

Papers Published in 2016 by Principal Investigator[1)]

Julian Adamek, University of Geneva

J. Adamek, D. Daverio, R. Durrer, M. Kunz, Gevolution: a cosmological N-body code based on General Relativity, Journal of Cosmology and Astroparticle Physics, DOI 10.1088/1475-7516/2016/07/053.

Constantia Alexandrou, University of Cyprus and the Cyprus Institute

C. Alexandrou, K. Hadjiyiannakou, C. Kallidonis, Axial charges of hyperons and charmed baryons using N_f=2+1+1 twisted mass fermions, Physical Review D, DOI 10.1103/PhysRevD.94.034502.

C. Alexandrou, M. Constantinou, G. Koutsou, K. Ottnad, M. Petschlies, Position space method for the nucleon magnetic moment in lattice QCD, Physical Review D, DOI 10.1103/PhysRevD.94.074508.

A. Abdel-Rehim, C. Alexandrou, M. Constantinou, K. Hadjiyiannakou, K. Jansen, C. Kallidonis, G. Koutsou, A. V. Avilés-Casco, Direct evaluation of the quark content of nucleons from Lattice QCD at the physical point, Physical Review Letters, DOI 10.1103/PhysRevLett.116.252001.

C. Alexandrou, Parton distribution functions from Lattice QCD, Few-Body Systems, DOI 10.1007/s00601-016-1073-5.

C. Alexandrou, A. Athenodorou, M. Constantinou, K. Hadjiyiannakou, K. Jansen, G. Koutsou, K. Ottnad, M. Petschlies, Neutron electric dipole moment using N_f=2+1+1 twisted mass fermions, Physical Review D, DOI 10.1103/PhysRevD.93.074503.

C. Alexandrou, Novel applications of Lattice QCD: parton distribution functions, proton charge radius and neutron electric dipole moment, Plenary talk at XII Quark Confinement, arXiv:1612.04644.

N.G. Stefanis, C. Alexandrou, T. Horn, H. Moutarde, I. Scimemi, Nucleon tomography. What can we do better today than Rutherford 100 years ago?, Plenary Round Table at XII Quark Confinement and the Hadron Spectrum, arXiv:1612.03077.

C. Alexandrou, M. Constantinou, K. Hadjiyiannakou, C. Kallidonis, G. Koutsou, K. Jansen, C. Wiese, A. Vaquero Avilés-Casco, Nucleon spin and quark content at the physical point, Talk presented at the 34th annual International Symposium on Lattice Field Theory, arXiv:1611.09163.

A. Abdel-Rehim, C. Alexandrou, M. Constantinou, J. Finkenrath, K. Hadjiyiannakou, K. Jansen, C. Kallidonis, G. Koutsou, A. Vaquero Avilés-Casco, J. Volmer, Disconnected diagrams with twisted-mass fermions, PoS LATTICE2016.

C. Alexandrou, M. Constantinou, K. Hadjiyiannakou, C. Kallidonis, G. Koutsou, K. Jansen, H. Panagopoulos, F. Steffens, A. Vaquero, C. Wiese, Recent results for the proton spin decomposition from lattice QCD, PoS DIS2016.

Maximilian Amsler, Northwestern University

S. M. Clarke, J. P. S. Walsh, M. Amsler, C. D. Malliakas, T. Yu, S. Goedecker, Y. B. Wang, C. Wolverton, D. E. Freedman, Discovery of a superconducting Cu-Bi intermetallic compound by high-pressure synthesis, Angewandte Chemie-International Edition, DOI 10.1002/anie.201605902.

J. G. He, M. Amsler, Y. Xia, S. S. Naghavi, V. I. Hegde, S. Q. Hao, S. Goedecker, V. Ozolins, C. Wolverton, Ultralow thermal conductivity in full Heusler semiconductors, Physical Review Letters, DOI 10.1103/PhysRevLett.117.046602.

J. A. Flores-Livas, M. Amsler, C. Heil, A. Sanna, L. Boeri, G. Profeta, C. Wolverton, S. Goedecker, E. K. U. Gross, Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure, Physical Review B, DOI 10.1103/PhysRevB.93.020508.

M. Amsler, S. Goedecker, W. G. Zeier, G. J. Snyder, C. Wolverton, L. Chaput, ZnSb polymorphs with improved thermoelectric properties, Chemistry of Materials, DOI 10.1021/acs.chemmater.5b03856.

L. Zhu, M. Amsler, T. Fuhrer, B. Schaefer, S. Faraji, S. Rostami, S. A. Ghasemi, A. Sadeghi, M. Grauzinyte, C. Wolverton, S. Goedecker, A fingerprint based metric for measuring similarities of crystalline structures, Journal of Chemical Physics, DOI 10.1063/1.4940026.

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

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

Charalampos Anastasiou, ETH Zurich

C. Anastasiou, C. Duhr, F. Dulat, E. Furlan, T. Gehrmann, F. Herzog, A. Lazopoulos, B. Mistlberger, CP-even scalar boson production via gluon fusion at the LHC, Journal of High Energy Physics, DOI 10.1007/Jhep09(2016)037.

C. Anastasiou, C. Duhr, F. Dulat, E. Furlan, T. Gehrmann, F. Herzog, A. Lazopoulos, B. Mistlberger, High precision determination of the gluon fusion Higgs boson cross-section at the LHC, Journal of High Energy Physics, DOI 10.1007/Jhep05(2016)058.

Wanda Andreoni, EPF Lausanne

J. M. H. Kroes, F. Pietrucci, K. Chikkadi, C. Roman, C. Hierold, W. Andreoni, The response of single-walled carbon nanotubes to NO2 and the search for a long-living adsorbed species, Applied Physics Letters, DOI 10.1063/1.4940422.

Stephan Brunner, EPF Lausanne

G. Merlo, O. Sauter, S. Brunner, A. Burckel, Y. Camenen, F. J. Casson, W. Dorland, E. Fable, T. Gorler, F. Jenko, A. G. Peeters, D. Told, L. Villard, Linear multispecies gyrokinetic flux tube benchmarks in shaped tokamak plasmas, Physics of Plasmas, DOI 10.1063/1.4942539.

A. Mariani, G. Merlo, S. Brunner, A. Merle, O. Sauter, T. Görler, F. Jenko, D. Told, Characterization with microturbulence simulations of the zero particle flux condition in case of a TCV discharge showing toroidal rotation reversal, Journal of Physics Conference Series, DOI 10.1088/1742-6596/775/1/012007.

Rubén Cabezón, University of Basel

D. García-Senz, R. M. Cabezón, I. Domínguez, F. K. Thielemann, Type Ia supernovae: can Coriolis force break the symmetry of the gravitational confined detonation explosion mechanism?, The Astrophysical Journal, DOI 10.3847/0004-637x/819/2/132.

Michele Ceriotti, EPF Lausanne

Y. X. Chen, H. I. Okur, N. Gomopoulos, C. Macias-Romero, P. S. Cremer, P. B. Petersen, G. Tocci, D. M. Wilkins, C. W. Liang, M. Ceriotti, S. Roke, Electrolytes induce long-range orientational order and free energy changes in the H-bond network of bulk water, Science Advances, DOI 10.1126/sciadv.1501891.

P. Gasparotto, A. A. Hassanali, M. Ceriotti, Probing defects and correlations in the hydrogen-bond network of ab-inizio water, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.5b01138.

V. Kapil, J. Behler, M. Ceriotti, High order path integrals made easy, Journal of Chemical Physics, DOI 10.1063/1.4971438.

V. Kapil, J. VandeVondele, M. Ceriotti, Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods, Journal of Chemical Physics, DOI 10.1063/1.4941091.

M. Rossi, P. Gasparotto, M. Ceriotti, Anharmonic and quantum fluctuations in molecular crystals: a first-principles study of the stability of paracetamol, Physical Review Letters, DOI 10.1103/PhysRevLett.117.115702.

G. Tocci, C. Liang, D. M. Wilkins, S. Roke, M. Ceriotti, Second-harmonic scattering as a probe of structural correlations in liquids, The Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.6b01851.

K. Voïtchovsky, D. Giofrè, J. J. Segura, F. Stellacci, M. Ceriotti, Thermally-nucleated self-assembly of water and alcohol into stable structures at hydrophobic interfaces, Nature Communications, DOI 10.1038/ncomms13064.

Shyam S. Chikatamarla, ETH Zurich

C. Antonini, S. Jung, A. Wetzel, E. Heer, P. Schoch, A. M. Moqaddam, S. S. Chikatamarla, I. Karlin, M. Marengo, D. Poulikakos, Contactless prompt tumbling rebound of drops from a sublimating slope, Physical Review Fluids, DOI 10.1103/PhysRevFluids.1.013903.

B. Dorschner, F. Bosch, S. S. Chikatamarla, K. Boulouchos, I. V. Karlin, Entropic multi-relaxation time lattice Boltzmann model for complex flows, Journal of Fluid Mechanics, DOI 10.1017/jfm.2016.448.

B. Dorschner, N. Frapolli, S. S. Chikatamarla, I. V. Karlin, Grid refinement for entropic lattice Boltzmann models, Physical Review E, DOI 10.1103/PhysRevE.94.053311.

N. Frapolli, S. S. Chikatamarla, I. V. Karlin, Lattice kinetic theory in a comoving Galilean reference frame, Physical Review Letters, DOI 10.1103/PhysRevLett.117.010604.

N. Frapolli, S. S. Chikatamarla, I. V. Karlin, Entropic lattice Boltzmann model for gas dynamics: theory, boundary conditions, and implementation, Physical Review E, DOI 10.1103/PhysRevE.93.063302.

A. M. Moqaddam, S. S. Chikatamarla, I. V. Karlin, Simulation of binary droplet collisions with the entropic lattice Boltzmann method, Physics of Fluids, DOI 10.1063/1.4942017.

G. Pareschi, N. Frapolli, S. S. Chikatamarla, I. V. Karlin, Conjugate heat transfer with the entropic lattice Boltzmann method, Physical Review E, DOI 10.1103/PhysRevE.94.013305.

Bastien Chopard, University of Geneva

P. Kunzli, K. Tsunematsu, P. Albuquerque, J. L. Falcone, B. Chopard, C. Bonadonna, Parallel simulation of particle transport in an advection field applied to volcanic explosive eruptions, Computers & Geosciences, DOI 10.1016/j.cageo.2016.02.005.

Aleix Comas-Vives, ETH Zurich

A. Comas-Vives, K. Furman, D. Gajan, M. C. Akatay, A. Lesage, F. H. Ribeiro, C. Copéret, Predictive morphology, stoichiometry and structure of surface species in supported Ru nanoparticles under H_2 and CO atmospheres from combined experimental and DFT studies, Physical Chemistry Chemical Physics, DOI 10.1039/c5cp06710c.

L. Foppa, C. Copéret, A. Comas-Vives, Increased back-bonding explains step-edge reactivity and particle size effect for CO activation on Ru nanoparticles, Journal of the American Chemical Society, DOI 10.1021/jacs.6b08697.

William A. Curtin, EPF Lausanne

Z. X. Wu, W. A. Curtin, Mechanism and energetics of < c + a > dislocation cross-slip in hcp metals, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1603966113.

Z. X. Wu, W. A. Curtin, Intrinsic structural transitions of the pyramidal I < c + a > dislocation in magnesium, Scripta Materialia, DOI 10.1016/j.scriptamat.2016.01.041.

Z. X. Wu, B. L. Yin, W. A. Curtin, Energetics of dislocation transformations in hcp metals, Acta Materialia, DOI 10.1016/j.actamat.2016.08.002.

Marco A. Deriu, SUPSI

M. A. Deriu, G. Grasso, J. A. Tuszynski, D. Gallo, U. Morbiducci, A. Danani, Josephin domain structural conformations explored by metadynamics in essential coordinates, Plos Computational Biology, DOI 10.1371/journal.pcbi.1004699.

M. A. Deriu, G. Grasso, J. A. Tuszynski, D. Massai, D. Gallo, U. Morbiducci, A. Danani, Characterization of the AXH domain of Ataxin-1 using enhanced sampling and functional mode analysis, Proteins-Structure Function and Bioinformatics, DOI 10.1002/prot.25017.

G. Grasso, M. A. Deriu, J. A. Tuszynski, D. Gallo, U. Morbiducci, A. Danani, Conformational fluctuations of the AXH monomer of Ataxin-1, Proteins-Structure Function and Bioinformatics, DOI 10.1002/prot.24954.

Xavier Deupi i Corral, Paul Scherrer Institute

M. Hilbert, A. Noga, D. Frey, V. Hamel, P. Guichard, S. H. W. Kraatz, M. Pfreundschuh, S. Hosner, I. Flückiger, R. Jaussi, M. M. Wieser, K. M. Thieltges, X. Deupi, D. J. Müller, R. A. Kammerer, P. Gönczy, M. Hirono, M. O. Steinmetz, SAS-6 engineering reveals interdependence between cartwheel and microtubules in determining centriole architecture, Nature Cell Biology, DOI 10.1038/ncb3362.

A. Singhal, Y. Guo, M. Matkovic, G. Schertler, X. Deupi, E. C. Y. Yan, J. Standfuss, Structural role of the T94I rhodopsin mutation in congenital stationary night blindness, Embo Reports, DOI 10.15252/embr.201642671.

Jiannong Fang, EPF Lausanne

M. Abkar, A. Sharifi, F. Porté-Agel, Wake flow in a wind farm during a diurnal cycle, Journal of Turbulence, DOI 10.1080/14685248.2015.1127379.

W. C. Cheng, F. Porté-Agel, Large-Eddy simulation of flow and scalar dispersion in rural-to-urban transition regions, International Journal of Heat and Fluid Flow, DOI 10.1016/j.ijheatfluidflow.2016.04.004.

S. Shamsoddin, F. Porté-Agel, A Large-Eddy simulation study of vertical axis wind turbine wakes in the atmospheric boundary layer, Energies, DOI 10.3390/en9050366.

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.

J. Fang, F. Porté-Agel, Intercomparison of terrain-following coordinate transformation and immersed boundary methods for large-eddy simulation of wind fields over complex terrain, Journal of Physics Conference Series, DOI 10.1088/1742-6596/753/8/082008.

M. Giometto, A. Christen, C. Meneveau, J. Fang, M. Krafczyk, M. B. Parlange, Spatial characteristics of roughness sublayer mean flow and turbulence over a realistic urban surface, Boundary Layer Meteorology, DOI 10.1007/s10546-016-0157-6.

Andreas Fichtner, ETH Zurich

M. Afanasiev, C. Boehm, A. Gokhberg, A. Fichtner, Automatic global multiscale seismic inversion: insights into model, data, and workflow management, Proceedings of the Platform for Advanced Scientific Computing Conference, DOI 10.1145/2929908.2929910.

C. Boehm, M. Hanzich, J. de la Puente, A. Fichtner, Wavefield compression for adjoint methods in full-waveform inversion, Geophysics, DOI 10.1190/geo2015-0653.1.

M. Afanasiev, D. Peter, K. Sager, S. Simutė, L. Ermert, L. Krischer, A. Fichtner, Foundations for a multiscale collaborative Earth model, Geophysical Journal International, DOI 10.1093/gji/ggv439.

L. Ermert, A. Villaseñor, A. Fichtner, Cross-correlation imaging of ambient noise sources, Geophysical Journal International, DOI 10.1093/gji/ggv460.

S. Simutė, H. Steptoe, L. Cobden, A. Gokhberg, A. Fichtner, Full-waveform inversion of the Japanese islands region, Journal of Geophysical Research, 10.1002/2016JB012802.

A. Gokhberg, A. Fichtner, Full-waveform inversion on heterogeneous HPC systems, Computers & Geosciences, DOI 10.1016/j.cageo.2015.12.013.

R. Maguire, J. Ritsema, P. E. van Keken, Andreas Fichtner, S. Goes, *P*- and *S*-wave delays caused by thermal plumes, Geophysical Journal International, DOI 10.1093/gji/ggw187.

Christos Frouzakis, ETH Zurich

M. Schmitt, C. E. Frouzakis, Y. M. Wright, A. G. Tomboulides, K. Boulouchos, Direct numerical simulation of the compression stroke under engine relevant conditions: local wall heat flux distribution, International Journal of Heat and Mass Transfer, DOI 718-731, 10.1016/j.ijheatmasstransfer.2015.08.074.

M. Schmitt, C. E. Frouzakis, Y. M. Wright, A. G. Tomboulides, K. Boulouchos, Investigation of wall heat transfer and thermal stratification under engine-relevant conditions using DNS, International Journal of Engine Research, DOI 10.1177/1468087415588710.

Thomas Gehrmann, University of Zurich

X. Chen, J. Cruz-Martinez, T. Gehrmann, E. Glover, M. Jaquier, NNLO QCD corrections to Higgs boson production at large transverse momentum, Journal of High Energy Physics, DOI 10.1007/Jhep10(2016)066.

J. Currie, T. Gehrmann, J. Niehues, Precise QCD predictions for the production of dijet final states in deep inelastic scattering, Physical Review Letters, DOI 10.1103/PhysRevLett.117.042001.

Stefan Goedecker, University of Basel

M. Amsler, S. Goedecker, W. G. Zeier, G. J. Snyder, C. Wolverton, L. Chaput, ZnSb polymorphs with improved thermoelectric properties, Chemistry of Materials, DOI 10.1021/acs.chemmater.5b03856.

S. M. Clarke, J. P. S. Walsh, M. Amsler, C. D. Malliakas, T. Yu, S. Goedecker, Y. B. Wang, C. Wolverton, D. E. Freedman, Discovery of a superconducting Cu-Bi intermetallic compound by high-pressure synthesis, Angewandte Chemie-International Edition, DOI 10.1002/anie.201605902.

J. A. Flores-Livas, M. Amsler, C. Heil, A. Sanna, L. Boeri, G. Profeta, C. Wolverton, S. Goedecker, E. K. U. Gross, Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure, Physical Review B, DOI 10.1103/PhysRevB.93.020508.

J. G. He, M. Amsler, Y. Xia, S. S. Naghavi, V. I. Hegde, S. Q. Hao, S. Goedecker, V. Ozolins, C. Wolverton, Ultralow thermal conductivity in full Heusler semiconductors, Physical Review Letters, DOI 10.1103/PhysRevLett.117.046602.

L. Zhu, M. Amsler, T. Fuhrer, B. Schaefer, S. Faraji, S. Rostami, S. A. Ghasemi, A. Sadeghi, M. Grauzinyte, C. Wolverton, S. Goedecker, A fingerprint based metric for measuring similarities of crystalline structures, Journal of Chemical Physics, DOI 10.1063/1.4940026.

G. Fisicaro, L. Genovese, O. Andreussi, N. Marzari, S. Goedecker, A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments, Journal of Chemical Physics, DOI 10.1063/1.4939125.

S. Kawai, A. Sadeghi, T. Okamoto, C. Mitsui, R. Pawlak, T. Meier, J. Takeya, S. Goedecker, E. Meyer, Organometallic bonding in an Ullmann-type on-surface chemical reaction studied by high-resolution atomic force microscopy, Small, DOI 10.1002/smll.201601216.

K. Lejaeghere, G. Bihlmayer, T. Bjorkman, P. Blaha, S. Blugel, et al., Reproducibility in density functional theory calculations of solids, Science, DOI 10.1126/science.aad3000.

B. Schaefer, S. Goedecker, Computationally efficient characterization of potential energy surfaces based on fingerprint distances, Journal of Chemical Physics, DOI 10.1063/1.4956461.

I. Valencia-Jaime, R. Sarmiento-Perez, S. Botti, M. a. L. Marques, M. Amsler, S. Goedecker, A. H. Romero, Novel crystal structures for lithium-silicon alloy predicted by minima hopping method, Journal of Alloys and Compounds, DOI 10.1016//j.jallcom.2015.09.101.

Jonathan P. Graves, EPF Lausanne

W. A. Cooper, D. Brunetti, B. P. Duval, J. M. Faustin, J. P. Graves, A. Kleiner, H. Patten, D. Pfefferle, L. Porte, M. Raghunathan, H. Reimerdes, O. Sauter, T. M. Tran, Saturated ideal kink/peeling formations described as three-dimensional magnetohydrodynamic tokamak equilibrium states, Physics of Plasmas, DOI 10.1063/1.4945743.

W. A. Cooper, J. P. Graves, B. P. Duval, O. Sauter, J. M. Faustin, A. Kleiner, S. Lanthaler, H. Patten, M. Raghunathan, T. M. Tran, T. Chapman, C. J. Ham, Three-dimensional magnetohydrodynamic equilibrium of quiescent H-modes in tokamak systems, Plasma Physics and Controlled Fusion, DOI 10.1088/0741-3335/58/6/064002.

J. M. Faustin, W. A. Cooper, J. P. Graves, D. Pfefferle, J. Geiger, Fast particle loss channels in Wendelstein 7-X, Nuclear Fusion, DOI 10.1088/0029-5515/56/9/092006.

J. M. Faustin, W. A. Cooper, J. P. Graves, D. Pfefferle, J. Geiger, ICRH induced particle losses in Wendelstein 7-X, Plasma Physics and Controlled Fusion, DOI 10.1088/0741-3335/58/7/074004.

D. Pfefferle, W. A. Cooper, A. Fasoli, J. P. Graves, Effects of magnetic ripple on 3D equilibrium and alpha particle confinement in the European DEMO, Nuclear Fusion, DOI 10.1088/0029-5515/56/11/112002.

M. Raghunathan, J. P. Graves, W. A. Cooper, M. Pedro, O. Sauter, Simulation of bootstrap current in 2D and 3D ideal magnetic fields in tokamaks, Nuclear Fusion, DOI 10.1088/0029-5515/56/9/092004.

Csaba Hetényi, Hungarian Academy of Science

N. Jeszenői, M. Bálint, I. Horváth, D. van der Spoel, C. Hetényi, Exploration of interfacial hydration networks of target-ligand complexes, Journal of Chemical Information and Modeling, DOI 10.1021/acs.jcim.5b00638.

Alexander Hobbs, University of Zurich

A. Hobbs, J. I. Read, O. Agertz, F. Iannuzzi, C. Power, Novel adaptive softening for collisionless N-body simulations: eliminating spurious haloes, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw251.

Torsten Hoefler, ETH Zurich

T. Gysi, J. Bär, T. Hoefler, dCUDA: hardware supported overlap of computation and communication, IEEE/ACM International Conference on High Performance Computing, Networking, Storage and Analysis (SC 16).

A. Calotoiu, D. Beckingsale, C. W. Earl, T. Hoefler, I. Karlin, M. Schulz, F. Wolf, Fast multi-parameter performance modeling, IEEE International Conference on Cluster Computing (Cluster), DOI 10.1109/Cluster.2016.57.

P. Schmid, M. Besta, T. Hoefler, High-performance distributed RMA locks, HPDC 16 Proceedings of the 25th ACM International Symposium on High-Performance Parallel and Distributed Computing, DOI 10.1145/2907294.2907323.

M. Martinasso, G. Kwasniewski, S. R. Alam, T. C. Schulthess, T. Hoefler, A PCIe congestion-aware performance model for densely populated accelerator servers, IEEE/ACM International Conference on High Peraformance Computing, Networking, Storage and Analysis (SC 16).

A. M. Dan, P. Lam, T. Hoefler, M. Vechev, Modeling and analysis of remote memory access programming, Proceedings of the 2016 ACM SIGPLAN International Conference on Object-Oriented Programming, Systems, Languages, and Applications.

W. Tang, B. Wang, S. Ethier, G. Kwasniewski, T. Hoefler, K. Ibrahim, K. Madduri, S. Williams, L. Oliker, C. Rosales-Fernandez, T. Williams, Extreme scale plasma turbulence simulations on top supercomputers worldwide, IEEE/ACM International Conference on High Performance Computing, Networking, Storage and Analysis (SC 16).

Ilia Horenko, Università della Svizzera italiana

T. J. O'kane, J. S. Risbey, D. P. Monselesan, I. Horenko, C. L. E. Franzke, On the dynamics of persistent states and their secular trends in the waveguides of the Southern Hemisphere troposphere, Climate Dynamics, DOI 10.1007/s00382-015-2786-8.

P. Gagliardini, E. Ossola, O. Scaillet, Time-varying risk premium in large cross-sectional equity data sets, Econometrica, DOI 10.3982/ECTA11069.

Jürg Hutter, University of Zurich

R. Koitz, J. Hutter, M. Iannuzzi, Formation and properties of a terpyridine-based 2D MOF on the surface of water, 2D Materials, DOI 10.1088/2053-1583/3/2/025026.

G. Mette, D. Sutter, Y. Gurdal, S. Schnidrig, B. Probst, M. Iannuzzi, J. Hutter, R. Alberto, J. Osterwalder, From porphyrins to pyrphyrins: adsorption study and metalation of a molecular catalyst on Au(111), Nanoscale, DOI 10.1039/c5nr08953k.

M. Schilling, G. R. Patzke, J. Hutter, S. Luber, Computational investigation and design of cobalt aqua complexes for homogeneous water oxidation, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.6b00712.

J. Wilhelm, M. Del Ben, J. Hutter, GW in the Gaussian and plane waves scheme with application to linear acenes, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00380.

J. Wilhelm, P. Seewald, M. Del Ben, J. Hutter, Large-scale cubic-scaling random phase approximation correlation energy calculations using a gaussian basis, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00840.

O. Schütt, P. Messmer, J. Hutter, J. VandeVondele, GPU-accelerated sparse matrix–matrix multiplication for linear scaling density functional theory, Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics (eds R. C. Walker and A. W. Götz), John Wiley & Sons, Ltd, Chichester, UK, DOI 10.1002/9781118670712.ch8.

Andrew Jackson, ETH Zurich

Y. F. Lin, P. Marti, J. Noir, A. Jackson, Precession-driven dynamos in a full sphere and the role of large scale cyclonic vortices, Physics of Fluids, DOI 10.1063/1.4954295.

P. Marti, A. Jackson, A fully spectral methodology for magnetohydrodynamic calculations in a whole sphere, Journal of Computational Physics, DOI 10.1016/j.jcp.2015.10.056.

S. Vantieghem, A. Sheyko, A. Jackson, Applications of a finite-volume algorithm for incompressible MHD problems, Geophysical Journal International, DOI 10.1093/gji/ggv527.

A. Sheyko, C. C. Finlay, A. Jackson, Magnetic reversals from planetary dynamo waves, Nature, DOI 10.1038/nature19842.

H. Matsui, E. Heien, J. Aubert, A. Jackson, et al., Performance benchmarks for a next generation numerical dynamo model, Geochemistry, Geophysics, Geosystems, DOI 10.1002/2015GC006159.

Fortunat Joos, University of Bern

C. Camenisch, K. M. Keller, M. Salvisberg, B. Amann, M. Bauch, et al., The 1430s: a cold period of extraordinary internal climate variability during the early Spörer Minimum with social and economic impacts in north-western and central Europe, Climate of the Past, DOI 10.5194/cp-12-2107-2016.

M. O. Chikamoto, A. Timmermann, M. Yoshimori, F. Lehner, A. Laurian, A. Abe-Ouchi, A. Mouchet, F. Joos, C. C. Raible, K. M. Cobb, Intensification of tropical Pacific biological productivity due to volcanic eruptions, Geophysical Research Letters, DOI 10.1002/2015gl067359.

S. G. Keel, F. Joos, R. Spahni, M. Saurer, R. B. Weigt, S. Klesse, Simulating oxygen isotope ratios in tree ring cellulose using a dynamic global vegetation model, Biogeosciences, DOI 10.5194/bg-13-3869-2016.

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-2016-515.

A. K. Magnan, M. Colombier, R. Bille, F. Joos, O. Hoegh-Guldberg, H.-O. Pörtner, H. Waisman, T. Spencer, J.-P. Gattuso, Implications of the Paris Agreement for the ocean, Nature Climate Change, DOI 10.1038/nclimate3038.

David Keyes, KAUST

D. Sukkari, H. Ltaief, D. Keyes, High performance polar decomposition for SVD solvers on distributed memory systems, International Euro-Par Conference, DOI 10.1007/978-3-319-43659-3_44.

Leonhard Kleiser, ETH Zurich

T. Luginsland, F. Gallaire, L. Kleiser, Impact of rotating and fixed nozzles on vortex breakdown in compressible swirling jet flows, European Journal of Mechanics B-Fluids, DOI 10.1016/j.euromechflu.2016.01.006.

M. O. John, D. Obrist, L. Kleiser, Secondary instability and subcritical transition of the leading-edge boundary layer, Journal of Fluid Mechanics, DOI 10.1017/jfm.2016.117.

M. Gloor, S. Bühler, L. Kleiser, Transition to turbulence and noise radiation in heated coaxial jet flows, Physics of Fluids, DOI 10.1063/1.4944753.

Petros Koumoutsakos, ETH Zurich

S. Wu, P. Angelikopoulos, G. Tauriello, C. Papadimitriou, P. Koumoutsakos, Fusing heterogeneous data for the calibration of molecular dynamics force fields using hierarchical Bayesian models, Journal of Chemical Physics, DOI 10.1063/1.4967956.

J. Chen, J. H. Walther, P. Koumoutsakos, Ultrafast cooling by covalently bonded graphene-carbon nanotube hybrid immersed in water, Nanotechnology, DOI 10.1088/0957-4484/27/46/465705.

M. Gazzola, A. A. Tchieu, D. Alexeev, A. De Brauer, P. Koumoutsakos, Learning to school in the presence of hydro dynamic interactions, Journal of Fluid Mechanics, DOI 10.1017/jfm.2015.686.

B. O. Andersen, N. F. Nielsen, J. H. Walther, Numerical and experimental study of pulse-jet cleaning in fabric filters, Powder Technology, DOI 10.1016/j.powtec.2015.12.028.

M. M. Hejlesen, J. H. Walther, A multiresolution method for solving the Poisson equation using high order regularization, Journal of Computational Physics, DOI 10.1016/j.jcp.2016.08.053.

C. S. Hemmingsen, K. M. Ingvorsen, S. Mayer, J. H. Walther, LES and URANS simulations of the swirling flow in a dynamic model of a uniflow-scavenged cylinder, International Journal of Heat and Fluid Flow, DOI 10.1016/j.ijheatfluidflow.2016.10.008.

E. Hovad, J. Spangenberg, P. Larsen, J. H. Walther, J. Thorborg, J. H. Hattel, Simulating the DISAMATIC process using the discrete element method - a dynamical study of granular flow, Powder Technology, DOI 10.1016/j.powtec.2016.09.039.

N. K. Karna, E. Oyarzua, J. H. Walther, H. A. Zambrano, Effect of the meniscus contact angle during early regimes of spontaneous imbibition in nanochannels, Physical Chemistry Chemical Physics, DOI 10.1039/c6cp06155a.

K. M. Pang, N. Karvounis, J. H. Walther, J. Schramm, Numerical investigation of soot formation and oxidation processes under large two-stroke marine diesel engine-like conditions using integrated CFD-chemical kinetics, Applied Energy, DOI 10.1016/j.apenergy.2016.02.081.

C. Wen, A. Q. Li, J. H. Walther, Y. Yang, Effect of swirling device on flow behavior in a supersonic separator for natural gas dehydration, Separation and Purification Technology, DOI 10.1016/j.seppur.2016.05.019.

C. Wen, Y. Yang, J. H. Walther, K. M. Pang, Y. Q. Feng, Effect of delta wing on the particle flow in a novel gas supersonic separator, Powder Technology, DOI 10.1016/j.powtec.2016.07.061.

F. Wermelinger, B. Hejazialhosseini, P. Hadjidoukas, D. Rossinelli, P. Koumoutsakos, An efficient compressible multicomponent flow solver for heterogeneous CPU/GPU architectures, Proceedings of the Platform for Advanced Scientific Computing Conference (PASC 16), DOI 10.1145/2929908.2929914.

L. Kulakova, P. Angelikopoulos, P. E. Hadjidoukas, C. Papadimitriou, P. Koumoutsakos, Approximate Bayesian computation for granular and molecular dynamics simulations, Proceedings of the Platform for Advanced Scientific Computing Conference (PASC 16), DOI 10.1145/2929908.2929918.

M. Zayernouri, A. Matzavinos, Fractional Adams-Bashforth/ Moulton methods: an application to the fractional Keller-Segel chemotaxis system, Journal of Computational Physics, DOI 10.1016/j.jcp.2016.04.041.

S. Mishra, C. Schwab, J. Sukys, Multi-level Monte Carlo finite volume methods for uncertainty quantification of acoustic wave propagation in random heterogeneous layerd medium, Journal of Computational Physics, DOI 10.1016/j.jcp.2016.02.014.

Matthias Krack, Paul Scherrer Institute

D. Bocharov, M. Krack, A. Kalinko, J. Purans, F. Rocca, S. E. Ali, A. Kuzmin, Ab initio molecular dynamics simulations of the Sc K-edge EXAFS of scandium trifluoride, 16th International Conference on X-Ray Absorption Fine Structure (Xafs16), DOI 10.1088/1742-6596/712/1/012009.

D. Bocharov, M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, A. Kuzmin, J. Purans, E. Kotomin, Interpretation of the U L-3-edge EXAFS in uranium dioxide using molecular dynamics and density functional theory simulations, 16th International Conference on X-Ray Absorption Fine Structure (Xafs16), DOI 10.1088/1742-6596/712/1/012091.

A. Stirling, T. Rozgonyi, M. Krack, M. Bernasconi, Prebiotic NH3 formation: insights from simulations, Inorganic Chemistry, DOI 10.1021/acs.inorgchem.5b02911.

Martin Kröger, ETH Zurich

S. H. Jeong, J. M. Kim, J. Yoon, C. Tzoumanekas, M. Kröger, C. Baig, Influence of molecular architecture on the entanglement network: topological analysis of linear, long- and short-chain branched polyethylene melts via Monte Carlo simulations, Soft Matter, DOI 10.1039/c5sm03016a.

A. Karatrantos, N. Clarke, M. Kröger, Modeling of polymer structure and conformations in polymer nanocomposites from atomistic to mesoscale: a review, Polymer Reviews, DOI 10.1080/15583724.2015.1090450.

Y. Li, S. Tang, M. Kröger, W. K. Liu, Molecular simulation guided constitutive modeling on finite strain viscoelasticity of elastomers, Journal of the Mechanics and Physics of Solids, DOI 10.1016/j.jmps.2015.12.007.

M. Schuppler, F. C. Keber, M. Kröger, A. R. Bausch, Boundaries steer the contraction of active gels, Nature Communications, DOI 10.1038/ncomms13120.

Z. Q. Shen, D. T. Loe, J. K. Awino, M. Kröger, J. L. Rouge, J. L. Rouge, Y. Li, Self-assembly of core-polyethylene glycol-lipid shell (CPLS) nanoparticles and their potential as drug delivery vehicles, Nanoscale, DOI 10.1039/c6nr04134e.

Y. R. Sliozberg, M. Kröger, T. L. Chantawansri, Fast equilibration protocol for million atom systems of highly entangled linear polyethylene chains, Journal of Chemical Physics, DOI 10.1063/1.4946802.

P. S. Stephanou, M. Kröger, Solution of the complete Curtiss-Bird model for polymeric liquids subjected to simple shear flow, Journal of Chemical Physics, DOI 10.1063/1.4944674.

M. K. Singh, P. Ilg, R. M. Espinosa-Marzal, M. Kröger, N. D. Spencer, Effect of crosslinking on the microtribological behavior of model polymer brushes, Tribology Letters, DOI10.1007/ s11249-016-0705-8.

M. K. Singh, P. Ilg, R. M. Espinosa-Marzal, N. D. Spencer, M. Kröger, Influence of chain stiffness, grafting density and normal load on the tribological and structural behavior of polymer brushes: a nonequilibrium-molecular-dynamics study, Polymers, DOI 10.3390/polym8070254.

C. Luo, M. Kröger, J.-U. Sommer, Entanglements and crystallization of concentrated polymer solutions: molecular dynamics simulations, Macromolecules, DOI 10.1021/acs.macromol. 6b02124.

Martin Kunz, University of Geneva

D. Daverio, M. Hindmarsh, M. Kunz, J. Lizarraga, J. Urrestilla, Energy-momentum correlations for Abelian Higgs cosmic strings, Physical Review, DOI 10.1103/PhysRevD.93.085014.

J. Adamek, D. Daverio, R. Durrer, M. Kunz, General relativity and cosmic structure formation, Nature Physics, DOI 10.1038/ Nphys3673.

J. Lizarraga, J. Urrestilla, D. Daverio, M. Hindmarsh, M. Kunz, New CMB constraints for Abelian Higgs cosmic strings, Journal of Cosmology and Astroparticle Physics, DOI 10.1088/1475-7516/2016/10/042.

Alexey Kuvshinov, ETH Zurich

M. Kruglyakov, A. Geraskin, A. Kuvshinov, Novel accurate and scalable 3-D MT forward solver based on a contracting integral equation method, Computers & Geosciences, DOI 10.1016/j.cageo.2016.08.017.

Matthias Liebendörfer, University of Basel

K. C. Pan, M. Liebendörfer, M. Hempel, F. K. Thielemann, Two-dimensional core-collapse supernova simulations with the isotropic diffusion source approximation for neutrino transport, The Astrophysical Journal, DOI 10.3847/0004-637x/817/1/72.

A. Perego, R. M. Cabezón, R. Käppeli, An advanced leakage scheme for neutrino treatment in astrophysical simulations, Astrophysical Journal Supplement Series, DOI 10.3847/0067-0049/223/2/22.

R. Käppeli, S. Mishra, A well-balanced finite volume scheme for the Euler equations with gravitation - The exact preservation of hydrostatic equilibrium with arbitrary entropy stratification, Astronomy & Astrophysics, DOI 10.1051/0004-6361/201527815.

Vittorio Limongelli, Università della Svizzera italiana

M. Lelimousin, V. Limongelli, M. S. P. Sansom, Conformational changes in the epidermal growth factor receptor: role of the transmembrane domain investigated by coarse-grained metadynamics free energy, Journal of the American Chemical Society, DOI 10.1021/jacs.6b05602.

F. Comitani, V. Limongelli, C. Molteni, The free energy landscape of GABA binding to a pentameric ligand-gated ion channel and its disruption by mutations, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00303.

Ulrike Lohmann, ETH Zurich

B. Gasparini, U. Lohmann, Why cirrus cloud seeding cannot substantially cool the planet, Journal of Geophysical Research-Atmospheres, DOI 10.1002/2015jd024666.

F. Glassmeier, U. Lohmann, Constraining precipitation susceptibility of warm-, ice-, and mixed-phase clouds with microphysical equations, Journal of the Atmospheric Sciences, DOI 10.1175/Jas-D-16-0008.1.

U. Lohmann, J. Henneberger, O. Henneberg, J. P. Fugal, J. Buhl, Z. A. Kanji, Persistence of orographic mixed-phase clouds, Geophysical Research Letters, DOI 10.1002/2016gl071036.

T. N. Dallafior, D. Folini, R. Knutti, M. Wild, Mixed-layer ocean responses to anthropogenic aerosol dimming from 1870 to 2000, Journal of Geophysical Research-Atmospheres, DOI 10.1002/2015jd024070.

V. Lembo, D. Folini, M. Wild, P. Lionello, Energy budgets and transports: global evolution and spatial patterns during the twentieth century as estimated in two AMIP-like experiments, Climate Dynamics, DOI 10.1007/s00382-016-3173-9.

Alessandro Lomi, Università della Svizzera italiana

M. Byshkin, A. Stivala, A. Mira, R. Krause, G. Robins, A. Lomi, Auxiliary parameter MCMC for exponential random graph models, Journal of Statistical Physics, DOI 10.1007/s10955-016-1650-5.

Sandra Luber, University of Zurich

F. H. Hodel, S. Luber, Redox-inert cations enhancing water oxidation activity: the crucial role of flexibility, ACS Catalysis, DOI 10.1021/acscatal.6b01218.

F. H. Hodel, S. Luber, What influences the water oxidation activity of a bioinspired molecular (Co4O4)-O-II cubane? An in-depth exploration of catalytic pathways, ACS Catalysis, DOI 10.1021/acscatal.5b02507.

Y. Li, O. Blacque, T. Fox, S. Luber, W. Polit, R. F. Winter, K. Venkatesan, H. Berke, Electronic communication in phosphine substituted bridged dirhenium complexes - clarifying ambiguities raised by the redox non-innocence of the C4H2- and C-4-bridges, Dalton Transactions, DOI 10.1039/c5dt04768d.

S. Luber, Sum frequency generation of acetonitrile on a rutile (110) surface from density functional theory-based molecular dynamics, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.6b02530.

P. Oulevey, S. Luber, B. Varnholt, T. Burgi, Symmetry breaking in chiral ionic liquids evidenced by vibrational optical activity, Angewandte Chemie-International Edition, DOI 10.1002/anie.201605792.

D. Scherrer, M. Schilling, S. Luber, T. Fox, B. Spingler, R. Alberto, C. J. Richmond, Ruthenium water oxidation catalysts containing the non-planar tetradentate ligand, biisoquinoline dicarboxylic acid ($biqaH_2$), Dalton Transactions, DOI 10.1039/c6dt03880h.

M. Schilling, G. R. Patzke, J. Hutter, S. Luber, Computational investigation and design of cobalt aqua complexes for homogeneous water oxidation, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.6b00712.

Mathieu Luisier, ETH Zurich

D. Bozyigit, N. Yazdani, M. Yarema, O. Yarema, W. M. M. Lin, S. Volk, K. Vuttivorakulchai, M. Luisier, F. Juranyi, V. Wood, Soft surfaces of nanomaterials enable strong phonon interactions, Nature, DOI 10.1038/nature16977.

A. Emboras, B. Cheng, P. Ma, C. Haffner, Y. Salamin, C. Hoessbacher, W. Heni, Y. Fedoryshyn, A. Pedersen, M. Luisier, J. Leuthold, Atomic scale plasmonic switch, Nano Letters, DOI 10.1021/acs.nanolett.5b04537.

M. Luisier, R. Rhyner, A. Szabo, A. Pedersen, Atomistic simulation of nanodevices, International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), DOI 10.1109/SISPAD.2016.7605202.

R. Rhyner, M. Luisier, Minimizing self-heating and heat dissipation in ultrascaled nanowire transistors, Nano Letters, DOI 10.1021/acs.nanolett.5b04071.

A. Ziegler, M. Frey, L. Smith, M. Luisier, A nonparabolic bandstructure model for computationally efficient quantum transport simulations, IEEE Transactions on Electron Devices, DOI 10.1109/Ted.2016.2542522.

Nicola Marzari, EPF Lausanne

A. Cepellotti, N. Marzari, Thermal transport in crystals as a kinetic theory of relaxons, Physical Review X, DOI 10.1103/PhysRevX.6.041013.

A. Chandrasekaran, X. K. Wei, L. Feigl, D. Damjanovic, N. Setter, N. Marzari, Asymmetric structure of 90 degrees domain walls and interactions with defects in $PbTiO_3$, Physical Review B, DOI 10.1103/PhysRevB.93.144102.

G. Fisicaro, L. Genovese, O. Andreussi, N. Marzari, S. Goedecker, A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments, Journal of Chemical Physics, DOI 10.1063/1.4939125.

M. Fronzi, Y. Tateyama, N. Marzari, M. Nolan, E. Traversa, First-principles molecular dynamics simulations of proton diffusion in cubic $BaZrO_3$ perovskite under strain conditions, Materials for Renewable and Sustainable Energy, DOI 10.1007/s40243-016-0078-9.

J. B. Hu, G. M. Vanacore, A. Cepellotti, N. Marzari, A. H. Zewail, Rippling ultrafast dynamics of suspended 2D monolayers, graphene, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1613818113.

T. Y. Kim, C. H. Park, N. Marzari, The electronic thermal conductivity of graphene, Nano Letters, DOI 10.1021/acs.nanolett.5b05288.

K. Lejaeghere, G. Bihlmayer, T. Bjorkman, P. Blaha, S. Blugel, et al., Reproducibility in density functional theory calculations of solids, Science, DOI 10.1126/science.aad3000.

N. Marzari, Materials modelling: the frontiers and the challenges, Nature Materials, DOI 10.1038/nmat4613.

N. L. Nguyen, G. Borghi, A. Ferretti, N. Marzari, First-principles photoemission spectroscopy of dna and rna nucleobases from koopmans-compliant functionals, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00145.

G. Pizzi, A. Cepellotti, R. Sabatini, N. Marzari, B. Kozinsky, AiiDA: automated interactive infrastructure and database for computational science, Computational Materials Science, DOI 10.1016/j.commatsci.2015.09.013.

G. Pizzi, M. Gibertini, E. Dib, N. Marzari, G. Iannaccone, G. Fiori, Performance of arsenene and antimonene double-gate MOSFETs from first principles, Nature Communications, DOI 10.1038/ncomms12585.

Lucio Mayer, University of Zurich

S. Bonoli, L. Mayer, S. Kazantzidis, P. Madau, J. Bellovary, et al., Black hole starvation and bulge evolution in a Milky Way-like galaxy, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw694.

J. H. Kim, O. Agertz, R. Teyssier, M. J. Butler, D. Ceverino, et al., The Agora high-resolution galaxy simulations comparison project. Ii. Isolated disk test, Astrophysical Journal, DOI 10.3847/1538-4357/833/2/202.

A. Lupi, F. Haardt, M. Dotti, D. Fiacconi, L. Mayer, P. Madau, Growing massive black holes through supercritical accretion of stellar-mass seeds, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stv2877.

L. Mayer, T. Peters, J. E. Pineda, J. Wadsley, P. Rogers, Direct detection of precursors of gas giants formed by gravitational instability with the Atacama large millimeter/submillimeter array, Astrophysical Journal Letters, DOI 10.3847/2041-8205/823/2/L36.

L. Mayer, V. Tamburello, A. Lupi, B. Keller, J. Wadsley, P. Madau, Clumpy disks as a testbed for feedback-regulated galaxy formation, Astrophysical Journal Letters, DOI 10.3847/2041-8205/830/1/L13.

K. C. Pan, M. Liebendorfer, M. Hempel, F. K. Thielemann, Two-dimensional core-collapse supernova simulations with the isotropic diffusion source approximation for neutrino transport, the Astrophysical Journal, DOI 10.3847/0004-637x/817/1/72.

A. Sokolowska, L. Mayer, A. Babul, P. Madau, S. Shen, Diffuse coronae in cosmological simulations of milky way-sized galaxies, The Astrophysical Journal, DOI 10.3847/0004-637x/819/1/21.

C. Surville, L. Mayer, D. N. C. Lin, Dust capture and long-lived density enhancements triggered by vortices in 2D protoplanetary disks, The Astrophysical Journal, DOI 10.3847/0004-637x/831/1/82.

M. Tomozeiu, L. Mayer, T. Quinn, Tidal stirring of satellites with shallow density profiles prevents them from being too big to fail, Astrophysical Journal Letters, DOI 10.3847/2041-8205/827/1/L15.

M. Tomozeiu, L. Mayer, T. Quinn, The evolution of dwarf galaxy satellites with different dark matter density profiles in the erismod simulations. I. The early infalls, The Astrophysical Journal, DOI 10.3847/0004-637x/818/2/193.

F. M. Khan, D. Fiacconi, L. Mayer, P. Berczik, A. Just, Swift coalescence of supermassive black holes in cosmological mergers of massive galaxies, The Astrophysical Journal, DOI 10.3847/0004-637X/828/2/73.

D. Fiacconi, P. Madau, D. Potter, J. Stadel, Cold dark matter substructures in early-type galaxy halos, The Astrophysical Journal, DOI 10.3847/0004-637X/824/2/144.

Simon McIntosh-Smith, University of Bristol

D. Curran, C. B. Allen, S. McIntosh-Smith, D. Beckingsale, Towards portability for a compressible finite-volume CFD code, 54th AIAA Aerospace Sciences Meeting, AIAA SciTech Forum, DOI 10.2514/6.2016-1813.

T. Deakin, S. McIntosh-Smith, W. Gaudin, Many-core acceleration of a discrete ordinates transport mini-app at extreme scale, High Performance Computing: 31st International Conference, ISC High Performance 2016, Frankfurt, Germany, June 19-23, 2016, Proceedings, M. J. Kunkel, P. Balaji, and J. Dongarra, Eds. Cham: Springer International Publishing, DOI 10.1007/978-3-319-41321-1_22.

Siddhartha Mishra, ETH Zurich

R. Käppeli, S. Mishra, A well-balanced finite volume scheme for the Euler equations with gravitation –The exact preservation of hydrostatic equilibrium with arbitrary entropy stratification, Astronomy & Astrophysics, DOI 10.1051/0004-6361/201527815.

F. Leonardi, S. Mishra, C. Schwab, Numerical approximation of statistical solutions of planar, incompressible flows, Mathematical Models & Methods in Applied Sciences, DOI 10.1142/S0218202516500597.

S. Mishra, C. Schwab, J. Šukys, Multi-level Monte Carlo finite volume methods for uncertainty quantification of acoustic wave propagation in random heterogeneous layered medium, Journal of Computational Physics, DOI 10.1016/j.jcp.2016.02.014.

A. Perego, R. M. Cabezón, R. Käppeli, An advanced leakage scheme for neutrino treatment in astrophysical simulations, Astrophysical Journal Supplement Series, DOI 10.3847/0067-0049/223/2/22.

R. N. Gantner, A generic C++ library for multilevel quasi-Monte Carlo, Proceedings of the Platform for Advanced Scientific Computing Conference (PASC 16), DOI 10.1145/2929908.2929915.

MeteoSwiss

J. Bhend, I. Mahlstein, M. A. Liniger, Predictive skill of climate indices compared to mean quantities in seasonal forecasts. Quarterly Journal of the Royal Meteorological Society, DOI 10.1002/qj.2908.

Keller, D., A. Fischer, M. A. Liniger, C. Appenzeller, R. Knutti, Testing a weather generator for downscaling climate change projections over Switzerland, International Journal of Climatology, DOI 10.1002/joc.4750.

L. Panziera, M. Gabella, S. Zanini, A. Hering, U. Germann, A. Berne, A radar-based regional extreme rainfall analysis to derive the thresholds for a novel automatic alert system in Switzerland, Hydrology and Earth System Science, DOI 10.5194/hess-20-2317-2016.

Francesco Miniati, ETH Zurich

A. Beresnyak, F. Miniati, Turbulent amplification and structure of the intracluster magnetic field, The Astrophysical Journal, DOI 10.3847/0004-637X/817/2/127.

Dominik Obrist, University of Bern

M. O. John, D. Obrist, L. Kleiser, Secondary instability and subcritical transition of the leading-edge boundary layer, Journal of Fluid Mechanics, DOI 10.1017/jfm.2016.117.

D. Hupp, P. Arbenz, D. Obrist, A parallel Navier-Stokes solver using spectral discretisation in time, International Journal of Computational Fluid Dynamics, DOI 10.1080/10618562.2016.1242725.

Kiryl Pakrouski, ETH Zurich

K. Pakrouski, M. Troyer, Y.-L. Wu, S. Das Sarma, M. R. Peterson, Enigmatic 12/5 fractional quantum Hall effect, Physical Review B, DOI 10.1103/PhysRevB.94.075108.

Andrea Parmigiani, Paul Scherrer Institute

A. Parmigiani, S. Faroughi, C. Huber, O. Bachmann, Y. Su, Bubble accumulation and its role in the evolution of magma reservoirs in the upper crust, Nature, DOI 10.1038/nature17401.

Michele Parrinello, Università della Svizzera italiana

C. Perego, F. Giberti, M. Parrinello, Chemical potential calculations in dense liquids using metadynamics, European Physical Journal-Special Topics, DOI 10.1140/epjst/e2016-60094-x.

J. Mccarty, O. Valsson, M. Parrinello, Bespoke bias for obtaining free energy differences within variationally enhanced sampling, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00125.

M. Salvalaglio, P. Tiwary, G. M. Maggioni, M. Mazzotti, M. Parrinello, Overcoming time scale and finite size limitations to compute nucleation rates from small scale well tempered metadynamics simulations, Journal of Chemical Physics, DOI 10.1063/1.4966265.

P. Shaffer, O. Valsson, M. Parrinello, Hierarchical protein free energy landscapes from variationally enhanced sampling, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00786.

F. Palazzesi, M. Salvalaglio, A. Barducci, M. Parrinello, Communication: role of explicit water models in the helix folding/unfolding processes, Journal of Chemical Physics, DOI 10.1063/1.4963340.

M. Bon, T. Laino, A. Curioni, M. Parrinello, Characterization of vanadium species in mixed chloride-sulfate solutions: an abinizio metadynamics study, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.6b02642.

A. Ardevol, F. Palazzesi, G. A. Tribello, M. Parrinello, General protein data bank-based collective variables for protein folding, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.5b00714.

Alfredo Pasquarello, EPF Lausanne

J. Wiktor, A. Pasquarello, Absolute deformation potentials of two-dimensional materials, Physical Review B, DOI 10.1103/PhysRevB.94.245411.

W. Chen, F. Ambrosio, G. Miceli, A. Pasquarello, Ab initio electronic structure of liquid water, Physical Review Letters, DOI 10.1103/PhysRevLett.117.186401.

Z. D. Guo, F. Ambrosio, A. Pasquarello, Oxygen defects in amorphous Al2O3: a hybrid functional study, Applied Physics Letters, DOI 10.1063/1.4961125.

G. Miceli, J. Hutter, A. Pasquarello, Liquid water through density-functional molecular dynamics: plane-wave vs atomic-orbital basis sets, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00271.

F. Ambrosio, G. Miceli, A. Pasquarello, Structural, dynamical, and electronic properties of liquid water: a hybrid functional study, Journal of Physical Chemistry B, DOI 10.1021/acs.jpcb.6b03876.

G. Miceli, A. Pasquarello, Self-compensation due to point defects in Mg-doped GaN, Physical Review B, DOI 10.1103/PhysRevB.93.165207.

D. Colleoni, A. Pasquarello, Oxygen defects in GaAs: a hybrid functional study, Physical Review B, DOI 10.1103/PhysRevB.93.125208.

Andreas Pedersen, ETH Zurich

T. Bunjaku, A. Pedersen, M. Luisier, Diffusion mechanisms in $Li_{0.5}CoO_2$ – A computational study, Applied Physics Letters, DOI 10.1063/1.4945689.

Albino Perego, University of Basel

A. Perego, R. M. Cabezón, R. Käppeli, An advanced leakage scheme for neutrino treatment in astrophysical simulations, Astrophysical Journal Supplement Series, DOI 10.3847/0067-0049/223/2/22.

Y. L. Zhu, A. Perego, G. C. McLaughlin, Matter-neutrino resonance transitions above a neutron star merger remnant, Physical Review D, DOI 10.1103/PhysRevD.94.105006.

Carlo A. Pignedoli, EMPA

A. Verdini, P. Shinde, G. L. Montanari, S. T. Suran-Brunelli, M. Caputo, et al., Water formation for the metalation of porphyrin molecules on oxidized Cu(111), Chemistry-a European Journal, DOI 10.1002/chem.201602105.

S. Y. Wang, L. Talirz, C. A. Pignedoli, X. L. Feng, K. Mullen, et al., Giant edge state splitting at atomically precise graphene zigzag edges, Nature Communications, DOI 10.1038/ncomms11507.

P. Ruffieux, S. Y. Wang, B. Yang, C. Sanchez-Sanchez, J. Liu, et al., On-surface synthesis of graphene nanoribbons with zigzag edge topology, Nature, DOI 10.1038/nature17151.

A. Basagni, G. Vasseur, C. A. Pignedoli, M. Vilas-Varela, D. Pena, et al., Tunable band alignment with unperturbed carrier mobility of on-surface synthesized organic semiconducting wires, ACS Nano, DOI 10.1021/acsnano.5b07683.

L. Talirz, P. Shinde, D. Passerone, C. A. Pignedoli, Synthesis of atomically precise graphene-based nanostructures: a simulation point of view, On-Surface Synthesis, DOI 10.1007/978-3-319-26600-8_12.

Igor Pivkin, Università della Svizzera italiana

I. V. Pivkin, Z. Peng, G. E. Karniadakis, P. A. Buffet, M. Dao, S. Suresh, Biomechanics of red blood cells in human spleen and consequences for physiology and disease, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.1606751113.

E. K. Peter, I. V. Pivkin, J. E. Shea, A canonical replica exchange molecular dynamics implementation with normal pressure in each replica, Journal of Chemical Physics, DOI 10.1063/1.4958325.

E. K. Peter, J. E. Shea, I. V. Pivkin, Coarse kMC-based replica exchange algorithms for the accelerated simulation of protein folding in explicit solvent, Physical Chemistry Chemical Physics, DOI 10.1039/c5cp06867c.

Alfio Quarteroni, EPF Lausanne

S. Deparis, D. Forti, P. Gervasio, A. Quarteroni, INTERNODES: an accurate interpolation-based method for coupling the Galerkin solutions of PDEs on subdomains featuring non-conforming interfaces, Computers & Fluids, DOI 10.1016/j.compfluid.2016.03.033.

S. Deparis, D. Forti, G. Grandperrin, A. Quarteroni, FaCSI: A block parallel preconditioner for fluid-structure interaction in hemodynamics, Journal of Computational Physics, DOI 10.1016/j.jcp.2016.10.005.

S. Deparis, D. Forti, A. Quarteroni, A fluid-structure interaction algorithm using radial basis function interpolation between non-conforming interfaces. in advances in computational fluid-structure interaction and flow simulation: new methods and challenging computations, Y. Bazilevs and K. Takizawa eds., DOI 10.1007/978-3-319-40827-9_34.

Christoph C. Raible, University of Bern

C. Camenisch, K. M. Keller, M. Salvisberg, B. Amann, M. Bauch, et al., The 1430s: a cold period of extraordinary internal climate variability during the early Sporer Minimum with social and economic impacts in north-western and central Europe, Climate of the Past, DOI 10.5194/cp-12-2107-2016.

A. Landais, V. Masson-Delmotte, E. Capron, P. M. Langebroek, P. Bakker, E. J. Stone, N. Merz, C. C. Raible, H. Fischer, A. Orsi, F. Prie, B. Vinther, D. Dahl-Jensen, How warm was Greenland during the last interglacial period?, Climate of the Past, DOI 10.5194/cp-12-1933-2016.

N. Merz, A. Born, C. C. Raible, T. F. Stocker, Warm Greenland during the last interglacial: the role of regional changes in sea ice cover, Climate of the Past, DOI 10.5194/cp-12-2011-2016.

C. C. Raible, S. Brönnimann, R. Auchmann, P. Brohan, T. L. Frolicher, H. F. Graf, P. Jones, J. Luterbacher, S. Muthers, R. Neukom, A. Robock, S. Self, A. Sudrajat, C. Timmreck, M. Wegmann, Tambora 1815 as a test case for high impact volcanic eruptions: Earth system effects, Wiley Interdisciplinary Reviews-Climate Change, DOI 10.1002/wcc.407.

P. Stucki, S. Dierer, C. Welker, J. J. Gómez-Navarro, C. C. Raible, O. Martius, S. Brönnimann, Evaluation of downscaled wind speeds and parameterised gusts for recent and historical windstorms in Switzerland, Tellus Series a-Dynamic Meteorology and Oceanography, DOI 10.3402/tellusa.v68.31820.

M. O. Chikamoto, A. Timmermann, M. Yoshimori, F. Lehner, A. Laurian, A. Abe-Ouchi, A. Mouchet, F. Joos, C. C. Raible, K. M. Cobb, Intensification of tropical Pacific biological productivity due to volcanic eruptions, Geophysical Research Letters, DOI 10.1002/2015GL067359.

Paolo Ricci, EPF Lausanne

R. Jorge, P. Ricci, F. D. Halpern, N. F. Loureiro, C. Silva, Plasma turbulence in the scrape-off layer of the ISTTOK tokamak, Physics of Plasmas, DOI 10.1063/1.4964783.

F. Militello, N. R. Walkden, T. Farley, W. A. Gracias, J. Olsen, F. Riva, L. Easy, N. Fedorczak, I. Lupelli, J. Madsen, A. H. Nielsen, P. Ricci, P. Tamain, J. Young, Multi-code analysis of scrape-off layer filament dynamics in MAST, Plasma Physics and Controlled Fusion, DOI 10.1088/0741-3335/58/10/105002.

F. D. Halpern, P. Ricci, S. Jolliet, J. Loizu, J. Morales, A. Mosetto, F. Musil, F. Riva, T. M.. Tran, C. Wersal, The GBS code for tokamak scrape-off layer simulations, Journal of Computational Physics, DOI 10.1016/j.jcp.2016.03.040.

F. Riva, C. Colin, J. Denis, L. Easy, I. Furno, J. Madsen, F. Militello, V. Naulin, A. H. Nielsen, J. M. B. Olsen, J. T. Omotani, J. J. Rasmussen, P. Ricci, E. Serre, P. Tamain, C. Theiler, Blob dynamics in the TORPEX experiment: a multi-code validation, Plasma Physics and Controlled Fusion, DOI 10.1088/0741-3335/58/4/044005.

Marcello Righi, Zurich University of Applied Science

M. Righi, RANS-LES hybrid turbulence modelling for aeroelastic problems: test case 3, the Second AIAA Aeroelastic Prediction Workshop, 34th AIAA Applied Aerodynamics Conference. AIAA AVIATION Forum, American Institute of Aeronautics and Astronautics, DOI 10.2514/6.2016-3264.

M. Righi, M. Berci, M. Franciolini, A. Da Ronch, A subsonic indicial aerodynamics for the unsteady loads of trapezoidal wings, 34th AIAA Applied Aerodynamics Conference. AIAA AVIATION Forum. American Institute of Aeronautics and Astronautics, DOI 10.2514/6.2016-4165.

Ursula Röthlisberger, EPF Lausanne

E. Brunk, M. a. S. Perez, P. Athri, U. Röthlisberger, Genetic-algorithm-based optimization of a peptidic scaffold for sequestration and hydration of CO_2, ChemPhysChem, DOI 10.1002/cphc.201601034.

Z. J. Ma, G. Palermo, Z. Adhireksan, B. S. Murray, T. Von Erlach, P. J. Dyson, U. Röthlisberger, C. A. Davey, An Organometallic compound which exhibits a DNA topology-dependent one-stranded intercalation mode, Angewandte Chemie-International Edition, DOI 10.1002/anie.201602145.

G. Palermo, A. Magistrato, T. Riedel, T. Von Erlach, C. A. Davey, P. J. Dyson, U. Röthlisberger, Fighting cancer with transition metal complexes: from naked DNA to protein and chromatin targeting strategies, ChemMedChem, DOI 10.1002/cmdc.201500478.

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?, The Journal of Physical Chemistry B, DOI 10.1021/acs.jpcb.6b08339.

L. Casalino, G. Palermo, N. Abdurakhmonova, U. Röthlisberger, A. Magistrato, Development of site-specific Mg2+-RNA force field parameters, a dream or a reality? Guidelines from combined molecular dynamics and quantum mechanics simulations, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00905.

S. C. van Keulen, U. Röthlisberger, Effect of N-terminal myristoylation on the active conformation of Gαi1-GTP, Biochemistry, DOI 0.1021/acs.biochem.6b00388.

M. I. Dar, G. Jacopin, S. Meloni, A. Mattoni, N. Arora, A. Boziki, S. M. Zakeeruddin, U. Röthlisberger, M. Grätzel, Origin of unusual bandgap shift and dual emission in organic-inorganic lead halide perovskites, Science Advances, DOI 10.1126/sciadv.1601156.

W. Tress, B. Beyer, N. A. Astani, F. Gao, S. Meloni, U. Röthlisberger, Extended intermolecular interactions governing photocurrent-voltage relations in ternary organic solar cells, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.6b01962.

S. Meloni, G. Palermo, N. Ashari-Astani, M. Grätzel, U. Röthlisberger, Valence and conduction band tuning in halide perovskites for solar cell applications, Journal of Materials Chemistry A, DOI 10.1039/c6ta04949d.

C. Y. Yi, J. S. Luo, S. Meloni, A. Boziki, N. Ashari-Astani, C. Grätzel, S. M. Zakeeruddin, U. Röthlisberger, M. Grätzel, Entropic stabilization of mixed A-cation ABX_3 metal halide perovskites for high performance perovskite solar cells, Energy & Environmental Science, DOI 10.1039/c5ee03255e.

S. Meloni, T. Moehl, W. Tress, M. Franckevičius, M. Saliba, Y. H. Lee, P. Gao, M. K. Nazeeruddin, S. M. Zakeeruddin, U. Röthlisberger, M. Grätzel, Ionic polarization-induced current-voltage hysteresis in CH3NH3PbX3 perovskite solar cells, Nature Communications, DOI 10.1038/ncomms10334.

S. Mathew, N. A. Astani, B. F. E. Curchod, J. H. Delcamp, M. Marszalek, J. Frey, U. Röthlisberger, M. K. Nazeeruddin, M. Grätzel, Synthesis, characterization and ab-inizio investigation of a panchromatic ullazine-porphyrin photosensitizer for dye-sensitized solar cells, Journal of Materials Chemistry A, DOI 10.1039/c5ta08728g.

Yohei Sato, Paul Scherrer Institute

J. Murallidharan, G. Giustini, Y. Sato, B. Niceno, V. Badalassi, S. P. Walker, CFD simulation of single bubble growth under high pressure pool boiling conditions, Nuclear Engineering and Technology, DOI 10.1016/j.net.2016.06.004.

Christoph Schär, ETH Zurich

O. Bellprat, S. Kotlarski, D. Lüthi, R. De Elia, A. Frigon, R. Laprise, C. Schär, Objective calibration of regional climate models: application over Europe and North America, Journal of Climate, DOI 10.1175/Jcli-D-15-0302.1.

F. Giorgi, C. Torma, E. Coppola, N. Ban, C. Schär, S. Somot, Enhanced summer convective rainfall at Alpine high elevations in response to climate warming, Nature Geoscience, DOI 10.1038/Ngeo2761.

H. Hassanzadeh, J. Schmidli, W. Langhans, L. Schlemmer, C. Schär, Impact of topography on the diurnal cycle of summertime moist convection in idealized simulations, Meteorologische Zeitschrift, DOI 10.1127/metz/2015/0653.

M. Keller, O. Fuhrer, J. Schmidli, M. Stengel, R. Stockli, C. Schär, Evaluation of convection-resolving models using satellite data: the diurnal cycle of summer convection over the Alps, Meteorologische Zeitschrift, DOI 10.1127/metz/2015/0715.

D. Leutwyler, O. Fuhrer, X. Lapillonne, D. Lüthi, C. Schär, Towards European-scale convection-resolving climate simulations with GPUs: a study with COSMO 4.19, Geoscientific Model Development, DOI 10.5194/gmd-9-3393-2016.

A. Possner, E. Zubler, U. Lohmann, C. Schär, The resolution dependence of cloud effects and ship-induced aerosol-cloud interactions in marine stratocumulus, Journal of Geophysical Research-Atmospheres, DOI 10.1002/2015jd024685.

C. Schär, N. Ban, E. M. Fischer, J. Rajczak, J. Schmidli, Frei, C. F. Giorgi, T. R. Karl, E. J. Kendon, A. M. G. K. Tank, P. A. O'Gorman, J. Sillmann, X. B. Zhang, F. W. Percentile indices for assessing changes in heavy precipitation events, Climatic Change, DOI 10.1007/s10584-016-1669-2.

A. Casanueva, S. Kotlarski, S. Herrera, J. Fernandez, J.M. Gutierrez, F. Boberg, A. Colette, O.B. Christensen, K. Goergen, D. Jacob, K. Keuler, G. Nikulin, C. Teichmann, R. Vautard, Daily precipitation statistics in a EURO-CORDEX RCM ensemble: added value of raw and bias-corrected high-resolution simulations. Climate Dynamics, DOI 10.1007/s00382-015-2865-x.

T. N. Dallafior, D. Folini, R. Knutti, M. Wild, Mixed-layer ocean responses to anthropogenic aerosol dimming from 1870 to 2000, Journal of Geophysical Research Atmospheres, DOI 10.1002/2015JD024070.

F. Hourdin, T. Mauritsen, A. Gettelmann, J.-C. Golaz, V. Balaji, Q. Duan, D. Folini, D. Ji, D. Klocke, Y. Qian, F. Rauser, C. Rio, L. Tomassini, M. Watanabe, D. Williamson, The art and sciences of climate model tuning, Bulletin of the American Meteorological Society: BAMS, DOI 10.1175/BAMS-D-15-00135.1.

K. Keuler, K. Radtke, S. Kotlarski, D. Lüthi, Regional climate change over Europe in COSMO-CLM: influence of emission scenario and driving global model, Meteorologische Zeitschrift, DOI 10.1127/metz/2016/0662.

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

V. Lembo, D. Folini, M. Wild, Martin, P. Lionello, Energy budgets and transports: global evolution and spatial patterns during the twentieth century as estimated in two AMIP-like experiments, Climate Dynamics, DOI 10.1007/s00382-016-3173-9.

A. Meyer, D. S. Folini, U. Lohmann, T. Peter, Thomas, Tropical temperature and precipitation responses to large volcanic eruptions: observations and AMIP5 simulations, Journal of Climate, DOI 10.1175/JCLI-D-15-0034.1.

D. Panosetti, S. Böing, L. Schlemmer, J. Schmidli, Idealized large-eddy and convection-resolving simulations of moist convection over mountainous terrain, Journal of the Atmospehric Sciences, DOI 10.1175/JAS-D-15-0341.1.

J. Rajczak, S. Kotlarski, C. Schär, Does quantile mapping of simulated precipitation correct for biases in transition probabilities and spell lengths?, Journal of Climate, DOI 10.1175/Jcli-D-15-0162.1.

I. Tobin, S. Jerez, R. Vautard, F. Thais, E. van Meijgaard, A. Prein, M. Deque, S. Kotlarski, C.F. Maule, G. Nikulin, T. Noel, C. Teichmann, Climate change impacts on the power generation potential of a European mid-century wind farms scenario, Environmental Research Letters, DOI 10.1088/1748-9326/11/3/034013.

K. J. P. M. Winter, S. Kotlarski, S. C. Scherrer, C. Schär, The Alpine snow-Albedo feedback in regional climate models, Climate Dynamics, DOI 10.1007/s00382-016-3130-7.

Olaf Schenk, Università della Svizzera italiana

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. De Coninck, B. Baets, D. Kourounis, F. Verbosio, O. Schenk, S. Maenhout, J. Fostier, Needles: large-scale genomic prediction with marker-by-environment interaction, Journal of Genetics, DOI 10.1534/genetics.115.179887.

L. Riha, T. Brzobohaty, A. Markopoulos, T. Kozubek, O. Schenk, W. Vanroose, Efficient implementation of FETI solver for multi and many-core architectures using Schur complements, Proceedings of the International Conference on High Performance Computing in Science and Engineering, HPCSE2015, Lecture Notes in Computer Science (LNCS), DOI 10.1007/978-3-319-40361-8_6.

Aurel Schneider, University of Zurich

A. Schneider, R. Teyssier, D. Potter, J. Stadel, J. Onions, D. S. Reed, R. E. Smith, V. Springel, F. R. Pearce, R. Scoccimarro, Matter power spectrum and the challenge of percent accuracy Journal of Cosmology and Astroparticle Physics, DOI 10.1088/1475-7516/2016/04/047.

Julien Seguinot, ETH Zurich

J. Seguinot, I. Rogozhina, A. P. Stroeven, M. Margold, and J. Kleman, Numerical simulations of the Cordilleran ice sheet through the last glacial cycle, The Cryosphere, DOI 10.5194/tc-10-639-2016, 2016.

Sonia I. Seneviratne, ETH Zurich

W. Thiery, E. L. Davin, S. I. Seneviratne, K. Bedka, S. Lhermitte, N. P. M. van Lipzig Hazardous thunderstorm intensification over Lake Victoria, Nature Communications, DOI 10.1038/ncomms 12786.

S. Mystakidis, E. L. Davin, N. Gruber, S. I. Seneviratne, Constraining future terrestrial carbon cycle projections using observation-based water and carbon flux estimates, Global Change Biology, DOI 10.1111/gcb.13217.

E. L. Davin, E. Maisonnave, S. I. Seneviratne, Is land surface processes representation a possible weak link in current Regional Climate Models?, Environmental Research Letters, DOI 10.1088/1748-9326/11/7/074027.

James J. Shepherd, MIT

F. D. Malone, N. S. Blunt, E. W. Brown, D. K. K. Lee, J. S. Spencer, W. M. C. Foulkes, J. J. Shepherd, Accurate exchange-correlation energies for the warm dense electron gas, Physical Review Letters, DOI 10.1103/PhysRevLett.117.115701.

T. Dornheim, S. Groth, T. Sjostrom, F. D. Malone, W. M. C. Foulkes, M. Bonitz, Ab Initio quantum Monte Carlo simulation of the warm dense electron gas in the thermodynamic limit, Physical Review Letters, DOI 10.1103/PhysRevLett.117.156403.

Gabriele Sosso, University College London

G.C. Sosso, T. Li, D. Donadio, G. A. Tribello, A. Michaelides, Microscopic mechanism and kinetics of ice formation at complex interfaces: zooming in on kaolinite, The Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.6b01013.

Nicola A. Spaldin, ETH Zurich

F. Thöle, M. Fechner, N. A. Spaldin, First-principles calculation of the bulk magnetoelectric monopole density: Berry phase and Wannier function approaches, Physical Review B, DOI 10.1103/PhysRevB.93.195167.

G. H. Olsen, U. Aschauer, N. A. Spaldin, S. M. Selbach, T. Grande, Origin of ferroelectric polarization in tetragonal tungsten-bronze-type oxides, Physical Review B, DOI 10.1103/PhysRevB.93.180101.

M. Fechner, M. J. A. Fierz, F. Thöle, U. Staub, N. A. Spaldin, Quasistatic magnetoelectric multipoles as order parameter for pseudogap phase in cuprate superconductors, Physical Review B, DOI 10.1103/PhysRevB.93.174419.

D. Mazumdar, R. Knut, F. Thöle, M. Gorgoi, S. Faleev, O. N. Mryasov, V. Shelke, C. Ederer, N. A. Spaldin, A. Gupta, O. Karis, The valence band electronic structure of rhombohedral-like and tetragonal-like $BiFeO_3$ thin films from hard X-ray photoelectron spectroscopy and first-principles theory, Journal of Electron Spectroscopy and Related Phenomena, DOI 10.1016/j.elspec.2015.10.002.

M. Ruminy, M. N. Valdez, B. Wehinger, A. Bosak, D. T. Adroja, U. Stuhr, K. Kamazawa, E. Pomjakushina, D. Prabakharan, M. K. Haas, L. Bovo, D. Sheptyakov, A. Cervellino, R. J. Cava, M. Kenzelmann, N. A. Spaldin, T. Fennell, First-principles calculation and experimental investigation of lattice dynamics in the rare-earth pyrochlores $R_2Ti_2O_7$ (R = Tb, Dy, Ho), Physical Review B, DOI 10.1103/PhysRevB.93.214308.

J. Heidler, M. Fechner, R. V. Chopdekar, C. Piamonteze, J. Dreiser, C. A. Jenkins, E. A. Arenholz, S. Rusponi, H. Brune, N. A. Spaldin, F. Nolting, Magnetoelectroelastic control of magnetism in an artificial multiferroic, Physical Review B, DOI 10.1103/PhysRevB.94.014401.

A. Marthinsen, C. Faber, U. Aschauer, N. A. Spaldin, S. M. Selbach, Coupling and competition between ferroelectricity, magnetism, strain, and oxygen vacancies in AMnO3 perovskites, MRS Communications, DOI 10.1557/mrc.2016.30.

P. Giraldo-Gallo, B. Sangiorgio, P. Walmsley, H. J. Silverstein, M. Fechner, S. C. Riggs, T. H. Geballe, N. A. Spaldin, I. R. Fisher, Fermi surface evolution of Na-doped PbTe studied through density functional theory calculations and Shubnikov-de Haas measurements, Physical Review B, DOI 10.1103/PhysRevB.94.195141.

U. Aschauer, R. Braddell, S. A. Brechbühl, P. M. Derlet, N. A. Spaldin, Strain-induced structural instability in FeRh, Physical Review B Condensed Matter and Materials Physics, DOI 10.1103/PhysRevB.94.014109.

G. Sclauzero, K. Dymkowski, C. Ederer, Tuning the metal-insulator transition in d1 and d2 perovskites by epitaxial strain: A first-principles-based study, Physical Review B, DOI 10.1103/PhysRevB.94.245109.

A. Y. Birenbaum, C. Ederer, Controlling the cation distribution and electric polarization with epitaxial strain in Aurivillius-phase Bi5FeTi3O15, Applied Physics Letters, DOI 10.1063/1.4942668.

Oskar Steiner, IRSOL

F. Calvo, O. Steiner, B. Freytag, Non-magnetic photospheric bright points in 3D simulations of the solar atmosphere, Astronomy & Astrophysics, DOI 10.1051/0004-6361/201628649.

Andras Stirling, Hungarian Academy of Sciences

A. Stirling, T. Rozgonyi, M. Krack, M. Bernasconi, Prebiotic NH_3 formation: insights from simulations, Inorganic Chemistry, DOI 10.1021/acs.inorgchem.5b02911.

Paul Tackley, ETH Zurich

D. A. May, P. Sanan, K. Rupp, M. G. Knepley, B. F. Smith, Extreme-scale multigrid components within PETSc, Proceedings of the Platform for Advanced Scientific Computing Conference (PASC 16), DOI 10.1145/2929908.2929913.

P. Sanan, S. M. Schnepp, D. A. May, Pipelined, flexible Krylov subspace methods, SIAM Journal on Scientific Computing, DOI 10.1137/15M1049130.

H. Morgan, M. G. Knepley, P. Sanan, L. R. Scott, A stochastic performance model for pipelined Krylov methods, Concurrency Computation Practice and Experience, DOI 10.1002/cpe.3820.

Matthias Troyer, ETH Zurich

J. Imriška, L. Wang, M. Troyer, First-order topological phase transition of the Haldane-Hubbard model, Physical Review B, DOI 10.1103/PhysRevB.94.035109.

J. Imriška, E. Gull, M. Troyer, Thermodynamics of the Hubbard model on stacked honeycomb and square lattices, The European Physical Journal B, DOI 10.1140/epjb/e2016-70146-y.

William Tang, PPPL

W. Tang, B. Wang, S. Ethier, G. Kwasniewski, T. Hoefler, K. Ibrahim, K. Madduri, S. Williams, L. Oliker, C. Rosales-Fernandez, T. Williams, Extreme scale plasma turbulence simulations on top supercomputers worldwide, IEEE/ACM International Conference on High Performance Computing, Networking, Storage and Analysis (SC 16).

Romain Teyssier, University of Zurich

J. H. Kim, O. Agertz, R. Teyssier, M. J. Butler, D. Ceverino, et al., The Agora high-resolution galaxy simulations comparison project. Ii. Isolated disk test, The Astrophysical Journal, DOI 10.3847/1538-4357/833/2/202.

D. Martizzi, O. Hahn, H. Y. Wu, A. E. Evrard, R. Teyssier, R. H. Wechsler, Rhapsody-G simulations - II. Baryonic growth and metal enrichment in massive galaxy clusters, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw897.

F. Sembolini, P. J. Elahi, F. R. Pearce, C. Power, A. Knebe, et al., nIFTy galaxy cluster simulations - II. Radiative models, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw800.

W. G. Cui, C. Power, A. Knebe, S. T. Kay, F. Sembolini, et al., nIFTy galaxy cluster simulations - IV. Quantifying the influence of baryons on halo properties, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw603.

P. J. Elahi, A. Knebe, F. R. Pearce, C. Power, G. Yepes, et al., nIFTY galaxy cluster simulations - III. The similarity and diversity of galaxies and subhaloes, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw338.

F. Sembolini, G. Yepes, F. R. Pearce, A. Knebe, S. T. Kay, et al., nIFTy galaxy cluster simulations - I. Dark matter and non-radiative models, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw250.

M. Rieder, R. Teyssier, A small-scale dynamo in feedback-dominated galaxies as the origin of cosmic magnetic fields - I. The kinematic phase, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stv2985.

A. Schneider, R. Teyssier, D. Potter, J. Stadel, J. Onions, D. S. Reed, R. E. Smith, V. Springel, F. R. Pearce, R. Scoccimarro, Matter power spectrum and the challenge of percent accuracy, Journal of Cosmology and Astroparticle Physics, DOI 10.1088/1475-7516/2016/04/047.

Davide Tiana, EPF Lausanne

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

Joost VandeVondele, ETH Zurich

S. Andermatt, J. Cha, F. Schiffmann, J. Vandevondele, Combining linear-scaling dft with subsystem DFT in Born Oppenheimer and ehrenfest molecular dynamics simulations: from molecules to a virus in solution, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00398.

V. V. Rybkin, J. Vandevondele, Spin-unrestricted second-order Moller-Plesset (MP2) forces for the condensed phase: from molecular radicals to F-centers in solids, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.6b00015.

J. Cheng, J. Vandevondele, Calculation of electrochemical energy levels in water using the random phase approximation and a double hybrid functional, Physical Review Letters, DOI 10.1103/PhysRevLett.116.086402.

V. Kapil, J. Vandevondele, M. Ceriotti, Accurate molecular dynamics and nuclear quantum effects at low cost by multiple steps in real and imaginary time: Using density functional theory to accelerate wavefunction methods, Journal of Chemical Physics, DOI 10.1063/1.4941091.

M. H. Bani-Hashemian, S. Bruck, M. Luisier, J. Vandevondele, A generalized Poisson solver for first-principles device simulations, Journal of Chemical Physics, DOI 10.1063/1.4940796.

Martin van Driel, ETH Zurich

A. Khan, M. Van Driel, M. Bose, D. Giardini, S. Ceylan, Yan, J. Clinton, F. Euchner, P. Lognonne, N. Murdoch, D. Mimoun, M. Panning, M. Knapmeyer, W. B. Banerdt, Single-station and single-event marsquake location and inversion for structure using synthetic Martian waveforms, Physics of the Earth and Planetary Interiors, DOI 10.1016/j.pepi.2016.05.017.

K. D. Leng, T. Nissen-Meyer, M. Van Driel, Efficient global wave propagation adapted to 3-D structural complexity: a pseudospectral/spectral-element approach, Geophysical Journal International, DOI 10.1093/gji/ggw363.

P. M. Mai, D. Schorlemmer, M. Page, J. P. Ampuero, K. Asano, et al., The earthquake-source inversion validation (SIV) project, Seismological Research Letters, DOI 10.1785/0220150231.

Harry van Lenthe, ETH Zurich

S. D. Badilatti, P. Christen, I. Parkinson, R. Müller, Load-adaptive bone remodeling simulations reveal osteoporotic microstructural and mechanical changes in whole human vertebrae, Journal of Biomechanics, DOI 10.1016/j.jbiomech.2016.10.002.

S. D. Badilatti, P. Christen, A. Levchuk, J. H. Marangalou, B. Van Rietbergen, I. Parkinson, R. Müller, Large-scale microstructural simulation of load-adaptive bone remodeling in whole human vertebrae, Biomechanics and Modeling in Mechanobiology, DOI 10.1007/s10237-015-0715-8.

P. Christen, F. A. Schulte, A. Zwahlen, B. Van Rietbergen, S. Boutroy, L. J. Melton, S. Amin, S. Khosla, J. Goldhahn, R. Müller, Voxel size dependency, reproducibility and sensitivity of an in vivo bone loading estimation algorithm, Journal of the Royal Society Interface, DOI 10.1098/rsif.2015.0991.

M. R. Rubin, A. Zwahlen, D. W. Dempster, H. Zhou, N. E. Cusano, C. C. Zhang, R. Müller, J. P. Bilezikian, Effects of parathyroid hormone administration on bone strength in hypoparathyroidism, Journal of Bone and Mineral Research, DOI 10.1002/jbmr.2777.

N. Ohs, F. Keller, O. Blank, W.-Y. W. Lee, C.-Y. J. Cheng, P. Arbenz, R. Müller, P. Christen, Towards in silico prognosis using big data, Current Directions in Biomedical Engineering, DOI 10.1515/cdbme-2016-0016.

Franco Vazza, Hamburg Observatory

D. Wittor, F. Vazza, M. Brüggen, Studying the effect of shock obliquity on the gamma-ray and diffuse radio emission in galaxy clusters, Galaxies, DOI 10.3390/galaxies4040071.

S. Hackstein, F. Vazza, M. Brüggen, G. Sigl, A. Dundovic, Propagation of ultrahigh energy cosmic rays in extragalactic magnetic fields: a view from cosmological simulations, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw1903.

F. Vazza, D. Wittor, M. Brüggen, C. Gheller, On the non-thermal energy content of cosmic structures, Galaxies, DOI10.3390/galaxies4040060.

C. Gheller, F. Vazza, M. Brüggen, M. Alpaslan, B. W. Holwerda, A. M. Hopkins, J. Liske, Evolution of cosmic filaments and of their galaxy population from MHD cosmological simulations, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw1595.

F. Vazza, M. Bruggen, D. Wittor, C. Gheller, D. Eckert, M. Stubbe, Constraining the efficiency of cosmic ray acceleration by cluster shocks, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stw584.

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.

Laurent Villard, EPF Lausanne

A. Fasoli, S. Brunner, W. A. Cooper, J. P. Graves, P. Ricci, O. Sauter, L. Villard, Computational challenges in magnetic-confinement fusion physics, Nature Physics, DOI 10.1038/Nphys3744.

G. Merlo, O. Sauter, S. Brunner, A. Burckel, Y. Camenen, F. J. Casson, W. Dorland, E. Fable, T. Görler, F. Jenko, A.G. Peeters, D. Told, L. Villard, Linear multispecies gyrokinetic flux tube benchmarks in shaped tokamak plasmas, Physics of Plasmas, DOI 10.1063/1.4942539.

F. Hariri, T. M. Tran, A. Jocksch, E. Lanti, J. Progsch, P. Messmer, S. Brunner, C. Gheller, L. Villard, A portable platform for accelerated PIC codes and its application to GPUs using OpenACC, Computer Physics Communications, DOI 10.1016/j.cpc.2016.05.008.

N. Ohana, A. Jocksch, E. Lanti, T. M. Tran, S. Brunner, C. Gheller, F. Hariri, L. Villard, Towards the optimization of a gyrokinetic Particle-In-Cell (PIC) code on large-scale hybrid architectures, Journal of Physics: Conference Series, DOI 10.1088/1742-6596/775/1/012010.

E. Lanti, J. Dominski, S. Brunner, B. F. McMillan, L. Villard, Padé approximation of the adiabatic electron contribution to the gyrokinetic quasi-neutrality equation in the ORB5 code, Journal of Physics: Conference Series, DOI 10.1088/1742-6596/775/1/012006.

A. Mariani, G. Merlo, S. Brunner, A. Merle, O. Sauter, T. Görler, F. Jenko, D. Told, Characterization with microturbulence simulations of the zero particle flux condition in case of a TCV discharge showing toroidal rotation reversal, Journal of Physics: Conference Series, DOI 10.1088/1742-6596/775/1/012007.

A. Jocksch, F. Hariri, T.-M. Tran, S. Brunner, C. Gheller, L. Villard, A bucket sort algorithm for the particle-in-cell method on manycore architectures, Parallel Processing and Applied Mathematics, PPAM 2015. Lecture Notes in Computer Science, DOI 10.1007/978-3-319-32149-3_5.

Peter E. Vincent, Imperial College London

P. Vincent, F. Witherden, B Vermeire, J. S. Park, A. Iyer, Towards green aviation with Python at petascale, SC 16: International Conference for High Performance Computing, Networking, Storage and Analysis (SC 16), DOI 10.1109/SC.2016.1.

Oleg V. Yazyev, EPF Lausanne

G. Manzoni, L. Gragnaniello, G. Autes, T. Kuhn, A. Sterzi, F. Cilento, M. Zacchigna, V. Enenkel, I. Vobornik, L. Barba, F. Bisti, P. Bugnon, A. Magrez, V. N. Strocov, H. Berger, O. V. Yazyev, M. Fonin, F. Parmigiani, A. Crepaldi, Evidence for a strong topological insulator phase in $ZrTe_5$, Physical Review Letters, DOI 10.1103/PhysRevLett.117.237601.

B. Náfrádi, P. Szirmai, M. Spina, H. Lee, O. V. Yazyev, A. Arakcheeva, D. Chernyshov, M. Gibert, L. Forró and E. Horváth, Optically switched magnetism in photovoltaic perovskite $CH_3NH_3(Mn:Pb)I_3$, Nature Communications, DOI 10.1038/ncomms13406.

A. Luican-Mayer, J. E. Barrios-Vargas, J. T. Falkenberg, G. Autès, A. W. Cummings, D. Soriano, G. Li, M. Brandbyge, O. V. Yazyev, S. Roche, E. Y. Andrei, Localized electronic states at grain boundaries on the surface of graphene and graphite, 2D Materials 3, DOI 10.1088/2053-1583/3/3/031005.

G. Autès, D. Gresch, M. Troyer, A. A. Soluyanov, O. V. Yazyev, Robust type-II Weyl semimetal phase in transition metal diphosphides XP_2 (X=Mo, W), Physical Review Letters, DOI 10.1103/PhysRevLett.117.066402.

N. Virk, O. V. Yazyev, Dirac fermions at high-index surfaces of bismuth chalcogenide topological insulator nanostructures, Scientific Reports, DOI 10.1038/srep20220.

A. Pulkin, O. V. Yazyev, Spin- and valley-polarized transport across line defects in monolayer MoS_2, Physical Review B, DOI 10.1103/PhysRevB.93.041419.

Gerhard Wellein, Friedrich-Alexander University of Erlangen-Nuremberg

M. Kreutzer, J. Thies, A. Pieper, A. Alvermann, M. Galgon, M. Röhrig-Zöllner, F. Shahzad, A. Basermann, A. R. Bishop, H. Fehske, G. Hager, B. Lang, G. Wellein, Performance engineering and energy efficiency of building blocks for large, sparse eigenvalue computations on heterogeneous supercomputers, Software for Exascale Computing – SPPEXA, Lecture Notes in Computational Science and Engineering, DOI 10.1007/978-3-319-40528-5_14.

“Metadynamics simulations allow us to explore complex chemical or physical processes such as protein folding, phase transitions or changes in crystalline structure, which usually cannot be observed on the time scale of normal molecular dynamics simulations”.
Matthias Krack, Paul Scherrer Institute

Name
Matthias Krack

Position
Group leader

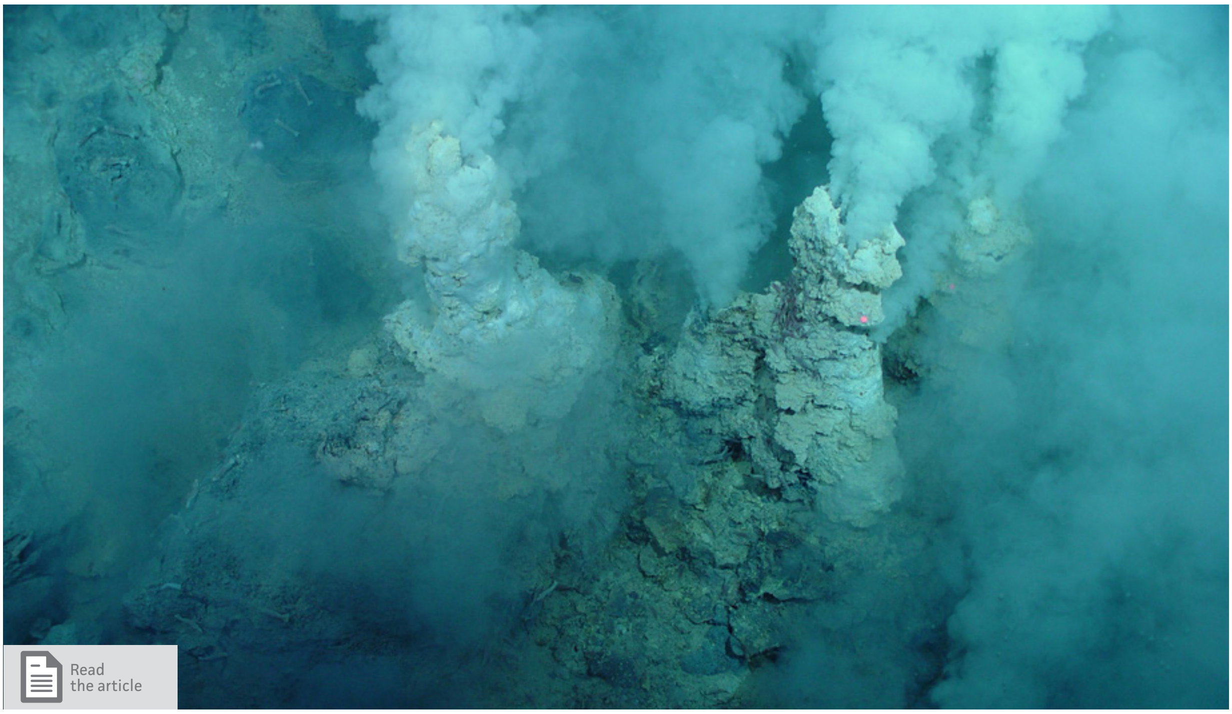
Institution
Paul Scherrer Institute

Background
1983–1989 Studies in chemistry, University of Hannover, Germany
1989–1993 Doctorate in theoretical chemistry, University of Hannover, Germany
1993–1998 Research associate, University of Hannover, Germany
1998–2001 Research associate, MPI for solid state research, Stuttgart, Germany
2001–2007 Senior research associate, ETH Zurich (CSCS)
2007–2015 Materials scientist, Paul Scherrer Institute

Area of research
Materials science, chemistry, multiscale modelling.

Specialised in
Development and application of atomistic simulation methods based on empirical potentials and density functional theory.

HPC means for me
A virtual laboratory that enables the modelling of complex chemical processes in silico as an important complement to experimental studies.



Simulating chemical evolution

Extreme temperature and pressure conditions as well as the mineralogical composition of hydrothermal vents in the deep ocean could have been the ideal environment for chemoautotrophic origin of life. Researchers using ab-initio computational methods and metadynamics simulation techniques on "Piz Daint" have for the first time simulated the detailed reaction chain that enables the formation of prebiotic ammonia molecules.
(Image: P. Rona, NOAA Photo Library)

Twenty-five years supporting Switzerland as a research hub

The guests listening to the presentation of CSCS director and ETH professor Thomas Schulthess.

In 2016 the Swiss National Supercomputing Centre was turning twenty-five. Having established itself on the international stage, it operates supercomputers of the latest generation, supports users from Swiss and international institutions in their top-flight research and runs computers as a service facility for research associations and MeteoSwiss.

On 19 October around 60 representatives from politics, industry and science celebrated the 25th anniversary of Switzerland's National Supercomputing Centre. The visitors were welcomed by CSCS Director Thomas Schulthess, after which Thomas Schulthess and Ticino's former National Councillor Fulvio Caccia provided a look back at 25 years of CSCS as well as a look ahead to the future. After the subsequent tour of the centre, the ceremony continued, accompanied by official speeches with lunch and refreshments in Fattoria Moncucchetto. Perhaps it was once the culinary benefits of the Ticino location compared to other parts of the country that swayed the decision to locate the National Supercomputing Centre in the most southerly Swiss canton. ETH President Lino Guzzella jokingly alluded to this in his speech. The lunch provided would certainly support this theory.

From left to right: Flavio Cotti, Christian Vitta, Manuele Bertoli and Paolo Beltraminelli.

From left to right: Piero Martinoli and Ralph Eichler.

A group of guests during the guided tour of the center with Michele De Lorenzi.

From left to right: Flavio Cotti, Boas Erez, Manuele Bertoli, Christian Vitta and Paolo Beltraminelli in front of a blade of supercomputer "Piz Daint".

From left to right: Thomas Schulthess (CSCS), Lino Guzzella (ETH Zurich) and Boas Erez (USI).

Fulvio Caccia.

Beatrice Fasana, member of the ETH Board.

Lino Guzzella, president of ETH Zurich.

Paolo Beltraminelli, president of the Ticino State Council.

Cristina Zanini Barzaghi, city of Lugano.

Anwar Osseyran, director of SURFsara and chairman of CSCS advisory board.

Boas Erez, rector of Università della Svizzera italiana.

The beginning
Thirty-five years ago, the Swiss government decided to establish a national computer centre in Switzerland and acquire a high-performance computer that all universities could use. As the Message on Special Measures read in 1985: "The high-performance computer should plug a major gap for promising research projects, and a national university and research IT network guarantee the exchange of information and data transfer between the individual universities and connection with international networks." CHF 40 million were earmarked for the procurement of a high-performance computer. Meanwhile, the foundation SWITCH was formed in 1987 with a view to networking the universities and guaranteeing the transfer of data with the computer centre.

After six years of discussions regarding its location, the Swiss National Supercomputing Centre was opened in Manno (Ticino) in 1991. The centre is run by ETH Zurich and its first supercomputer was an NEC SX-3 with two processors. With a processing power of 5.5 gigaflops, it could carry out 5.5 milliard computer operations per second, which is about the same power as an iPad today. The computer supported Swiss research primarily in the domains of climate, astronomy and engineering – for instance in the simulation of fluid dynamics processes.

Since supercomputers become outdated every three to four years, they have to be replaced or overhauled with new, more powerful technologies. This is what happened at CSCS in 2002, when the centre procured its first massively parallel computer. The IBM SP4 had 256 processors and was capable of performing 1.3 trillion calculations a second. The supercomputer was almost ten times more powerful than its predecessor (NEC SX-5) and, moreover, was useful for solving problems in new application domains such as molecular dynamics. When the IBM computer was eventually replaced with a Cray XT3, which was even more general purpose, in 2005, application fields became still more diverse. Today, high-performance computing (HPC) is a key technology that allows researchers to make new discoveries and come up with new solutions to highly complex issues in the fields of physics, chemistry, environmental science, energy, health and economics.

In December 2009, the Swiss parliament approved a strategy for high-performance computing and networking (HPCN) drawn up by the ETH Board on behalf of the Swiss State Secretariat for Education, Research and Innovation (SBFI).

The Swiss federal government, ETH domain and universities thereby laid the foundation for an internationally competitive Swiss supercomputing network. Three years later, CSCS moved into a state-of-the-art new building in Lugano and took receipt of "Piz Daint", a Cray XC30 supercomputer that was Switzerland's first petaflop machine and can perform millions of billions of calculations a second. One of the goals of the HPCN strategy was to support top-level research in Switzerland and thereby secure the country's competitiveness.

Today: Most powerful supercomputer in Europe
After an upgrade of "Piz Daint" at the end of 2016 to a Cray XC50/XC40, Switzerland currently possesses Europe's most powerful supercomputer, used by some 600 researchers in Switzerland and abroad. The computer allows for an even more realistic and efficient simulation of highly complex problems. It can also structure and analyse large quantities of unstructured data, such as that produced by CERN's Large Hadron Collider (LHC).

The HPCN strategy has also yielded successful initiatives in which researchers have cooperated with hardware and software developers to allow for more efficient use of new and future supercomputer architectures. These initiatives led for instance to an optimized weather code and a new computer for MeteoSwiss. Since the summer of 2016, these solutions have made it possible to make weather forecasts in greater detail than ever before while still being energy efficient. Close ties have also been established with USI Università della Svizzera italiana, particularly in data science.

In the 25 years since it was established, CSCS has had a colourful history with nine directors. Thanks in no small part to the HPCN strategy, CSCS is regarded as a scientific computing centre with an international reputation. It offers its users a comprehensive range of hardware and software services. As well as "Piz Daint", CSCS also runs the abovementioned weather computer for MeteoSwiss the compute cluster of the Swiss Institute of Particle Physics (CHIPP) and, since 2013, the supercomputer of the Blue Brain Project.

More computing power for Swiss research

A hardware upgrade in the final quarter of 2016 saw "Piz Daint", Europe's most powerful supercomputer, more than double its computing performance. ETH Zurich invested around CHF 40 million in the upgrade, enabling researchers to perform simulations, data analysis and visualisation more efficiently than ever before.

With a peak performance of seven petaflops, "Piz Daint" has been Europe's most powerful supercomputer since its debut in November 2013. And it is set to remain number one for the foreseeable future thanks to a hardware upgrade in late 2016, which has increased its peak performance to around 20 petaflops. This increase in performance is vital for enabling higher-resolution simulations as well as in the rapidly developing field of data science. Both of these involve the processing of vast amounts of data, and it is in these areas that ETH Zurich is establishing a research strength. Modern materials science, geophysics, life sciences and climate science all require simulations that are both computing and data intensive, and the new hardware enables researchers to run these simulations more realistically and more efficiently. In the future, big science experiments such as the Large Hadron Collider at CERN will also see their data analysis support provided by "Piz Daint".

ETH Zurich has invested CHF 40 million in the upgrade of "Piz Daint" – from a Cray XC30 to a Cray XC50 – in order to provide an infrastructure that will accommodate the increasing demands in high performance computing (HPC) up until the end of the decade. The upgrade involved replacing two types of compute nodes as well as the deployment of a novel technology from Cray Inc. known as DataWarp. DataWarp's 'burst buffer mode' quadruples the effective bandwidth to and from storage devices, markedly accelerating data input and output rates and so facilitating the analysis of millions of small, unstructured files. Thus, "Piz Daint" is able to analyse the results of its computations on the fly. The revamped "Piz Daint" remains an extremely energy-efficient and balanced system where simulations and data analyses are scalable from a few to thousands of compute nodes.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"'Piz Daint' has enabled our group to build a 'multiscale-scope' for computational science to study phenomena from the atomistic to the macroscale. 'Piz Daint' has been instrumental to our research efforts ranging from the detection of metastatic cancer cells to revealing the hydrodynamics behind the beauty of fish schools."
Petros Koumoutsakos, ETH Zurich

Name
Petros Koumoutsakos

Position
Professor

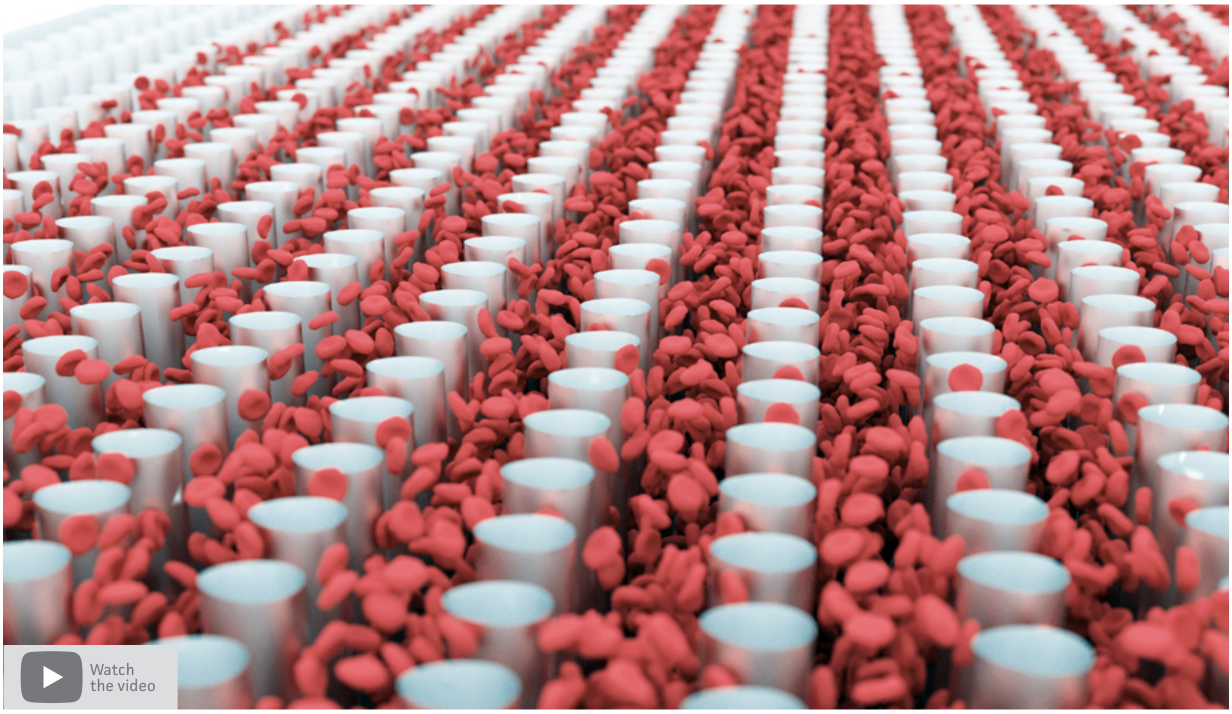
Institution
ETH Zurich

Background
1993-1994 Post-doc fellow, California Institute of Technology, USA
1994-1996 Post-doc fellow, Stanford University, USA
1996-2001 Research associate, NASA Ames, USA
1997-2000 Assistant professor of computational fluid dynamics, ETH Zurich
2016-2021 Fellow, Collegium Heleveticum
Since 2000 Professorship for computational science, ETH Zurich

Area of research
Computing.

Specialised in
Computational science and engineering, supercomputing, fluid mechanics, particle methods, uncertainty quantification.

HPC means for me
Thinking and curiosity assisted by (super)computers for discovery and prediction.



In silico lab-on-a-chip

State-of-the-art simulations of the flow of micron-sized red blood cells and tumour cells through mm-long microfluidic channels. The so-called "in-silico lab-on-a-chip" emulates laboratory experiments looking at how rare tumour cells could be filtered out of the blood thus allowing for the early diagnosis of metastatic cancer. (Image: Christian Conti, CSElab)

Finances

Expenditures

	CHF
Investments	**40 023 532.86**
Equipment and Furniture	**8 035.15**
Personnel	8 313 178.80
Payroll	6 469 583.30
Employer s contributions	1 113 631.20
Further education, Travel, Recruitment	729 964.30
Other Material Expenses	**6 234 696.37**
Maintenance building & Technical Infrastructure	655 516.81
Energy	1 499 835.87
Administrativ expenses	11 565.79
Hardware, Software, Services	3 529 306.73
Remunerations, Marketing Workshops, Services	522 197.97
Other	16 273.20
Extraordinary Income / Expenditures	**50 362.37**
Membership fees	50 362.37

Income

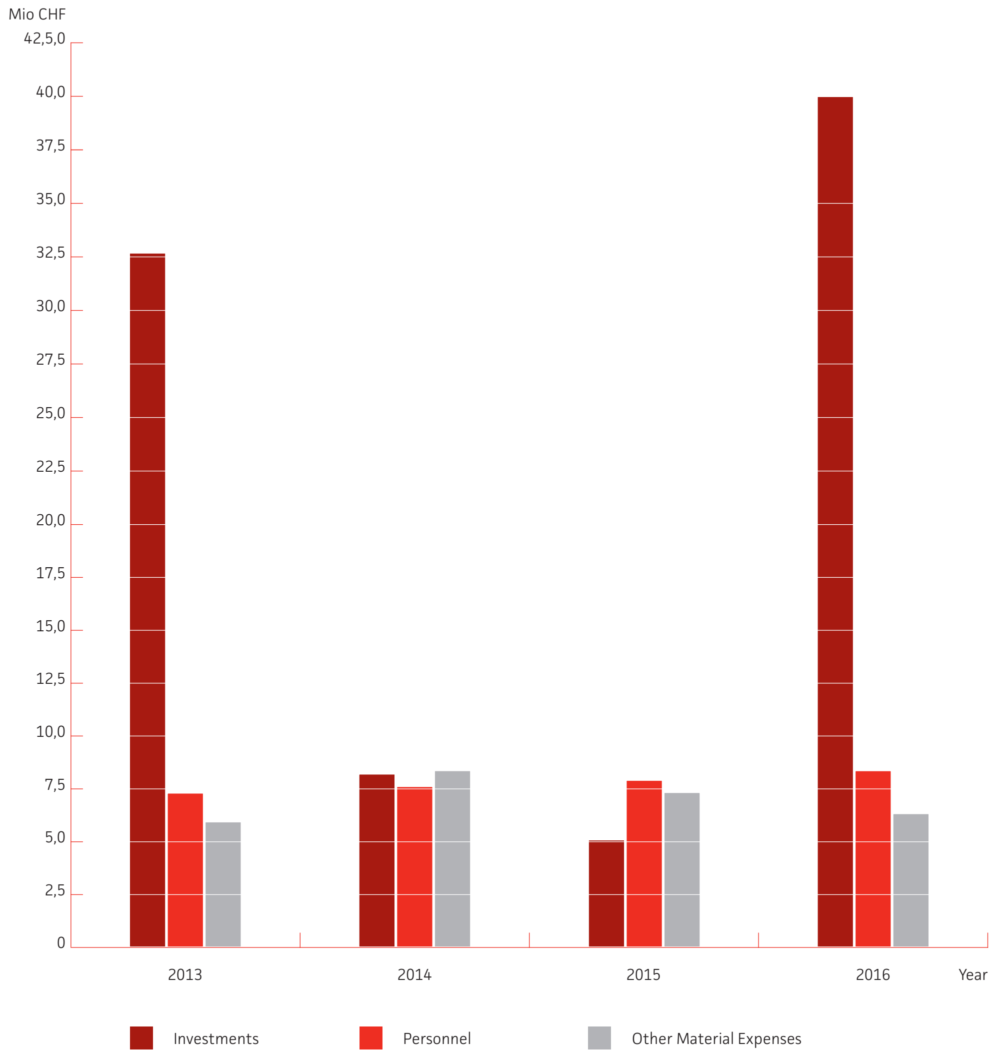
	CHF
Basic Budget	**52 819 584.26**
Contribution ETH Zurich	52 819 584.26
Other Income	**164 687.02**
Services / Courses	61 929.55
Reimbursements	8 517.97
Other Income	94 239.50

Total Expenses	**54 629 805.55**	**Total Income**	**52 984 271.28**
Balance current year			**-1 645 534.27**
Rollover Project Fund Investments 2016			2 879 930.61
Total Balance User Lab 2016			**1 234 396.34**
./. Rollover Project Fund Investments 2017			29 561.50
Balance operational Funds CSCS - Rollover to ETH 2016			1 204 834.84

Third-Party Contributions	
MeteoSwiss	1 190 750.00
Paul Scherrer Institute	1 148 000.00
CHIPP	843 345.00
Blue Brain	818 856.10
EU Projects (excl. 2/3 overhead ETHZ)	803 504.00
University of Zurich	616 000.00
Euler Cluster	327 807.00
Monch Cluster	325 000.00
C2SM	288 000.00
Università della Svizzera italiana	265 000.00
Marvel	205 000.00
Hilti	169 560.00
Partner Re	18 000.00

Development of Overall Expenses

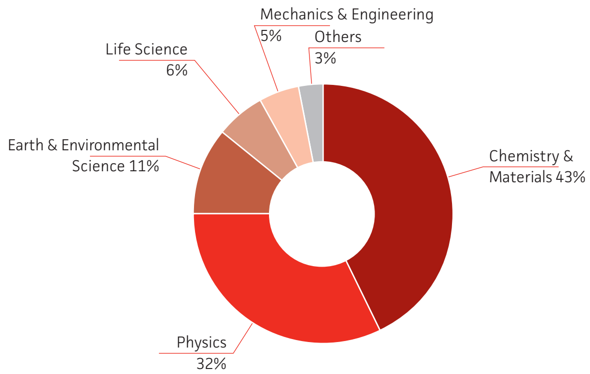
	2013	2014	2015	2016
Investments	32 555 142	8 118 445	5 042 501	40 023 533
Personnel	7 249 675	7 538 405	7 842 930	8 313 178
Other Material Expenses	5 900 556	8 268 005	7 271 103	6 293 094



Usage Statistics

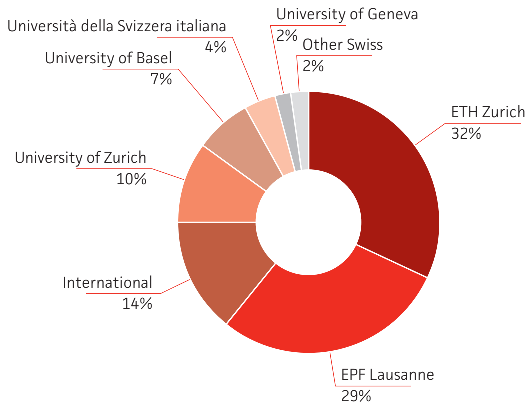
Usage by Research Field

Research Field	CPU h	%
Chemistry & Materials	11 482 049	43
Physics	8 664 124	32
Earth & Environmental Science	2 826 961	11
Life Science	1 568 041	6
Mechanics & Engineering	1 275 781	5
Others	951 620	3
Total Usage	**26 768 576**	**100**



Usage by Institution

Institution	CPU h	%
ETH Zurich	8 467 682	32
EPF Lausanne	7 801 865	29
International	3 715 101	14
University of Zurich	2 748 650	10
University of Basel	2 005 133	7
Università della Svizzera italiana	969 233	4
University of Geneva	476 510	2
Other Swiss	584 402	2
Total Usage	**26 768 576**	**100**



Compute Infrastructure

HPC Systems

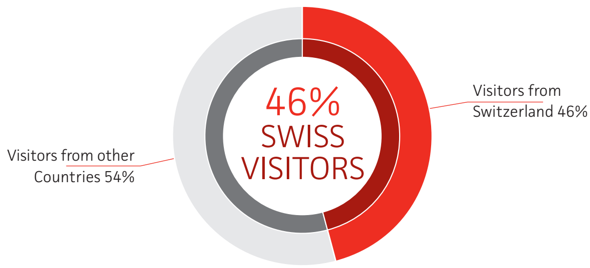
Name	Model	Interconnect Type	CPU Type	Node Specifications		
				No. Cores	No. Sockets	No. Nodes
Piz Daint	Cray XC50 Cray XC40	Cray Aries	Intel Xeon E5-2690 v3 + Nvidia P100 Intel Xeon E5-2695 v4	12 18	1 2	4 936 1 431
Blue Brain BG/Q	IBM BG/Q	IBM BGQ 3D Torus	PowerPC A2	16	1	4 096
Blue Brain Viz	IBM Cluster	Infiniband FDR	Intel Xeon E5-2670	8	2	40
Monch	NEC Cluster	Infiniband FDR	Intel Xeon E5-2660 v2	10	2	376
Phoenix	x86 Cluster	Infiniband FDR	Intel Xeon E5-2670	8	2	64
Piz Kesch	Cray CS-Storm	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2	12
Piz Escha	Cray CS-Storm	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2	12
Monte Leone	HP DL 360 HP DL 360 HP DL 380	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	20 7 4
Pilatus	x86 Cluster	Infiniband FDR	Intel Xeon E5-2670	8	2	38

Website cscs.ch

	2015	2016
Total Website Visitors	72 991	69 833
Average Website Visits (Minutes)	2.43	2.84

New visitors

Visitors origin



Top 5 most visited website pages

1. CSCS Homepage www.cscs.ch
2. Staff www.cscs.ch/about/staff
3. Open Positions www.cscs.ch/about/working_at_cscs/open_positions
4. Events www.cscs.ch/events
5. Piz Daint and Piz Dora www.cscs.ch/computers/piz_daint_piz_dora

Twitter

	2015	2016
Followers	375	592

LinkedIn

	2015	2016
Followers	3 830	5 831

YouTube
Published videos

	2015	2016
Watch Time (Minutes)	402 370.00	424 011.00
Average View Duration (Minutes)	4.45	4.00
Number of Views	84 438.00	105 797.00

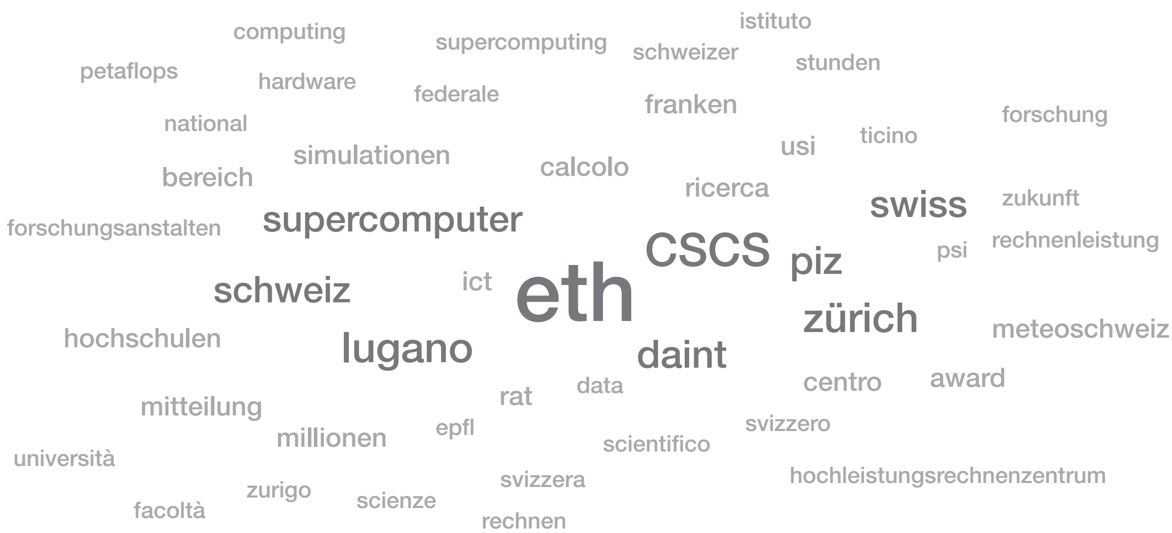
Facebook
November 2015: creation of the CSCS page

	2015	2016
Followers	-	89

CSCS in the News

	2015	2016
News websites	335	406
Print	176	186
Radio & TV	10	15

Word Cloud of News Related to CSCS

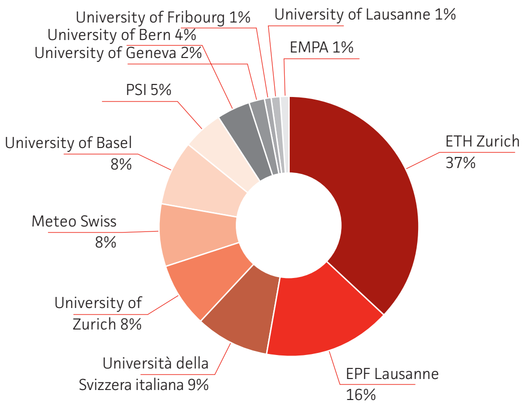


User Satisfaction

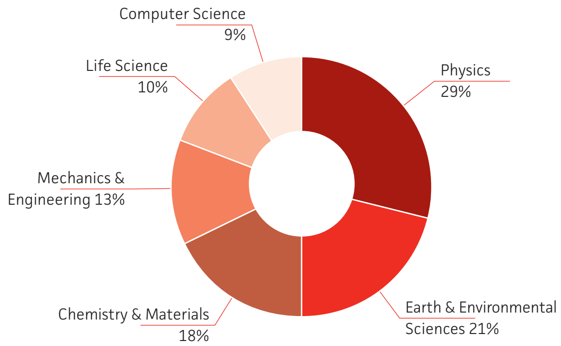
A user satisfaction survey was submitted to 1190 users in January 2017. The response rate was of 17.5% (208 answers).

User Profile

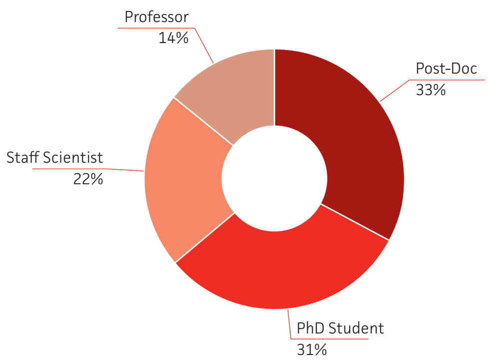
Your institution



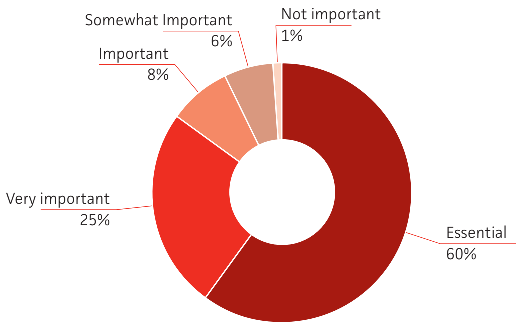
Your scientific field



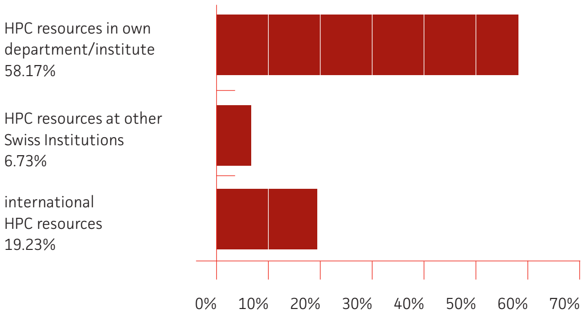
Your position



For my research, CSCS resources are:



Which HPC resources are you using besides CSCS?



User Support

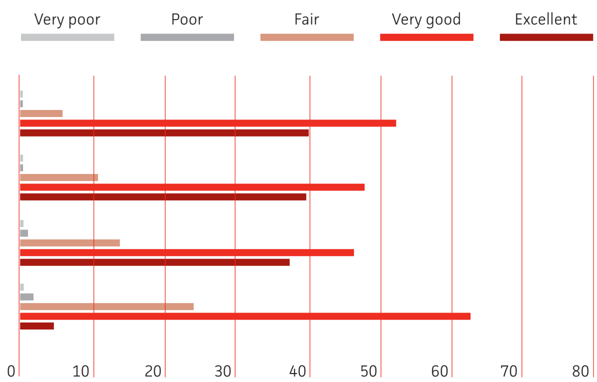
How do you rate the quality of...

Helpdesk support

System support

Application support

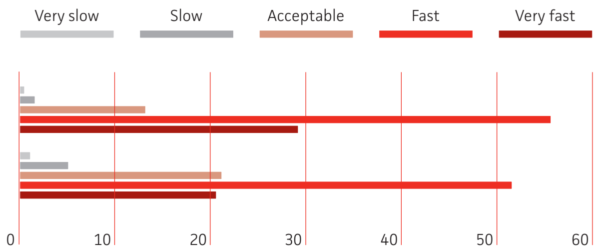
The offer of training courses and user events



How fast does support handle your request?

The reaction time of the helpdesk is

The time to solution for the support requests is



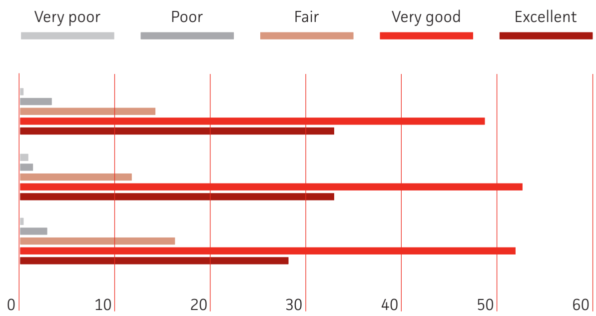
System Availability, Stability and Usability

How you perceive...

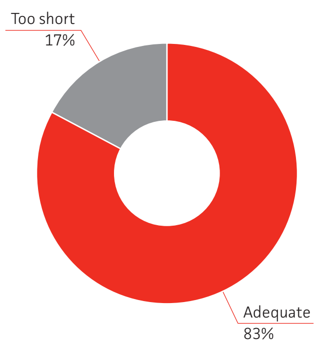
The availability of CSCS systems?

The stability of CSCS systems?

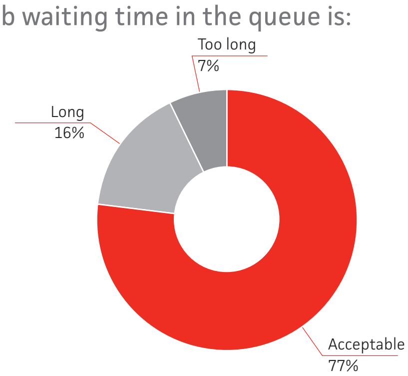
The ease of use of CSCS systems?



The run time limits for batch jobs are:

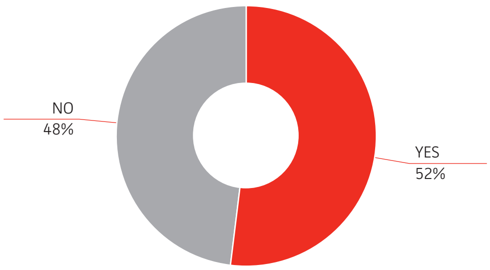


The job waiting time in the queue is:

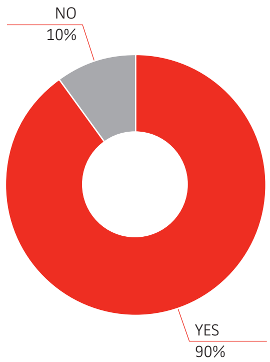


Project Proposal Process

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?

The submission portal is

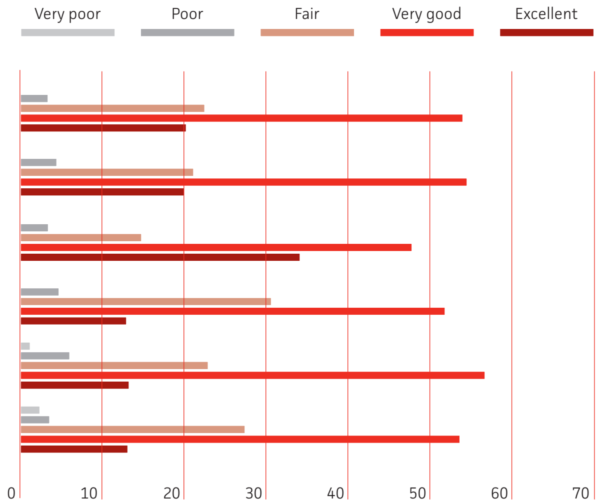
The quality of the submission form is

The support provided during the call is

The feedback from scientific reviewers is

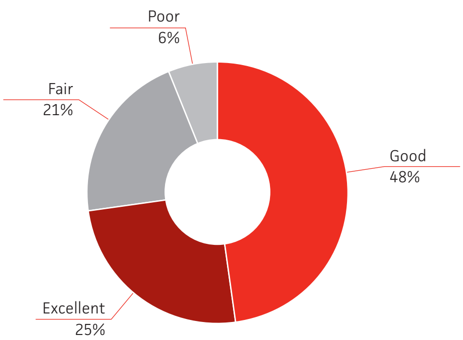
The feedback from technical reviewers is (when given)

The information provided by the panel committee is

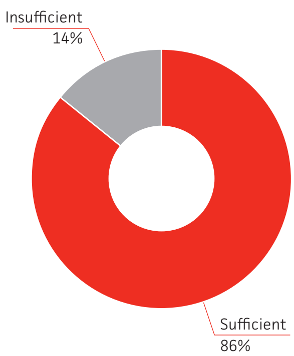


Adequacy of Allocated Resources

The resources assigned to my project are:

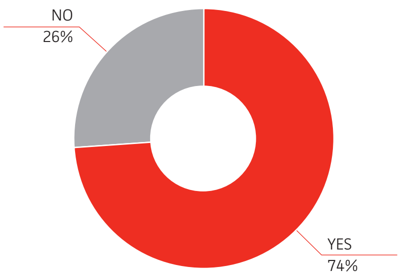


My storage allocation on “project” is:

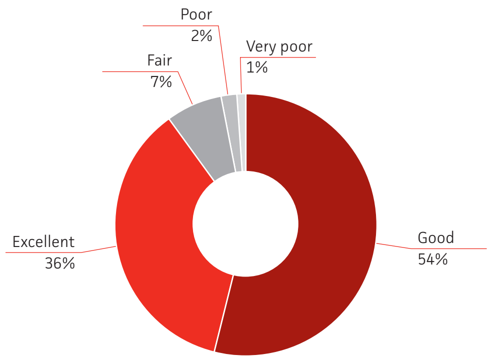


Application Development

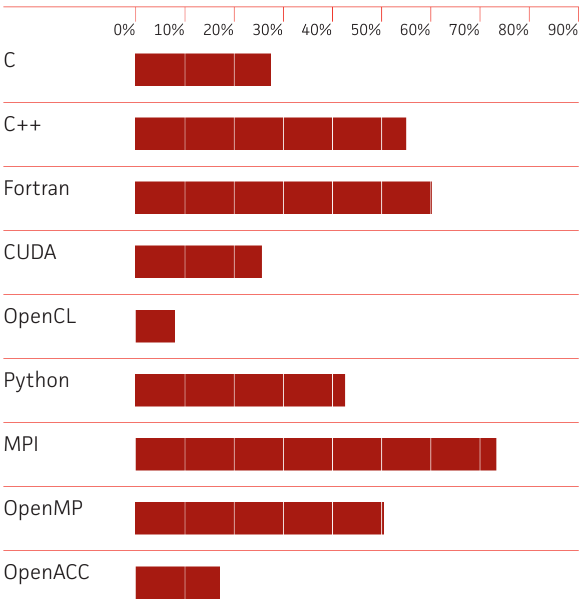
Do you develop and maintain application codes?



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

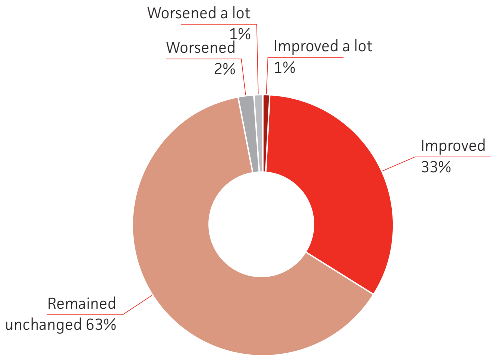
Your consumption of your allocation

Upcoming events and courses

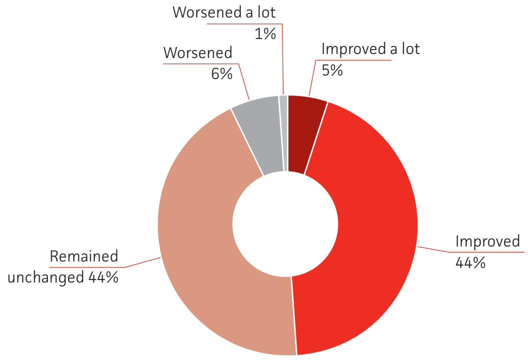
Future developments at CSCS

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:



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