CSCS

Annual Report
2013

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

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Welcome from the Director

Thomas Schulthess, Director of CSCS.

Welcome to this review of the Swiss National Supercomputer Centre (CSCS) in 2013, a year of further growth in our programs during which we transcended the peta-scale computing barrier.

The long-sought goal of the Swiss High-Performance Computing and Networking initiative was the installation of a peta-scale computing system at CSCS by 2014. This was accomplished with the upgrade of "Piz Daint" to 28 cabinets and 5'272 hybrid CPU-GPU compute nodes. At Supercomputing 2014 in Denver the resulting system secured the attributes "greenest petaflops-scale supercomputer" in the world and "most powerful supercomputer in Europe". Indeed, "Piz Daint" and "Juqueen", a 28-cabinets IBM BG/Q system at Julich Supercomputing Center (JSC), are currently the only open-access supercomputers in Europe that can deliver five or more petaflop/s on compute intensive applications. Regional climate simulations of the CSCS user program consume 7 times less energy to solution on "Piz Daint" compared to CSCS' current flagship system "Monte Rosa", or 4 times less if "Piz Daint" were running the simulations without GPUs.

The success of "Piz Daint" would not have been possible without the sustained investments in application software development carried out by projects funded by the Swiss Platform for High-Performance and High-Productivity Computing (HP2C) since 2010. The application codes that came out of these projects along with a thorough evaluation of all available processor-options for the Cray XC30 culminated in the development of the compute nodes in "Piz Daint" and the ability to productively exploit energy efficient GPU co-processors.

The close collaboration with NVIDIA's software experts was also instrumental in the excellent application performance on "Piz Daint". In 2013 we formalized this within the framework of the NVIDIA "Co-Design Lab for Hybrid Computing" at ETH Zurich. In this lab software engineers from NVIDIA's DevTech team, who are located on ETH premises, collaborate closely with application developers in Swiss academia to design new algorithms and implement application software that can exploit heterogeneous architectures. Furthermore, the co-design lab will guide future developments of hybrid systems based on GPUs.

Another seminal milestone was reached with the installation of "Blue Brain 4", the new 4-cabinets IBM BG/Q system of EPF Lausanne's Blue Brain project at CSCS. This system is the fourth in a succession of IBM Blue Gene systems that have been in operation at EPF Lausanne since 2005. It highlights the strong collaboration between EPF Lausanne and CSCS in the development of supercomputing infrastructure for brain simulations. "Blue Brain 4" is the development system within Europe's "Human Brain Project", the main production system of which is being operated at JSC. Furthermore, in 2013 EPF Lausanne's Blue Brain Project and CSCS launched a collaborative project with IBM in order to develop active storage technologies indented to solve the memory challenges on the HBP's simulations roadmap.

I would like to thank CSCS, ETH Zurich, the University of Lugano, the engineers of Cray and NVIDIA, our collaborators at EPF Lausanne and IBM, as well as all persons and organizations that have supported us in recent years and particularly in 2013. We are excited about the possibilities these recent developments have opened up for science in Switzerland and Europe, and for the development of future computing systems as we approach the exascale era.

Prof. Thomas Schulthess
Director of CSCS

Content

KEY INFORMATION

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

Production Machines
Piz Daint, Cray XC30, 7.9 PFlops
Monte Rosa, Cray XE6, 402 TFlops

Computing Time for User Lab
2013: 459 333 565 CPU hrs
2012: 270 922 127 CPU hrs

User Community
2013: 90 Projects, 372 Users*
2012: 83 Projects, 842 Users

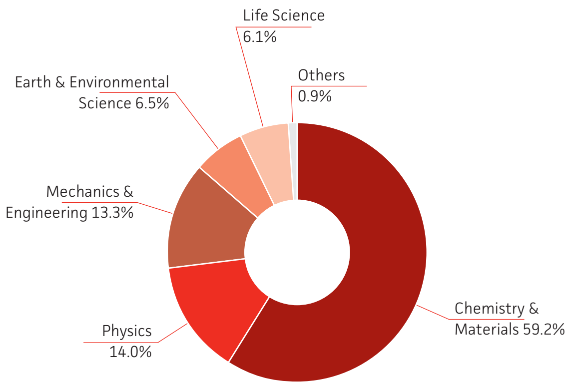
Investments
2013: 32.5 Mio CHF
2012: 17.3 Mio CHF

Employees
2013: 65
2012: 54

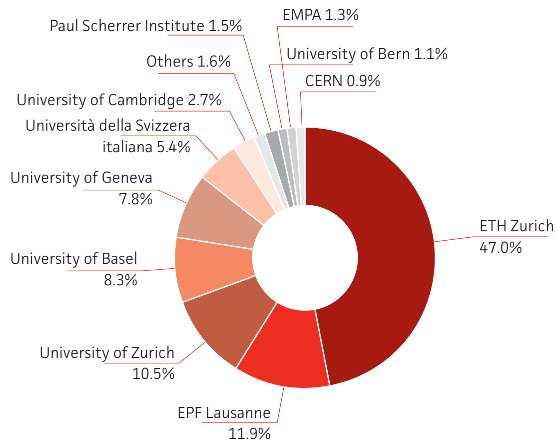
Operational Costs
2013: 13.1 Mio CHF
2012: 11.9 Mio CHF

* Respect to previous years, only the number of User Lab users is listed

Usage by Research Field



Usage by Institution



Computing Systems for User Lab

Name	Supplier & Model	Installation / Upgrade	User	Peak Performance (TFlops)
Piz Daint	Cray XC30	2012 / 2013	User Lab	7 787
Monte Rosa	Cray XE6	2009 / 2011	User Lab	402
Tödi	Cray XK7	2009 / 2012	R&D	393
Pilatus	DALCO Cluster	2012	User Lab	15
Rothorn	SGI UV 1000	2011	User Lab	3
Matterhorn	Cray XMT	2011	User Lab	NA

Computing Systems for Third Parties

Name	Supplier & Model	Installation / Upgrade	User	Peak Performance (TFlops)
Blue Brain 4	IBM BG/Q	2013	EPF Lausanne	839 + 13
Mönch	NEC Cluster	2013	ETH Zurich	139
Monte Lema	Cray XE6	2012	MeteoSwiss	34
Phoenix	Cluster	2007 / 2012	CHIPP (LHC Grid)	25
Albis	Cray XE6	2012	MeteoSwiss	15

January

CSCS, the coordinator of the HPC activities for the Human Brain Project

The European Commission awarded the Human Brain Project 1 billion euros over a 10-year period. One of the partners of the Human Brain Project led by Professor Henry Markram at EPF Lausanne is indeed CSCS. CSCS will coordinate the four supercomputer centers participating in the project, and will develop the simulation platform in collaboration with EPF Lausanne. This massive funding for an outstandingly ambitious computational project underlines the ever increasing role of supercomputers as new research instruments that complement traditional laboratory experiments.

HBP
Human Brain Project

CSCS among the partners of the Human Brain Project.

Dr. Diego Rossinelli talks to the public about computational fluid dynamics

After the major success of the scientific talks at the Open Day 2012, CSCS organized a series of seminars for a general public to demonstrate the importance of supercomputers for science and society. The invited speakers were indeed scientists from various Swiss research institutes and universities who are using CSCS' computational resources to carry out their research. In January Dr. Diego Rossinelli, from ETH Zurich, talked about "Supercomputers, instruments of modern science". In his excursus on computational fluid dynamics, his field of expertise, Diego stressed its importance in science and fascinated the audience with some of his spectacular visualizations.

February

Extension of the tape library to accommodate more data

The automated tape library (IBM TS3500) installed in 2012 was extended to take its storage capacity to about 27.4 PB of uncompressed data. The library is now composed of 16 frames plus 2 service bay cabinets and can hold up to 18'257 tapes moved by two robots (in the installed configuration there are 24 LTO5 drives). The library is part of the Backup System (IBM Tivoli Storage Manager) and is integrated into the Hierarchical Storage Management environment (HSM) that puts files on tapes that have not been accessed for a long time.

The upgraded IBM TS3500 tape library.

First course on OpenACC and CUDA programming on the Cray XK7 platform

CSCS upgraded its Cray XK6 platform to Cray XK7 by introducing NVIDIA K20X devices together with CUDA 5, and a new Cray programming environment that included OpenACC compilers. The goal of this 2-day training course was to introduce new features of the platform and its programming environment, and to provide hands-on training on CUDA5 and OpenACC programming. The course instructors were Alistair Hart from Cray and Peter Messmer from NVIDIA.

March

"Get up to speed with the Cray Cascade"

A four-day course introduced the user community to "Piz Daint", the first 12 cabinets Cray XC30 installed worldwide. The course aimed to show how to get the best performance out of the Intel Sandy Bridge processors, and how to take full advantage of the new powerful high-bandwidth, low-latency network.

Experts from Intel dived into the features of the Sandy Bridge processor and demonstrated the use of the Intel tools for generating optimized code and Cray specialists showed how to use their set of tools and numerical libraries and how to take full advantage of the MPI libraries and communication strategies.

Professor Dissertori talks to the public about supercomputers and particle physics

The second scientific talk of the year organized by CSCS for a general public to look at the importance of supercomputers and their use in the various scientific disciplines, was dedicated to Particle Physics. Professor Günther Dissertori from ETH Zurich showed in a brilliant presentation why without grid-computing it would have been impossible to discover the Higgs boson. To underline the importance of this discovery, the 2013 Nobel Prize for Physics was indeed awarded to Peter W. Higgs and François Englert.

HPC Advisory Council Switzerland 2013

It was in 2010 that Hussein Harake (CSCS), Brian Sparks (HPC Advisory Council) and Gilad Shainer (Chairman of the HPC Advisory Council) organized for the first time the HPC Advisory Council conference in Lugano. After four years, the conference has grown and become an important fixture in the HPC community. More than 100 participants attended the fourth workshop in Lugano. The conference focused on high-performance computing essentials, new developments and emerging technologies, best practices and hands-on training. As every year, the conference brought together system managers, researchers, developers, computational scientists, students and industry affiliates from Switzerland and abroad for cross-training and to discuss recent HPC developments and future advancements.

April

The new Cray XC30 “Piz Daint” goes into production

CSCS next flagship system “Piz Daint”, named after one of the highest mountains in Val Müstair, Grisons, was opened to the user community as a production system together with “Monte Rosa”. Its procurement and installation marks an important milestone in the implementation of the national high performance supercomputing strategy. The new machine is a Cray XC30 (Cascade) system with a peak performance of 750 Teraflops using Intel Sandy Bridge processors and with a new network interface chip and an advanced interconnect topology. At the time of installation, “Piz Daint” was the largest Cray XC30 in the world with 2’256 compute nodes, over 36’000 compute cores and 70 TB of memory with a five-fold increase in system bisection network bandwidth compared to “Monte Rosa”.

4th European HPC Centre Infrastructure Workshop

The 4th edition of this highly successful series of European Workshops on HPC Infrastructures was hosted by CSCS at the Hotel Cadro Panoramica, Lugano from April 22 to 24 2013. The workshop brought together 58 HPC infrastructure specialists from around the world to discuss the latest trends and technologies in designing and operating supercomputing centers. The program focused on updates from various sites in Europe and the USA, a vendor view of future challenges for HPC and its supporting infrastructures, presentations on energy efficiency and related standards as well as presentations from infrastructure technology vendors. The next meeting will be hosted by the French Alternative Energies and Atomic Energy Commission (CEA).

May

Hpc-ch forum on “HPC in the Swiss Industry” at Novartis

This meeting held at the Novartis headquarters in Basel aimed to bring together all members of the hpc-ch community from both academia and industry and to give them a unique networking opportunity and the chance to exchange best practices. The meeting allowed the participants to gain an overview of the HPC activities in several companies, to discuss the business applications of HPC, and to understand how HPC services are provided and what the HPC challenges are in industry.

Impressions from the HPC Advisory Council Switzerland 2013.

June

InfiniBand foundation course

CSCS together with Mellanox Training Centre organized a two-day introduction course to InfiniBand. This course provided the foundations for the InfiniBand technology from a usability point of view. 25 system administrators from different Swiss universities and industry attended the course. When asked about the course, Sergio Maffioletti, one of the participants from the University of Zurich commented: "A very interesting and very intense 2-day course on Infiniband. With a Mellanox expert who presented the technology and the key operation concepts, the course will be very useful for us and help us streamline the operation of our current IB deployment."

Participants in the InfiniBand foundation course.

Professor Auricchio talks to the public about cardiology and supercomputers

On June 7th, Professor Auricchio, from Cardiocentro Ticino, gave the last scientific talk of the first series of four conferences organized by CSCS to highlight the importance of supercomputers and their use in the various scientific disciplines. Professor Auricchio's presentation was "How supercomputers can give back harmony to the heart", a study in collaboration with Professor Rolf Krause and Dr. Mark Potse at Università della Svizzera italiana. The speaker explained how supercomputers have become "virtual laboratories" for medicine where researchers can extensively test therapies on failing hearts.

ISC13: a brand new booth for "HPC in Switzerland"

Encouraged by the positive feedback from visitors over the last few years, CSCS and hpc-ch again hosted their own booth at the International Supercomputing Conference, ISC13, held in Leipzig, Germany on 16-20 June. This year the booth was slightly larger and with a brand new layout: a large map giving an overview of Switzerland and its HPC players, and two large monitors to display movies and presentations on projects and activities. This year's motto was "implementing sustainable supercomputing" and the presentations were designed to show some examples of how Switzerland is addressing this important topic.

The front and the retro of the new booth for hpc-ch and CSCS at ISC13.

July

Assembling the "Blue Brain 4"

In July, an IBM Blue Gene/Q was acquired from the Blue Brain Project (EPF Lausanne) and installed at CSCS. The system, named "Blue Brain 4", is in fact a key scientific tool for the neuroscientific research done at EPF Lausanne within the Blue Brain Project. This system makes possible the simulation of larger neuron networks. A target for this system is to achieve the simulation of a brain at the rodent's scale (approximately 200 millions neurons). Launched by EPF Lausanne in 2005, the Blue Brain Project is the first ever attempt to reverse engineer the mammalian brain.

The IBM Blue Gene/Q "Blue Brain 4".

Summer School on Computer Simulations in Science and Engineering

On 8-19 July, CSCS in collaboration with Università della Svizzera italiana, and with the sponsorship of the Swiss Graduate Program FoMICS, hosted a two-week summer school on parallel programming aimed at graduate and PhD students who were new to the world of high performance computing and who wished to learn the basic skills required to write, develop and maintain parallel applications in scientific computing. The school covered topics such as the principles of parallel programming, distributed memory programming with MPI, shared memory programming using OpenMP, hybrid programming with MPI/OpenMP, as well as some advanced topics.

Hike to the Monte Boglia with the participants in the Summer School.

August

Assembling the NEC cluster "Mönch"

CSCS is going to operate for a group of professors of ETH Zurich a NEC cluster called "Mönch" which was assembled in August. The cluster is a 9 rack NEC-provided Intel-based system with 4 login nodes, 312 standard compute nodes, 24 large-memory compute nodes and 8 servers to provide I/O to Lustre. Each of the standard compute nodes consists of 2 Intel 10-core Ivy Bridge EP E5-2660v2 processors, offering 20 physical cores per node – with hyperthreading enabled, the system sees 40 cores.

The NEC Cluster "Mönch", named after a mountain in the Bernese Alps.

Participants in the CSCS User Meeting.

September

User Meeting in Lucerne

On September 6th, CSCS held the annual meeting with the user community in Lucerne welcoming 63 participants. After a standing lunch Thomas Schulhtess opened the event with an "Update on CSCS, 'Piz Daint' and PASC", followed by Maria Grazia Giuffreda who presented the new CSCS challenge to the Swiss scientific community: the CHRONOS Call for proposals. After the coffee break, Sadaf Alam gave an overview of "Piz Daint" Programming Environment and Enabling Technologies, with a special focus on the similarities and differences between "Piz Daint", the Cray XC30, and "Monte Rosa", the Cray XE6. CSCS' last presentation was "Training courses @CSCS". Themis Athanassiadou briefly presented the upcoming courses focused on the hybrid system and GPUs. The last hour of the meeting was an open discussion between CSCS and the User Community.

Autumn School on GPU-enabled numerical libraries

The Swiss Graduate Program FoMICS "Foundations in Mathematics and Informatics for Computer Simulations in Science and Engineering" initiative together with CSCS offered a 2-day intensive workshop on the use of numerical libraries for Graphical Processing Units (GPUs). The first day of the course included a fast-paced GPU programming tutorial, supplementing the GPU Programming Workshop and focusing on such advanced topics as exploiting different types of GPU memory, exploring CPU GPU bandwidth, and programming non-trivial algorithms.

The next $1^{1/2}$ days included tutorials on existing GPU-enabled libraries, such as CUBLAS, CUSPARSE, CUFFT, PARALUTION, and MAGMA.

October

Promising hybrid computer architecture

The supercomputer "Piz Daint", which has been in operation at CSCS since April, was extended with graphic processing units (GPU) from NVIDIA. In this extension, one of the two conventional processors (CPU) located on a compute node was replaced by a GPU. Compared to a conventional CPU, the GPU has reduced functionalities that are optimized for numerical calculations. In simple terms, this enables the GPU to compute much faster whilst saving energy. Furthermore, the new supercomputer sources much of its overall performance and efficiency from a novel interconnecting network between compute nodes designed by computer manufacturer Cray. The hybrid "Piz Daint" is still the first of its kind, and has been designed to help researchers solve more detailed, higher-resolution models – and all this while consuming less power.

Prof. Thomas Schulthess, director of CSCS, showing a computing blade of the hybrid Cray XC30 supercomputer "Piz Daint".

COSMO goes hybrid

COSMO is a model used by the German Meteorological Service (DWD), MeteoSwiss and other institutions as a basis for their daily weather forecasts. Over the last past three years, researchers from the Center for Climate Systems Modeling (C2SM) of ETH Zurich and MeteoSwiss worked for the High Performance and High Productivity Computing (HP2C) initiative to revise and refine the model's code and the algorithms used in it. Their goal was to make the software more efficient for regional weather and climate simulations and to adapt it to new computer architectures based on graphics processors (GPUs). The new software was tested successfully on a computer with graphics processors and the newly extended "Piz Daint", permitting the performance of simulations with greater efficiency and reduced energy consumption.

First CHRONOS Call for Proposals

It was June when CSCS launched its first CHRONOS call for proposals. **CHRONOS,** which stands for **C**omputationally-Intensive, **H**igh-Impact **R**esearch **O**n **N**ovel **O**utstanding **S**cience, is a new annual call for proposals issued by CSCS for high-impact, challenging and innovative research open to all fields of science from all over the world. On October 11th, the deadline for submission, seven project proposals were submitted for a total request of 11 million node hours (equivalent to 320 Mio core hours) on the hybrid Cray XC30 system, "Piz Daint".

November

Redesign of CSCS website

On November 11th, CSCS went online with its new website. The previous website was due for a makeover and therefore CSCS initiated a "web relaunch" project to develop a new, future-oriented website. The project involved both the main site (www.cscs.ch) and the user portal (user.cscs.ch). A lot of work was done to rationalize the content-management structure to ensure straightforward content creation, distribution and updating; to design a fully responsive website that is easy to read and navigate on any access device. And all this had to take account of the three entirely different audiences: CSCS staff, other academic/professional users, and the general public.

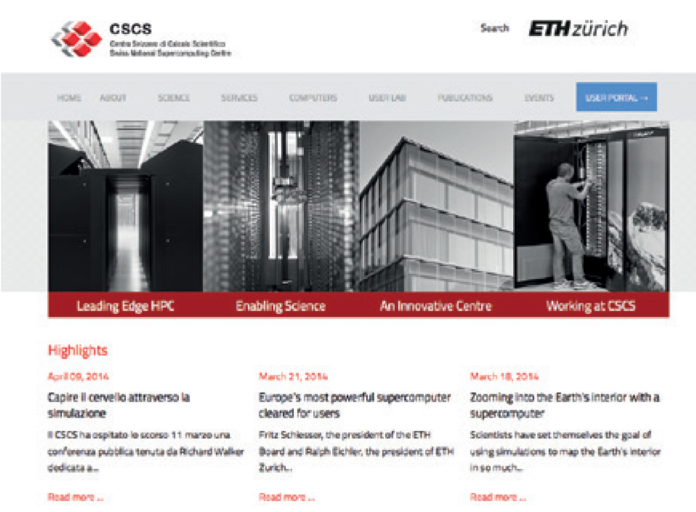
December

Let's learn more on programming for GPUs

On December 4-6, CSCS organized a 3-day training course on GPU programming. Themis Athanassiadou from CSCS welcomed the 22 participants and gave a short introduction of CSCS and the three-day course. One and half days were dedicated to Alistair Hart from Cray who introduced the audience to OpenACC, followed by Peter Messmer from NVIDIA who gave an overview on CUDA, CUDA toolkit and GPU optimization. The last afternoon was reserved for hybrid performance and debugging tools introduced by Jean-Guillaume Piccinali from CSCS.

NVIDIA Co-Design Lab Workshop

In November, NVIDIA announced the creation of the NVIDIA Co-Design Laboratory for Hybrid Multicore Computing at ETH Zurich. A project aimed to reinforce the collaboration between NVIDIA and CSCS, supplying computing resources and technical expertise to help domain scientists get up-and-running quickly and efficiently on the GPU-accelerated systems. The lab hosted an on-site workshop to introduce researchers to lab personnel and provide information on available training materials and supercomputing resources. The goal of this one-day workshop was to introduce the lab and its services, to offer a platform to exchange success stories and best practices for hybrid multicore computing, and to share ongoing GPU activities. The program was aimed at both seasoned GPU users and newcomers to accelerated computing, from all over Switzerland.



The homepage of the new CSCS website.

A new era for the User Lab

2013 was the first full year in the all-new building in Lugano. It was not a quiet year, though, as the acquisition of a new supercomputer had been on the agenda, which will eventually replace "Monte Rosa" (Cray XE6) as the flagship machine of CSCS.

The first 12 cabinets of this new computer, a Cray XC30, were installed in early 2013 and opened to the user community on April 1st. In good tradition the computer has been named after a prominent Swiss Mountain, and "Piz Daint" in the Munster Valley of the Swiss Ortler Alps was chosen as the namesake.

This installation just marked the beginning of a new era of supercomputing at CSCS. A major upgrade started already in October, and it more than doubled the size of the system to 28 cabinets. More importantly, the upgrade transformed the massively parallel CPU-based supercomputer into one that additionally included one NVIDIA GPU on every single node. In the final configuration, the 28 cabinets of "Piz Daint" accomodate 5'272 hybrid compute nodes, each equipped with one Intel Xeon E5 processor and one NVIDIA Tesla K20X GPU. "Piz Daint" is the first supercomputer at CSCS that was co-designed by scientists who contributed with numerous test runs of key scientific application codes.

CHRONOS, a new call for proposals

Anticipating the significant increase of compute power available in 2014 as well as the move toward hybrid CPU-GPU computing, CSCS has launched a new annual call for proposals dubbed CHRONOS, which specifically addresses these changes. Scientific projects were sought that tackle significant and high-impact problems, require substantial compute resources, and ideally profit optimally from the hybrid GPU-CPU architecture. The acronym **CHRONOS** emphasizes the essential requirements as it stands for "**C**omputationally-Intensive, **H**igh-Impact **R**esearch **O**n **N**ovel **O**utstanding **S**cience", and the call specifically encourages the use of GPU-enabled codes. The CHRONOS program solicits top-quality proposals from researchers all over the world, and so is not restricted to Swiss institutions.

The first call closed, and a total of seven proposals were received from Swiss (4) and German (1) research groups as well as from international collaborations (2) involving Swiss scientists. Following proposal review and panel committee deliberations, five of them were awarded a total of 265 Mio core hours per year on the upgraded "Piz Daint", available as of April 2014.

Resources allocated in 2013

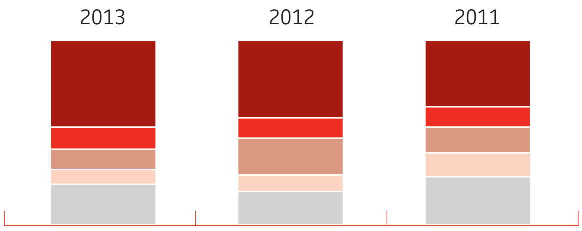
CHRONOS calls are made in addition to the standard semi-annual calls for production projects, which still dominate resource allocation at CSCS. In 2013, a total of 90 production proposals were active on "Monte Rosa" as well as the initial (non-GPU) version of "Piz Daint". Although the number of projects is slightly bigger than in 2012 (83), the total allocated time increased sharply from 271 Mio core hours to about 413 Mio core hours. This observation confirms our general experience that computational projects grow rapidly in complexity and demand, thus necessitating regular upgrades and expansion of supercomputer facilities. Design, acquisition, and installation of "Piz Daint" are just the most recent pieces in the chain of activities, by which CSCS meets this continuing challenge.

Resource distributions manifest a wide range of fields for which computational studies make important contributions. When compared to previous years, they may further identify particular needs of certain disciplines. In 2013 more than half of the allocation (59%, compared to 41% in 2012) went to Chemistry & Materials, a number that is due in no small part to today's chance to simulate molecular assemblies with quantum physical rather than empirical models, an opportunity that potentially increases accuracy and paves the way to novel insight, but is also very demanding on computational resources. Other fields, such as Earth & Enviromental Science seem to have lost in importance (6%, compared to 16% in 2012), but in reality, and in absolute terms, required similar amounts of computational resources as last year. The remaining fields, including Mechanics & Engineering (13%), Physics (14%), Life Science (6%), and Computer Science (1%), seem to show demands that rise continually over time, so that percentile numbers remain fairly constant.

Usage Statistics

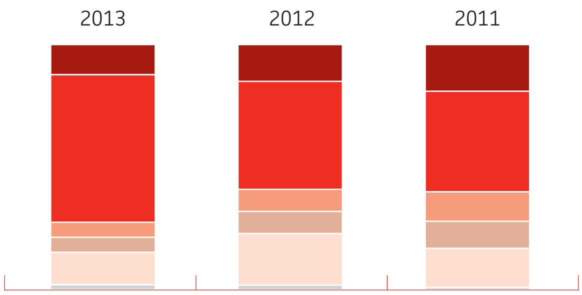
Usage by Institution (%)

Institution	2013	2012	2011
ETH Zurich	47	42	36
University of Zurich	12	20	14
EPF Lausanne	11	11	11
University of Basel	8	9	13
Others	22	18	26
Total Usage	**100**	**100**	**100**



Usage by Research Field (%)

Research Field	2013	2012	2011
Physics	14	15	19
Chemistry & Materials	59	44	41
Earth & Environ. Science	6	9	12
Life Science	6	9	11
Mechanics & Engineering	13	21	16
Others	2	2	1
Total Usage	**100**	**100**	**100**



10 Largest Projects

Principal Investigator	Organisation	Research Field	Project Title	Granted Allocation in core hrs (Mio CPU h)
Joost VandeVondele	ETH Zurich	Materials Science	Exploring frontiers in nanoscale simulation: new models and improved accuracy	46.00
Martin Kunz	University of Geneva	Astrophysics	Large field-theory simulations of cosmic strings and other topological defects	28.63
Christoph Schär	ETH Zurich	Climate	Towards high-resolution climate change scenarios on European to Alpine scales	15.00
Petros Koumoutsakos	ETH Zurich	Fluid Dynamics	Optimization of shape, motion and formation patterns of single and multiple swimmers	14.00
Leonhard Kleiser	ETH Zurich	Fluid Dynamics	Noise emission and vortex breakdown in round subsonic jets	13.00
Mathieu Luisier	ETH Zurich	Nanoscience	Quantum transport simulations of Si-InAs tunneling devices	13.00
Rubén Cabezón	University of Basel	Astrophysics	Matter accretion on compact objects: the role of neutrinos, magnetic field and equations of state	12.48
Petros Koumoutsakos	ETH Zurich	Fluid Dynamics	Compressible vortex reconnection at high reynolds numbers	12.07
Jürg Hutter	University of Zurich	Chemical Sciences	Atomistic simulation of molecules at interfaces	12.00
Andreas Hauser	University of Geneva	Chemical Sciences	Photophysics and photochemistry of transition metal compounds: Theoretical approaches/magnetic properties of the compound [Co(bpy)3][LixNa1-xRh(ox)3]	10.25

List of Projects by Institution

CERN

Lattice QCD at physical quark masses, Stefan Schaefer (Lattice Gauge Theory, 10.00 Mio CPU h)

EMPA

CarboCount CH, Dominik Brunner (Climate, 2.38 Mio CPU h)

EPF Lausanne

Top-down formation of carbon nanotubes from graphene: learning and designing with large-scale ab initio simulations Wanda Andreaoni (Materials Science, 7.24 Mio CPU h)

Characterization of the role of nucleotide binding domain in the allosteric mechanism of Hsp70 chaperone machinery, Alessandro Barducci (Biological Sciences, 0.96 Mio CPU h)

Understanding the effect of quantum nuclei on hydrogen bonding, charge transport and dissociation in liquid water, Michele Ceriotti (Chemical Sciences, 7.50 Mio CPU h)

Application of Large-Eddy simulation to atmospheric boundary layer flows above urban surfaces, Wai Chi Cheng (Geoscience, 1.97 Mio CPU h)

Energetic particle physics in magnetically confined configurations, Anthony W. Cooper (Plasma Physics, 1.00 Mio CPU h)

Characterization of the cytochrome bc1 complex and its interactions with cardiolipins, Matteo Dal Peraro (Biological Sciences, 2.15 Mio CPU h)

Large-Eddy simulation of diurnal cycles of alpine slope winds, Marc Parlange (Geoscience, 0.50 Mio CPU h)

Numerical simulations of vascular districts, Alfio Quarteroni (Fluid Dynamics, 6.00 Mio CPU h)

Simulation of plasma turbulence in the edge of tokamak devices, Paolo Ricci (Plasma Physics, 3.00 Mio CPU h)

Multiscale simulations of biological systems and bioinspired devices, Ursula Röthlisberger (Chemical Sciences, 6.44 Mio CPU h)

Variational Monte Carlo calculation of the square lattice Mott insulator magnetic excitation spectrum, Heinrik Ronnøw (Materials Science, 10.00 Mio CPU h)

Light-matter interaction from first principles: new developments in nonadiabatic dynamics with applications in energy production, saving, and storage, Ivano Tavernelli (Chemical Sciences, 1.75 Mio CPU h)

ORB5-Turbulence, Laurent Villard (Plasma Physics, 1.00 Mio CPU h)

Spin-orbit effects in Dirac fermion materials, Oleg Yazyev (Materials Science, 1.00 Mio CPU h)

ETH Zurich

Entropic lattice Boltzmann method for turbulent flow simulations, Shyam Chikatamarla (Fluid Dynamics, 1.00 Mio CPU h)

Knotted vortices: entropic lattice Boltzmann method for simulation of vortex dynamics, Shyam Chikatamarla (Fluid Dynamics, 3.66 Mio CPU h)

Computational science for the metrology of nanostructures, Mauro Ciappa (Engineering Physics, 0.40 Mio CPU h)

Development of a database of physics-based synthetic earthquakes for ground motion prediction, Luis Dalguer (Geo-science, 3.44 Mio CPU h)

Multi-scale full seismic waveform inversion, Andreas Fichtner (Geoscience, 6.20 Mio CPU h)

The next frontier in cosmological simulations of galaxy formation, Javiera Guedes (Astrophysics, 5.50 Mio CPU h)

Galaxy clusters as cosmological probes, Oliver Hahn (Astrophysics, 10.00 Mio CPU h)

Compressible vortex reconnection at high Reynolds numbers, Petros Koumoutsakos (Fluid Dynamics, 12.07 Mio CPU h)

Optimization of shape, motion and formation patterns of single and multiple swimmers, Petros Koumoutsakos (Fluid Dynamics, 14.00 CPU h)

Uncertainty quantification and propagation for large scale molecular dynamics simulations of nano-fluidics, Petros Koumoutsakos (Nanoscience, 4.00 Mio CPU h)

The role of aerosols in the climate system: a global Earth system perspective, Ulrike Lohmann (Climate, 8.00 Mio CPU h)

Quantum transport simulations of Si-InAs tunneling devices, Mathieu Luisier (Nanoscience, 13.00 Mio CPU h)

Saturated MHD turbulence in galaxy clusters, Francesco Miniati (Astrophysics, 1.00 Mio CPU h)

Towards high-resolution climate change scenarios on European to Alpine scales, Christoph Schär (Climate, 15.00 Mio CPU h)

Bandgap engineering in multi homojunction devices, Florian Schiffmann (Materials Science, 1.00 Mio CPU h)

Land-climate feedbacks in a changing climate, Sonia Seneviratne (Climate, 0.80 Mio CPU h)

High-order series expansions for quantum magnets, Matthias Troyer (Materials Science, 5.33 Mio CPU h)

Exploring frontiers in nanoscale simulation: new models and improved accuracy, Joost VandeVondele (Materials Science, 46.00 Mio CPU h)

Study dynamics of the unitary Fermi gas using time-dependent density-functional theory, Lei Wang (Materials Science, 1.50 Mio CPU h)

Theoretical modeling of tip enhanced Raman spectroscopy (TERS) Anti-Stokes studies, Renato Zenobi (Materials Science, 4.80 Mio CPU h)

Paul Scherrer Institute

Thermodynamic equilibrium in cement from molecular simulations, Sergey Churakov (Materials Science, 1.55 Mio CPU h)

Simulation of radiation damage in nuclear materials, Matthias Krack (Materials Science, 2.10 Mio CPU h)

Large-Eddy simulation of particle-laden flow in the steam generator bundle, Roman Mukin (Fluid Dynamics, 2.00 Mio CPU h)

Surface reactivity from first principles for the iron-sulfur world, Andras Stirling (Chemical Sciences, 3.40 Mio CPU h)

University of Basel

Gating mechanisms of the ASIC acid-sensing ion channel, Simon Bernèche (Biological Sciences, 1.00 Mio CPU h)

Matter accretion on compact objects: the role of neutrinos, magnetic field and equations of state, Rubén Cabezón (Astrophysics, 12.48 Mio CPU h)

Structure prediction of clusters, solids and surfaces, Stefan Goedecker (Nanoscience, 10.00 Mio CPU h)

Elephant: A three-dimensional supernova model for efficient parameter studies with spectral neutrino transport, Matthias Liebendörfer (Astrophysics, 3.50 Mio CPU h)

University of Bern

ISOCARB, Fortunat Joos (Climate, 0.88 Mio CPU h)

Time-slice and transient simulations of key periods in the past, Christoph Raible (Climate, 3.03 Mio CPU h)

Modeling disparate scales within BATS-R-US, Martin Rubin (Computer Science, 0.25 Mio CPU h)

University of Geneva

Interplay between structure and electronic properties in materials with strong correlations, Antoine Georges (Materials Science, 5.50 Mio CPU h)

Large field-theory simulations of cosmic strings and other topological defects, Martin Kunz (Astrophysics, 28.63 Mio CPU h)

University of Naples

Investigating the binding conformational flexibility of non-nucleoside reverse transcriptase inhibitors through metadynamics simulations principal, Agostino Bruno (Biological Sciences, 0.95 Mio CPU h)

Università della Svizzera italiana

Study of the functional protein motion in amyloid-beta peptide by means metadynamics & parallel tempering, Albert Ardèvol (Biological Sciences, 1.50 Mio CPU h)

Simulation of GeTe nanowires for phase change memories, Sebastiano Caravati (Materials Science, 3.14 Mio CPU h)

Simulation of large scale conformation fluctuations in Adenylate Kinase, Elena Formoso (Chemical Sciences, 0.90 Mio CPU h)

Fundamental studies of the air-water interface, Ali Hassanali (Materials Science, 0.50 Mio CPU h)

Combining all-atoms enhanced sampling techniques and NMR experimental data for a novel structure determination protocol, Michele Parrinello (Biological Sciences, 1.10 Mio CPU h)

Blood flow in microvessels and at bifurcations: parallel simulations, Igor Pivkin (Biological Sciences, 0.82 Mio CPU h)

Improving diagnosis of atrial fibrillation, Mark Potse (Medical/Life Science, 4.00 Mio CPU h)

Polyamorphism in the phase change compound GeTe, Gabriele Sosso (Materials Science, 0.50 Mio CPU h)

University of Zurich

Simulating the effects of a preheated universe on the baryon content of dwarfs and galaxies, Michael Busha (Astrophysics, 5.00 Mio CPU h)

The birth of the Milky Way: simulating galaxy assembly and supermassive black hole growth, Alexander Hobbs (Astrophysics, 3.80 Mio CPU h)

CP2K: program development, Jürg Hutter (Chemical Sciences, 2.40 Mio CPU h)

Atomistic simulation of molecules at interfaces, Jürg Hutter (Chemical Sciences, 12.00 Mio CPU h)

The tidal evolution of dwarf galaxies as a clue to the missing satellites problem; high resolution simulations, Lucio Mayer (Astrophysics, 2.20 Mio CPU h)

Feedback mechanisms in star formation: from molecular clouds to primordial minihalos, Thomas Peters (Astrophysics, 3.00 Mio CPU h)

Dark matter in cosmological simulations of dwarf galaxies, Justin Read (Astrophysics, 0.56 Mio CPU h)

Regulating baryons with feedback processes across the hubble sequence, Rok Roškar (Astrophysics, 4.25 Mio CPU h)

Curved aromatic systems in the solid-state for advanced applications, Laura Zoppi (Materials Science, 1.25 Mio CPU h)

Renewals

EMPA

Applied nanoscience: novel catalysts and bottom-up design of graphene-like nanostructures. Computational insight within a surface science laboratory, Daniele Passerone (Nanoscience, 5.00 Mio CPU h)

EPF Lausanne

Large-scale simulations of carbon nanotubes for NANOTERA device applications, Wanda Andreaoni (Materials Science, 4.40 Mio CPU h)

First-principles design and engineering of electronic and thermal transport – from nanoelectronics devices to novel thermoelectrics, Nicola Marzari (Materials Science, 2.00 Mio CPU h)

Defect levels at interfaces of high-mobility semiconductors through hybrid density functionals, Alfredo Pasquarello (Computational Condensed Matter Physics, 1.60 Mio CPU h)

Application of Large-Eddy simulation to atmospheric boundary layer flows, Fernando Porté-Agel (Geoscience, 1.30 Mio CPU h)

ETH Zurich

Direct numerical simulations of heat transfer and catalytic combustion in three-dimensional channels, Christos Frouzakis (Combustion, 1.88 Mio CPU h)

Direct numerical simulation of flow, heat transfer, and autoignition in engine-like geometries, Christos Frouzakis (Combustion, 2.50 Mio CPU h)

Exact diagonalization study of the fractional quantum Hall effect, Sergei Isakov (Materials Science, 8.74 Mio CPU h)

Noise emission and vortex breakdown in round subsonic jets, Leonhard Kleiser (Fluid Dynamics, 13.00 Mio CPU h)

Numerical simulation of particle-laden multi-phase flows, Leonhard Kleiser (Fluid Dynamics, 3.40 Mio CPU h)

SILENS - Subcritically bifurcating instability of the leading-edge boundary layer investigated by numerical simulations, Leonhard Kleiser (Fluid Dynamics, 1.75 Mio CPU h)

Massively parallel multilevel montecarlo finite volume simulations for uncertainty quantification in nonlinear wave propagation, Christoph Schwab (Applied Mathematics, 2.20 Mio CPU h)

Coupled and competing instabilities in complex oxides, Nicola Spaldin (Materials Science, 1.00 Mio CPU h)

Image-based analyses of bone structure and function, Harry van Lenthe (Biomedical Engineering, 2.00 Mio CPU h)

Precessionally driven turbulence and dynamos in spheroidal and cylindrical enclosures, Stijn Vantieghem (Geoscience, 4.80 Mio CPU h)

Simulating integrin junctions under tension: from the extracellular matrix to the cytoskeleton, Viola Vogel (Biological Sciences, 3.20 Mio CPU h)

Hydrocean

Simulation of ship survivability under wave impact by simulation with SPH-Flow, David Guibert (Fluid Dynamics, 0.75 Mio CPU h)

University of Basel

The role of dimerization in protein activation and signalling, Markus Meuwly (Chemical Sciences, 0.50 Mio CPU h)

University of Bern

Assessing climate variability from 800 to 2100 AD and decadal predictability, Christoph Raible (Climate, 3.50 Mio CPU h)

University of Geneva

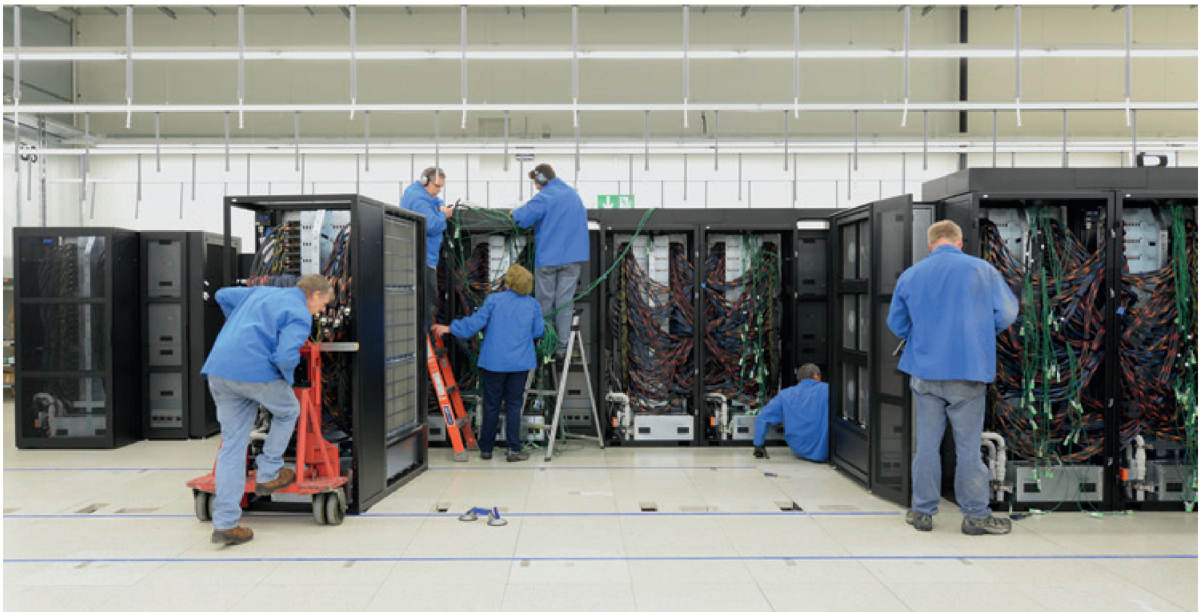
Photophysics and photochemistry of transition metal compounds: theoretical approaches/magnetic properties of the compounds [Co(bpy)3][LixNa1-xRh(ox)3], Andreas Hauser (Chemical Sciences, 10.25 Mio CPU h)

Accurate spin-state energetics of transition metal complexes, Max Lawson Daku (Chemical Sciences, 5.00 Mio CPU h)

Università della Svizzera italiana

Conformational study of p38 alpha MAP kinase in free and ligand bound forms, Michele Parrinello (Biological Sciences, 1.00 Mio CPU h)

Electrophysiology of heart failure, Mark Potse (Medical/Life Science, 0.72 Mio CPU h)



“Piz Daint” during its upgrade to 28 cabinets and 5’272 hybrid CPU-GPU compute nodes.

New Insight into the Earth's Deep Interior

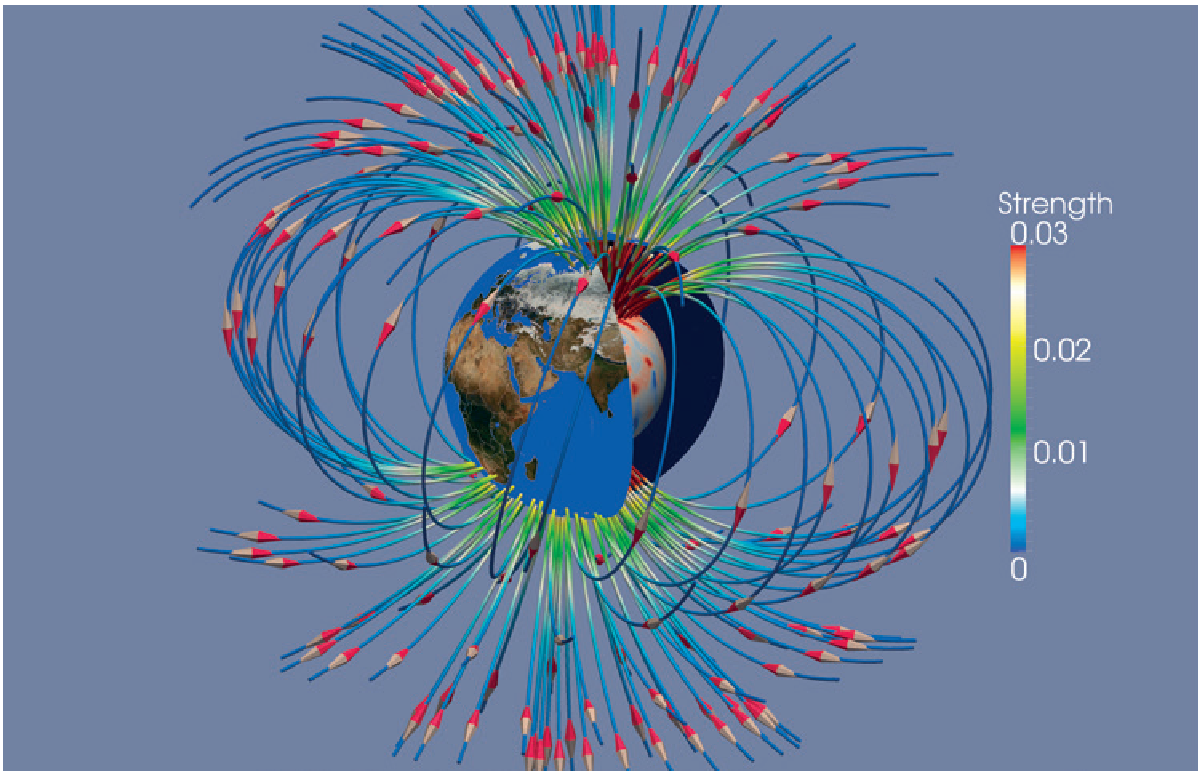
For 300 years we have known that the Earth's magnetic field moves gradually westward. Computer simulations on the CSCS supercomputer "Monte Rosa" by researchers at ETH Zurich and the University of Leeds explain why this happens.

The Earth's magnetic field surrounding our globe protects the Earth from harmful radiation and helps animals like birds or bats to get their bearings. The Earth's magnetic field is mainly generated by the so-called geodynamo processes in the liquid outer core and in the solid inner core. Philip Livermore from the University of Leeds along with Rainer Hollerbach and Andrew Jackson from ETH Zurich have now demonstrated for the first time, using computer simulations on the CSCS supercomputer "Monte Rosa", that the magnetic field in turn influences these dynamic processes in the Earth's core. Hence, the magnetic field leads to the solid inner core – which is about the size of the moon – rotating in an easterly direction and the outer core fluid and magnetic field being pushed westward. The latter was already observed back in 1692 by the discoverer of Halley's comet, the natural scientist Edmund Halley, but could not be explained up to now.

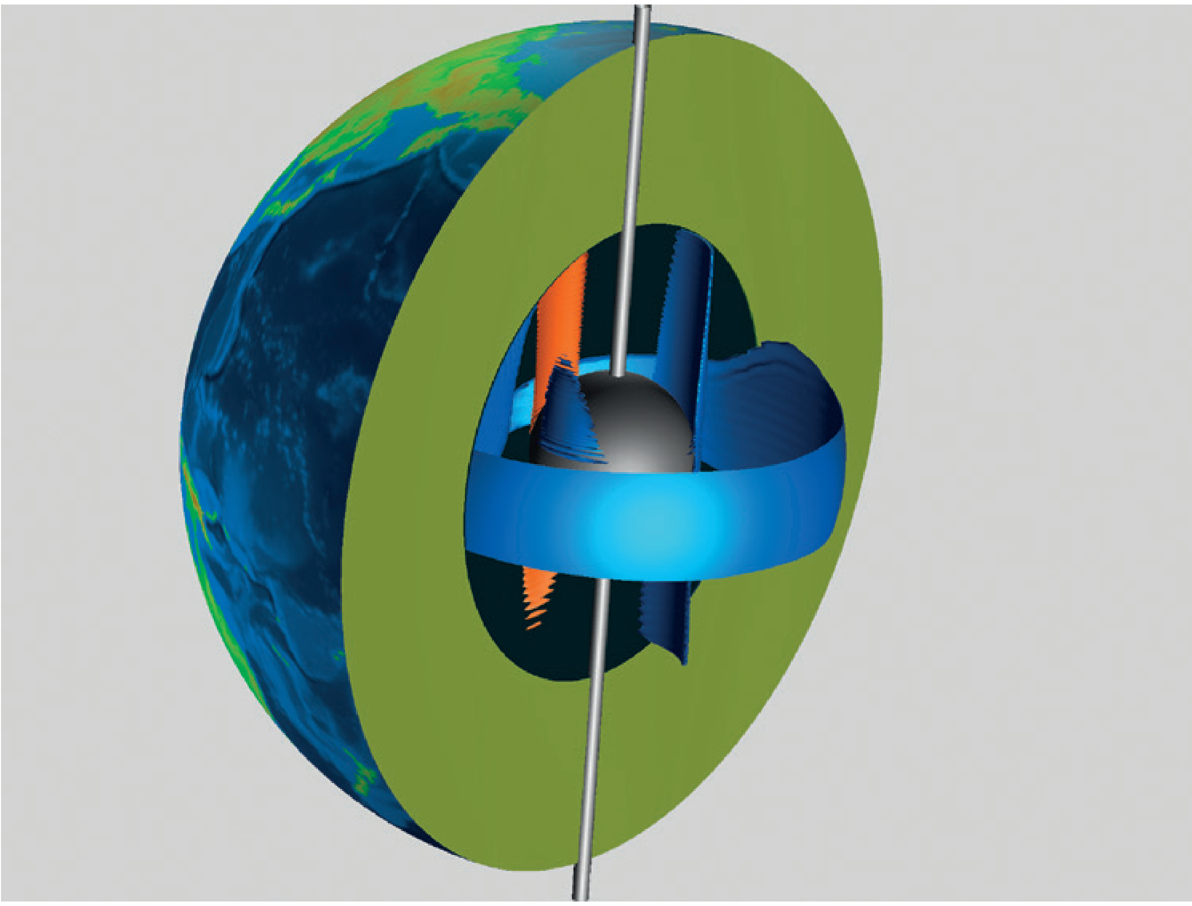
Thrust to the east and west

The scientists used new methods for their simulation and worked in particular with a viscosity that was two orders of magnitude lower and thus 100 times closer to reality than in previous models. The scientists said that this was how they had succeeded in achieving correspondingly higher resolutions of certain physical processes in the Earth's core.

The simulations show that the force of the Earth's magnetic field in the outermost region of the liquid core drives the magnetic field westwards. At the same time, these very forces give the solid inner core a thrust towards the east. This leads to Earth's inner core having a higher rotation speed than the Earth.



Earth's magnetic field is generated in its liquid iron core. Depicted are the results of a 3-D self-consistent computer simulation. Magnetic field lines are shown, with the strongest field near the poles being depicted in red and yellow.



The cut-away view of the earth is showing the inner core and rotation axis in grey. In blue the westward move of the outer magnetic field and in red the eastward move of the inner core.

Based on their study the researchers came to the conclusion that even subtle changes in the Earth's inner magnetic field can lead to the respective directions of movement being reversed. This, in turn, explains the observation that over the last 3'000 years the Earth's magnetic field has shifted on several occasions eastward instead of westward. It was likely that the Earth's inner core then rotated in a westerly direction, instead of eastwards.
According to the researchers even the smallest changes in the magnetic field could have led to different rotation speeds of the inner core. The research team of Hrvoje Tkalcic at the Australian National University recently made just such an observation of spin rate fluctuations over the last 50 years.

Sole opportunity for reconstruction

Numerical models of the Earth's magnetic field rank among the most computer-intensive simulations in high performance computing. In the simulations systems of equations governing fluid dynamics, classical mechanics and thermodynamics have to be solved. Together with seismic measurements, such simulations are the only tool for researching the Earth's interior from depths of 2'900 kilometres all the way to the Earth's centre at a depth of 6'378 kilometres. In recent decades studies of this kind have made enormous contributions to understanding what happens in the Earth's interior.

HPC Wire, one of the most important news and information resource about HPC, nominated this study as one of the 30 top supercomputing led discovery of 2013.

Sea-ice Formation Sustained the "Little Ice Age"

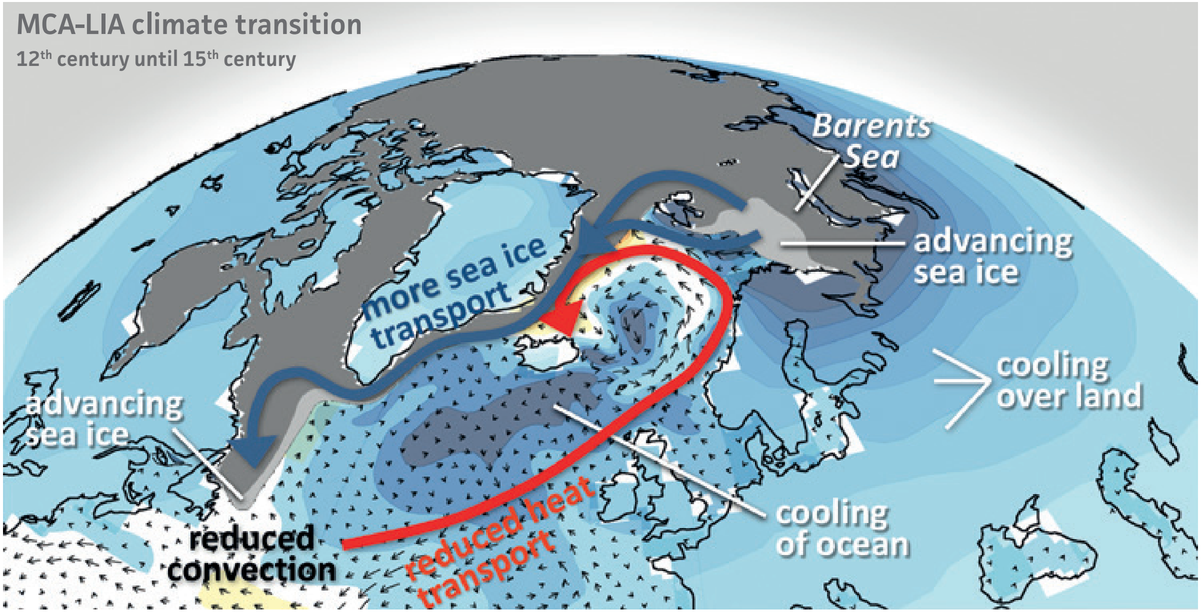
Volcanic eruptions and reduced solar radiation caused global cooling between the thirteenth and the fifteenth centuries. The resulting accelerated formation of sea ice in the Northern Seas triggered a positive feedback process that shaped the Little Ice Age, as a new study by climate scientists from the University of Bern and the Oeschger Centre for Climate Change Research reveals.

The winter weather in Europe is largely governed by the so-called North Atlantic Oscillation (NAO). This air pressure seesaw between the Azores High and the Icelandic Low produces mild winters in Central and Northern Europe if the two air pressure centres are particularly pronounced and cold winters if they are weak. Until now, the NAO was believed to be jointly responsible for the cooling in the early fifteenth century along with volcanic eruptions and weakened solar radiation. The subsequent Little Ice Age continued into the nineteenth century. Now, however, Bernese climate researchers Flavio Lehner, Andreas Born, Christoph Raible and Thomas Stocker reveal that the Little Ice Age was also able to take its course without the influence of the NAO, driven purely by the consequences of strong and frequent volcanic eruptions at the time, a reduced solar radiation, or both together.

Simulating feedback mechanism

Using simulations on the CSCS supercomputer "Monte Rosa", the climate researchers searched for a feedback process that was capable of triggering the Little Ice Age. As the driving forces of the climate, they applied volcanic eruptions and a weakening of solar radiation in their models. Although six slightly different starting conditions were selected for the simulations, every simulation initiated the same process: in the Barents Sea, the sea-ice masses grew and spread to the warmer sub-arctic area of the North Atlantic, where they melted. The freshwater inflow resulting from the meltwater altered the water stratification and thus the differences in density. As a result, the ocean convection, driven by the density differences, was weakened and less warm water was transported into the Nordic Seas, which in turn boosted the growth of sea ice. This so-called positive feedback process intensified the Little Ice Age especially in northern latitudes.

For the first time, the scientists verified their results with a synthetic ice formation simulation, in which they allowed sea ice to grow artificially in the Barents Sea without factoring in the consequences of volcanic activity or less solar radiation. "Starting with the Barents Sea, which is still one of the 'ice machines' of the Arctic today, we were able to trigger the same



This image depicts the feedback mechanism between cooling and sea-ice formation in the Barents Sea. As a result, the ocean circulation is weakened and less warm water reaches the North.

feedback process that we had previously observed in the simulations driven solely by volcanoes and solar radiation," says Lehner. According to the scientists, the feedback process in the models continued for up to seventy years even after the artificial ice growth had been "switched off".

For the scientists, the fact that all the slightly altered, realistic simulations and the synthetic ice simulation yielded consistent results is solid proof that the Little Ice Age was primarily governed by external triggers. Volcanic activity and less solar radiation initially caused an increase in sea-ice formation independently of atmospheric circulation. Due to the cooling, the mean sea level pressure gradually increased over the Barents Sea, which enabled the cold air to reach Europe. "However, this pressure response is clearly a delayed reaction of the atmosphere to the preceding processes in the ocean," says Raible.

New questions

For the Bernese climate researchers, the motivation behind this study was a previous project conducted in 2012, in which they used simulations to verify the hypothesis as to whether the North Atlantic Oscillation dominated the so-called Medieval Climate Anomaly (from around 800 to 1'100 years ago). The unusually warm period of the Medieval Climate Anomaly preceded the Little Ice Age. In 2009 another research team had postulated a persistent and very pronounced positive NAO during this warm period based on reconstructed precipitation data. Moreover, the researchers identified a clear transition to an oscillating, more negative NAO at the beginning of the Little Ice Age. Based on their results, they concluded that the NAO had a major influence on the Medieval Climate Anomaly and its transition to the Little Ice Age.

When the Bernese researchers failed to confirm these conclusions in their climate model simulations, they began to search for the plausible mechanism, now published in the *Journal of Climate of the American Meteorological Society,* which triggered the Little Ice Age irrespective of the NAO. The researchers are convinced that "by improving our understanding of past climate fluctuations and thus of the complex climate, we are able to gain valuable insights for possible future scenarios." The simulations the scientists used to identify the feedback mechanism cover a time period up to the year 1500, by which time the transition to the Little Ice Age was complete. Currently, simulations are running on Monte Rosa spanning from the Medieval Climate Anomaly, which started around the year 850, to 2100. The researchers expect the first results this winter.

The accelerated formation of sea ice in the Northern Seas triggered a positive feedback process that shaped the Little Ice Age that lasted about from 1500 to 1850.

Mechanical Stimulus Crucial for Bone Development

Researchers from ETH Zurich demonstrated for the first time *in vivo* how bone tissue responds to local mechanical stimuli that control bone formation.

It is common knowledge that mechanical stress on bones, such as through jogging or walking, encourages bone formation. Just how the bone-forming cells – but also their bone-resorbing counterparts in the absence of strain – in the bone marrow respond to mechanical stimuli, however, remained unclear. For the first time, researchers have now demonstrated how local mechanical stress and bone formation or resorption (bone breakdown) are linked by combining lab experiments and simulations on the CSCS supercomputer "Monte Rosa". This revealed that the build-up and breakdown of bone substance is eighty-per-cent controlled by mechanical stimuli.

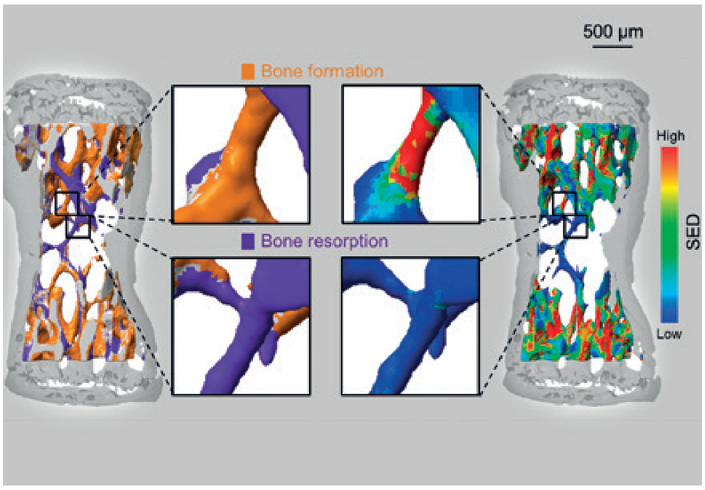


Image of the 3D simulation depicting the stress in the bone tissue calculated based on CT images. The red areas represent high mechanical stress and bone formation, the blue ones low stress and bone resorption.

Strain encourages balanced bone formation

The simulations reveal how the mechanical strain exerted locally in the lab – by stretching a vertebral body in a mouse tail – leads to the build-up of the bone substance in certain places and its resorption elsewhere. According to the researchers, the results also confirm the assumption that bone substance is formed where it is needed and resorbed where it is not. A well-balanced interplay between osteoblasts, which are responsible for bone formation, and osteoclasts, which resorb and break down bones, is important in a healthy organism. Both the over- and underproduction of these two kinds of cells leads to abnormal changes in the bone structure. "Our study is thus essential to gain a better understanding of bone diseases and how to develop new medications," Ralph Müller, the study director and a professor at ETH Zurich, is convinced.

The scientists used different groups of mice for their experiments. While a certain caudal vertebra segment was stressed mechanically three times a week for a period of four weeks in one group, this part of the experiment was omitted for the control group. Moreover, there was another test group where the ovaries were removed from the animals. The resulting lack of oestrogen has a negative impact on bone formation and leads to bone resorption – presumably one of the reasons why around thirty per cent of women develop osteoporosis after the menopause.

Experiment and simulation indicate correlation

During the experiments, the researchers regularly took high-resolution computed tomography images of the animals. Superimposed and processed into three-dimensional representations using imaging processing, the images produced spatial models displaying the areas of bone formation, bone resorption and areas where nothing has changed. The scientists then exposed these models virtually to different forces on the supercomputer and calculated what happens next for every area. Through these simulations, the researchers were able to study the link between local mechanical stress and its impact on the bone at the cellular level. "The results clearly show that the activity of both the osteoblasts and the osteoclasts is controlled by mechanical strain," says Müller. "High local strains lead to the formation of the bone and low strains provoke its resorption." According to the researchers' analyses, the probability of bone substance being resorbed under increasing mechanical strain decreases exponentially while bone formation increases exponentially. Moreover, bone resorption appears to be controlled mechanically considerably more than bone formation, especially in mice without ovaries, where non-specific bone resorption increases significantly in the absence of mechanical strain. In other words, bone substance is also resorbed in places where it is actually needed. For the scientists, the results echo the mounting evidence that oestrogen receptors are involved in the bone-cell response to mechanical stimuli. In other words, a lack of oestrogen receptors limits targeted bone resorption.

Detail showing the island in the distribution deck dedicated to “Piz Daint”: this is where the cold water preparation and electricity distribution happens.

Papers with Highest Journal Impact Factor[1)]

Science

Impact Factor: 31.20

M. Setvin, U. Aschauer, P. Scheiber, Y. F. Li, W. Y. Hou, et al., Reaction of O-2 with Subsurface Oxygen Vacancies on TiO2 Anatase (101), Science, Doi 10.1126/Science.1239879.

S. V. Kalinin, N. A. Spaldin, Functional Ion Defects in Transition Metal Oxides, Science, Doi 10.1126/Science.1243098.

Angewandte Chemie-International Edition

Impact Factor: 13.46

M. Salvalaglio, T. Vetter, M. Mazzotti, M. Parrinello, Controlling and Predicting Crystal Shapes: The Case of Urea, Angewandte Chemie-International Edition, Doi 10.1002/Anie.201304562.

V. Limongelli, S. De Tito, L. Cerofolini, M. Fragai, B. Pagano, et al., The G-Triplex DNA, Angewandte Chemie-International Edition, Doi 10.1002/Anie.201206522.

L. E. Polander, A. Yella, B. F. E. Curchod, N. A. Astani, J. Teuscher, et al., Towards Compatibility between Ruthenium Sensitizers and Cobalt Electrolytes in Dye-Sensitized Solar Cells, Angewandte Chemie-International Edition, Doi 10.1002/Anie.201304608.

Nano Letters

Impact Factor: 13.20

J. H. Walther, K. Ritos, E. R. Cruz-Chu, C. M. Megaridis, P. Koumoutsakos, Barriers to Superfast Water Transport in Carbon Nanotube Membranes, Nano Letters, Doi 10.1021/Nl304000k.

H. Y. Cun, M. Iannuzzi, A. Hemmi, S. Roth, J. Osterwalder, et al., Immobilizing Individual Atoms beneath a Corrugated Single Layer of Boron Nitride, Nano Letters, Doi 10.1021/Nl400449y.

Annual Review of Fluid Mechanics

Impact Factor: 12.77

P. Koumoutsakos, I. Pivkin, F. Milde, The Fluid Mechanics of Cancer and Its Therapy, Annual Review of Fluid Mechanics, Doi 10.1146/Annurev-Fluid-120710-101102.

Nature Geoscience

Impact Factor: 11.75

P. Regnier, P. Friedlingstein, P. Ciais, F. T. Mackenzie, N. Gruber, et al., Anthropogenic perturbation of the carbon fluxes from land to ocean, Nature Geoscience, Doi 10.1038/Ngeo1830.

ACS Nano

Impact Factor: 10.77

S. Kawai, A. Sadeghi, X. Feng, P. Lifen, R. Pawlak, et al., Obtaining Detailed Structural Information about Supramolecular Systems on Surfaces by Combining High-Resolution Force Microscopy with ab Initio Calculations, ACS Nano, Doi 10.1021/Nn403672m.

Journal of the American Chemical Society

Impact Factor: 9.91

Q. C. Sun, S. Mosquera-Vazquez, L. M. L. Daku, L. Guenee, H. A. Goodwin, et al., Experimental Evidence of Ultrafast Quenching of the (MLCT)-M-3 Luminescence in Ruthenium(II) Tris-bipyridyl Complexes via a (3)dd State, Journal of the American Chemical Society, Doi 10.1021/Ja407225t.

L. Talirz, H. Sode, J. M. Cai, P. Ruffieux, S. Blankenburg, et al., Termini of Bottom-Up Fabricated Graphene Nanoribbons, Journal of the American Chemical Society, Doi 10.1021/Ja311099k.

A. Shchyrba, M. T. Nguyen, C. Wackerlin, S. Martens, S. Nowakowska, et al., Chirality Transfer in 1D Self-Assemblies: Influence of H-Bonding vs Metal Coordination between Dicyano[7]helicene Enantiomers, Journal of the American Chemical Society, Doi 10.1021/Ja407315f.

T. Bauert, L. Zoppi, G. Koller, J. S. Siegel, K. K. Baldridge, et al., Quadruple Anionic Buckybowls by Solid-State Chemistry of Corannulene and Cesium, Journal of the American Chemical Society, Doi 10.1021/Ja4063103.

Proceedings of the National Academy of Sciences of The United Stated of America

Impact Factor: 9.74

Barducci, M. Bonomi, M. K. Prakash, M. Parrinello, Free-energy landscape of protein oligomerization from atomistic simulations, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1320077110.

F. Palazzesi, A. Barducci, M. Tollinger, M. Parrinello, The allosteric communication pathways in KIX domain of CBP, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1313548110.

[1)] 2013 JCR Science Edition, ISI Web of Knowledge SM

E. Demirci, T. Junne, S. Baday, S. Berneche, M. Spiess, Functional asymmetry within the Sec61p translocon, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1318432110.

M. Ceriotti, J. Cuny, M. Parrinello, D. E. Manolopoulos, Nuclear quantum effects and hydrogen bond fluctuations in water, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1308560110.

A. Hassanali, F. Giberti, J. Cuny, T. D. Kuhne, M. Parrinello, Proton transfer through the water gossamer, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1306642110.

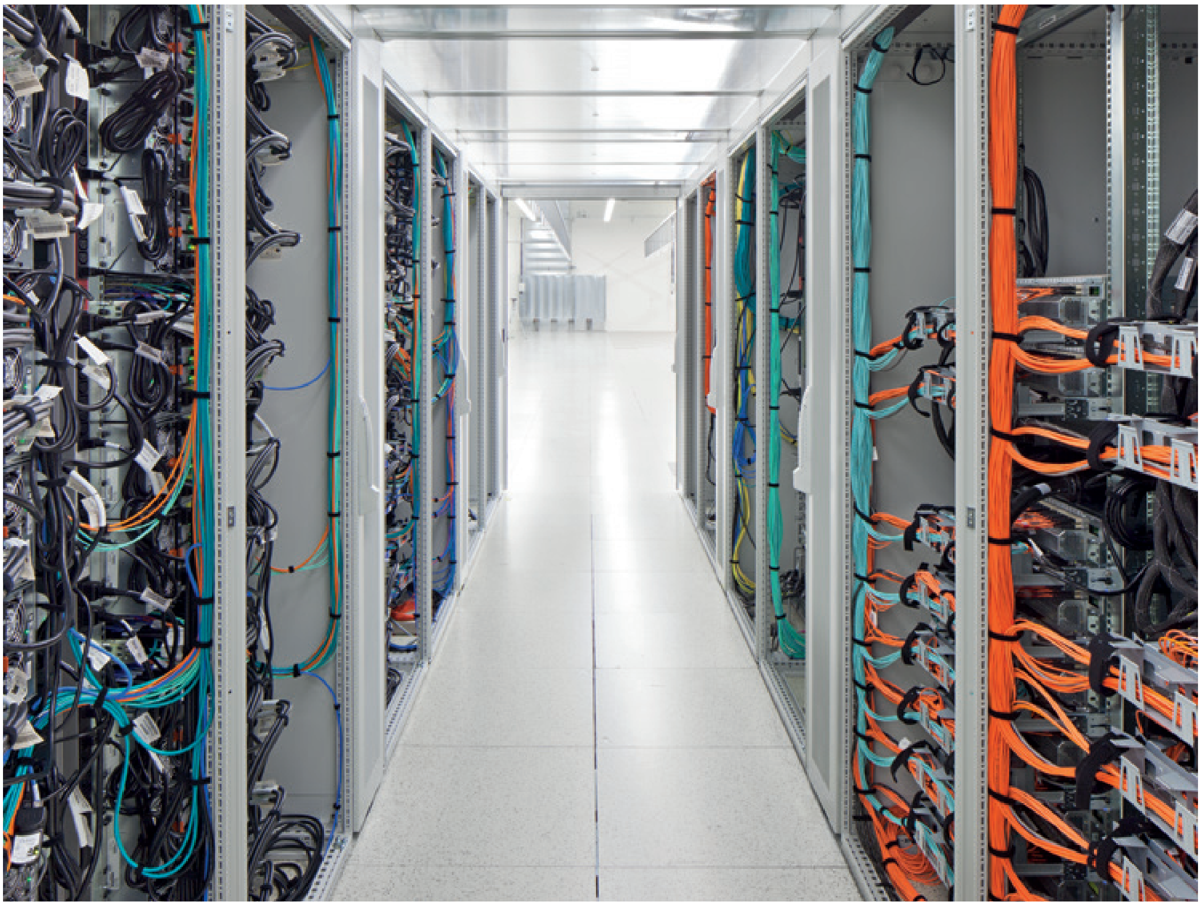
V. Limongelli, M. Bonomi, M. Parrinello, Funnel metadynamics as accurate binding free-energy method, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1303186110.

Z. L. Peng, X. J. Li, I. V. Pivkin, M. Dao, G. E. Karniadakis, et al., Lipid bilayer and cytoskeletal interactions in a red blood cell, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1311827110.

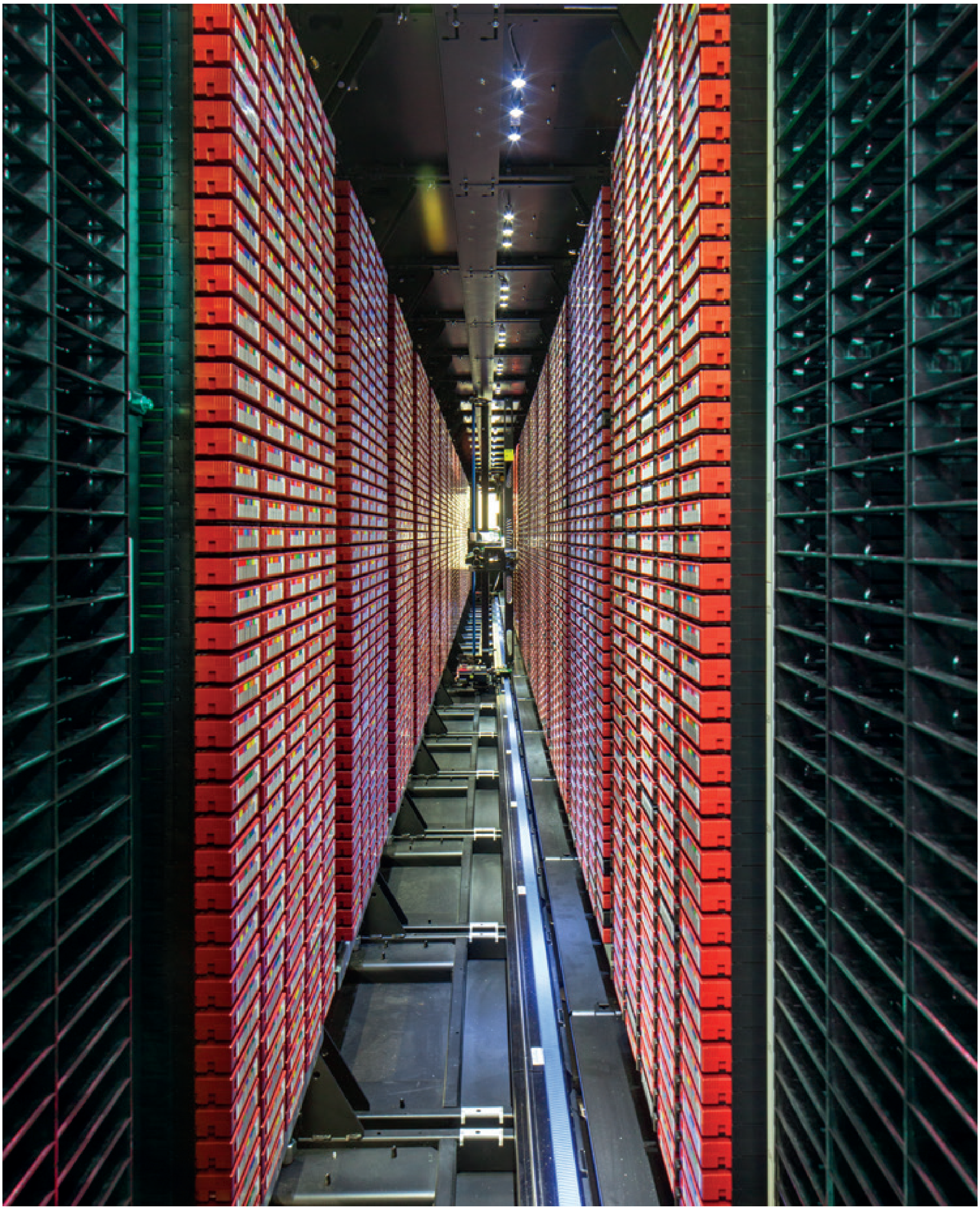
Nucleic Acids Research

Impact Factor: 8.03

S. Moretti, B. Laurenczy, W. H. Gharib, B. Castella, A. Kuzniar, et al., Selectome update: quality control and computational improvements to a database of positive selection, Nucleic Acids Research, Doi 10.1093/nar/gkt1065.



Inside the cooling island dedicated to the Blue Brain Project.



Inside the upgraded IBM TS3500 tape library.

Papers Published in 2013 by Principal Investigator[1)]

Wanda Andreoni, EPF Lausanne

J. M. H. Kroes, F. Pietrucci, A. Curioni, R. Jaafar, O. Gröning, et al., Atomic Oxygen Chemisorption on Carbon Nanotubes Revisited with Theory and Experiment, Journal of Physical Chemistry C, Doi 10.1021/Jp310332y.

Dirk Bakowies, ETH Zurich

D. Bakowies, Assessment of Density Functional Theory for Thermochemical Approaches Based on Bond Separation Reactions, Journal of Physical Chemistry A, Doi 10.1021/Jp310735h.

Alessandro Barducci, EPF Lausanne

Barducci, M. Bonomi, M. K. Prakash, M. Parrinello, Free-energy landscape of protein oligomerization from atomistic simulations, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1320077110.

F. Palazzesi, A. Barducci, M. Tollinger, M. Parrinello, The allosteric communication pathways in KIX domain of CBP, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1313548110.

Richard Barrett, SANDIA

R.F. Barrett, C.T. Vaughan, S.D. Hammond, D. Roweth, Reducing the Bulk of the Bulk Synchronous Parallel Model, Parallel Processing Letters, Doi 10.1142/S0129626413400100.

Simon Bernèche, University of Basel

S. Roy, C. Boiteux, O. Alijevic, C. W. Liang, S. Bernèche, et al., Molecular determinants of desensitization in an ENaC/degenerin channel, Faseb Journal, Doi 10.1096/Fj.13-230680.

E. Demirci, T. Junne, S. Baday, S. Bernèche, M. Spiess, Functional asymmetry within the Sec61p translocon, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1318432110.

S. Baday, S. H. Wang, G. Lamoureux, S. Bernèche, Different Hydration Patterns in the Pores of AmtB and RhCG Could Determine Their Transport Mechanisms, Biochemistry, Doi 10.1021/Bi400015f.

Shahid Bokhari, University of Ohio

S. H. Bokhari, Ü. V. Çatalyürek, M. N. Gurcan, Massively multithreaded maxflow for image segmentation on the Cray XMT-2. Concurrency Computat.: Pract. Exper., Doi: 10.1002/cpe.3181.

Dominik Brunner, EMPA

R. Lorenz, E. L. Davin, D. M. Lawrence, R. Stöckli, S. I. Seneviratne, How Important is Vegetation Phenology for European Climate and Heat Waves?, Journal of Climate, Doi 10.1175/Jcli-D-13-00040.1.

B. P. Guillod, E. L. Davin, C. Kundig, G. Smiatek, S. I. Seneviratne, Impact of soil map specifications for European climate simulations, Climate Dynamics, Doi 10.1007/S00382-012-1395-Z.

K. P. Bowman, J. C. Lin, A. Stohl, R. Draxler, P. Konopka, et al., Input Data Requirements Lagrangian Trajectory Models, Bulletin of the American Meteorological Society, Doi 10.1175/Bams-D-12-00076.1.

Sebastiano Caravati, Università della Svizzera italiana

G. C. Sosso, G. Miceli, S. Caravati, F. Giberti, J. Behler, et al., Fast Crystallization of the Phase Change Compound GeTe by Large-Scale Molecular Dynamics Simulations, Journal of Physical Chemistry Letters, Doi 10.1021/Jz402268v.

S. Caravati, G. C. Sosso, M. Bernasconi, M. Parrinello, Density functional simulations of hexagonal Ge2Sb2Te5 at high pressure, Physical Review B, Doi 10.1103/Physrevb.87.094117.

S. Caravati, G. C. Sosso, M. Bernasconi, M. Parrinello, Density functional simulations of hexagonal Ge2Sb2Te5 at high pressure, Physical Review B, Doi 10.1103/Physrevb.88.019903.

Michele Ceriotti, EPF Lausanne

M. Ceriotti, J. Cuny, M. Parrinello, D. E. Manolopoulos, Nuclear quantum effects and hydrogen bond fluctuations in water, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1308560110.

Wai Chi Cheng, EPF Lausanne

W. C. Cheng, F. Porté-Agel, Evaluation of subgrid-scale models in large-eddy simulation of flow past a two-dimensional block, International Journal of Heat and Fluid Flow, Doi 10.1016/J.Ijheatfluidflow.2013.06.007.

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

Shyam Chikatamarla, ETH Zurich

I. V. Karlin, D. Sichau, S. S. Chikatamarla, Consistent two-population lattice Boltzmann model for thermal flows, Physical Review E, Doi 10.1103/Physreve.88.063310.

S. S. Chikatamarla, I. V. Karlin, Entropic lattice Boltzmann method for turbulent flow simulations: Boundary conditions, Physica a-Statistical Mechanics and Its Applications, Doi 10.1016/J.Physa.2012.12.034.

Sergey Churakov, Paul Scherrer Institute

S. V. Churakov, Mobility of Na and Cs on Montmorillonite Surface under Partially Saturated Conditions, Environmental Science & Technology, Doi 10.1021/Es401530n.

Wilfred A. Cooper, EPF Lausanne

W. A. Cooper, I. T. Chapman, O. Schmitz, A. D. Turnbull, B. J. Tobias, et al., Bifurcated helical core equilibrium states in tokamaks, Nuclear Fusion, Doi 10.1088/0029-5515/53/7/073021.

I. T. Chapman, J. P. Graves, O. Sauter, C. Zucca, O. Asunta, et al., Power requirements for electron cyclotron current drive and ion cyclotron resonance heating for sawtooth control in ITER, Nuclear Fusion, Doi 10.1088/0029-5515/53/6/066001.

Luis Dalguer, ETH Zurich

S. G. Song, L. A. Dalguer, Importance of 1-point statistics in earthquake source modelling for ground motion simulation, Geophysical Journal International, Doi 10.1093/Gji/Ggs089.

Matteo Dal Peraro, EPF Lausanne

T. Lemmin, C. Bovigny, D. Lancon, M. Dal Peraro, Cardiolipin Models for Molecular Simulations of Bacterial and Mitochondrial Membranes, Journal of Chemical Theory and Computation, Doi 10.1021/Ct300590v.

T. Lemmin, C. S. Soto, G. Clinthorne, W. F. Degrado, M. Dal Peraro, Assembly of the Transmembrane Domain of E. coli PhoQ Histidine Kinase: Implications for Signal Transduction from Molecular Simulations, Plos Computational Biology, Doi 10.1371/Journal.Pcbi.1002878.

G. Palermo, M. Stenta, A. Cavalli, M. Dal Peraro, M. De Vivo, Molecular Simulations Highlight the Role of Metals in Catalysis and Inhibition of Type II Topoisomerase, Journal of Chemical Theory and Computation, Doi 10.1021/Ct300691u.

Andreas Fichtner, ETH Zurich

A. Fichtner, J. Trampert, P. Cupillard, E. Saygin, T. Taymaz, et al., Multiscale full waveform inversion, Geophysical Journal International, Doi 10.1093/Gji/Ggt118.

A. Fichtner, E. Saygin, T. Taymaz, P. Cupillard, Y. Capdeville, et al., The deep structure of the North Anatolian Fault Zone, Earth and Planetary Science Letters, Doi 10.1016/J.Epsl.2013.04.027.

L. Colli, A. Fichtner, H. P. Bunge, Full waveform tomography of the upper mantle in the South Atlantic region: Imaging a westward fluxing shallow asthenosphere?, Tectonophysics, Doi 10.1016/J.Tecto.2013.06.015.

Christos Frouzakis, ETH Zurich

F. Lucci, C. E. Frouzakis, J. Mantzaras, Three-dimensional direct numerical simulation of turbulent channel flow catalytic combustion of hydrogen over platinum, Proceedings of the Combustion Institute, Doi 10.1016/J.Proci.2012.06.110.

S. G. Kerkemeier, C. N. Markides, C. E. Frouzakis, K. Boulouchos, Direct numerical simulation of the autoignition of a hydrogen plume in a turbulent coflow of hot air, Journal of Fluid Mechanics, Doi 10.1017/Jfm.2013.22.

Stefan Goedecker, University of Basel

A. Willand, Y. O. Kvashnin, L. Genovese, A. Vazquez-Mayagoitia, A. K. Deb, et al., Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations, Journal of Chemical Physics, Doi 10.1063/1.4793260.

M. G. Vergniory, M. a. L. Marques, S. Botti, M. Amsler, S. Goedecker, et al., Comment on "Topological Insulators in Ternary Compounds with a Honeycomb Lattice", Physical Review Letters, Doi 10.1103/Physrevlett.110.129701.

R. Sarmiento-Perez, T. F. T. Cerqueira, I. Valencia-Jaime, M. Amsler, S. Goedecker, et al., Sodium-gold binaries: novel structures for ionic compounds from an ab initio structural search, New Journal of Physics, Doi 10.1088/1367-2630/15/11/115007.

A. Sadeghi, S. A. Ghasemi, B. Schaefer, S. Mohr, M. A. Lill, et al., Metrics for measuring distances in configuration spaces, Journal of Chemical Physics, Doi 10.1063/1.4828704.

A. Sadeghi, A. Baratoff, S. Goedecker, Electrostatic interactions with dielectric samples in scanning probe microscopies, Physical Review B, Doi 10.1103/Physrevb.88.035436.

S. Kawai, A. Sadeghi, X. Feng, P. Lifen, R. Pawlak, et al., Obtaining Detailed Structural Information about Supramolecular Systems on Surfaces by Combining High-Resolution Force Microscopy with ab Initio Calculations, ACS Nano, Doi 10.1021/Nn403672m.

T. D. Huan, M. Amsler, R. Sabatini, V. N. Tuoc, N. B. Le, et al., Thermodynamic stability of alkali-metal-zinc double-cation borohydrides at low temperatures, Physical Review B, Doi 10.1103/Physrevb.88.024108.

T. D. Huan, M. Amsler, M. a. L. Marques, S. Botti, A. Willand, et al., Low-Energy Polymeric Phases of Alanates, Physical Review Letters, Doi 10.1103/Physrevlett.110.135502.

N. Dugan, L. Genovese, S. Goedecker, A customized 3D GPU Poisson solver for free boundary conditions, Computer Physics Communications, Doi 10.1016/J.Cpc.2013.02.024.

T. F. T. Cerqueira, R. Sarmiento-Perez, F. Trani, M. Amsler, S. Goedecker, et al., The crystal structure of p-type transparent conductive oxide CuBO2, Mrs Communications, Doi 10.1557/Mrc.2013.21.

S. Botti, M. Amsler, J. A. Flores-Livas, P. Ceria, S. Goedecker, et al., Carbon structures and defect planes in diamond at high pressure, Physical Review B, Doi 10.1103/Physrevb.88.014102.

M. Amsler, J. A. Flores-Livas, M. a. L. Marques, S. Botti, S. Goedecker, Prediction of a novel monoclinic carbon allotrope, European Physical Journal B, Doi 10.1140/Epjb/E2013-40639-4.

M. Amsler, S. Botti, M. a. L. Marques, S. Goedecker, Conducting Boron Sheets Formed by the Reconstruction of the alpha-Boron (111) Surface, Physical Review Letters, Doi 10.1103/Physrevlett.111.136101.

Ali Hassanali, Università della Svizzera italiana

A. Hassanali, F. Giberti, J. Cuny, T. D. Kuhne, M. Parrinello, Proton transfer through the water gossamer, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1306642110.

Andreas Hauser, University of Geneva

A. Vargas, I. Krivokapic, A. Hauser, L. M. L. Daku, Towards accurate estimates of the spin-state energetics of spin-crossover complexes within density functional theory: a comparative case study of cobalt(II) complexes, Physical Chemistry Chemical Physics, Doi 10.1039/C3cp44336a.

Q. C. Sun, S. Mosquera-Vazquez, L. M. L. Daku, L. Guenee, H. A. Goodwin, et al., Experimental Evidence of Ultrafast Quenching of the (MLCT)-M-3 Luminescence in Ruthenium(II) Tris-bipyridyl Complexes via a (3)dd State, Journal of the American Chemical Society, Doi 10.1021/Ja407225t.

A. Portell, X. Alcobe, L. M. L. Daku, R. Cerny, R. Prohens, Crystal structure solution of an elusive polymorph of Dibenzylsquaramide, Powder Diffraction, Doi 10.1017/S0885715613000821.

Torsten Hoefler, ETH Zurich

T. Schneider, T. Hoefler, R. E. Grant, B. W. Barrett, R. Brightwell, Protocols for Fully Offloaded Collective Operations on Accelerated Network Adapters, 2013 42nd Annual International Conference on Parallel Processing (Icpp), Doi 10.1109/Icpp.2013.73.

B. Prisacari, G. Rodriguez, C. Minkenberg, T. Hoefler, Fast Pattern-Specific Routing for Fat Tree Networks, Acm Transactions on Architecture and Code Optimization, Doi 10.1145/2555289.2555293.

T. Hoefler, J. Dinan, D. Buntinas, P. Balaji, B. Barrett, et al., MPI + MPI: a new hybrid approach to parallel programming with MPI plus shared memory, Computing, Doi 10.1007/S00607-013-0324-2.

A. Friedley, T. Hoefler, G. Bronevetsky, A. Lumsdaine, C. C. Ma, Ownership Passing: Efficient Distributed Memory Programming on Multi-core Systems, Acm Sigplan Notices, Doi 10.1145/2517327.2442534.

R. Gerstenberger, M. Besta, T. Hoefler, Enabling highly-scalable remote memory access programming with MPI-3 one sided, SC '13 Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis, Doi 10.1145/2503210.2503286.

A. Calotoiu, T. Hoefler, M. Poke, F. Wolf, Using automated performance modeling to find scalability bugs in complex codes, SC '13 Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis, Doi 10.1145/2503210.2503277.

A. Friedley, G. Bronevetsky, T. Hoefler, A. Lumsdaine, Hybrid MPI: efficient message passing for multi-core systems, SC '13 Proceedings of the International Conference on High Performance Computing, Networking, Storage and Analysis, Doi 10.1145/2503210.2503294.

T. Schneider, F. Kjolstad, T. Hoefler, MPI datatype processing using runtime compilation, EuroMPI '13 Proceedings of the 20th European MPI Users' Group Meeting, Doi 10.1145/2488551.2488552.

T. Schneider, R. Gerstenberger, T. Hoefler, Application-oriented ping-pong benchmarking: how to assess the real communication overheads, Computing, Doi 10.1007/s00607-013-0330-4.

Jürg Hutter, University of Zurich

F. Tran, J. Hutter, Nonlocal van der Waals functionals: The case of rare-gas dimers and solids, Journal of Chemical Physics, Doi 10.1063/1.4807332.

R. Koitz, A. P. Seitsonen, M. Iannuzzi, J. Hutter, Structural and electronic properties of a large-scale Moire pattern of hexagonal boron nitride on Cu(111) studied with density functional theory, Nanoscale, Doi 10.1039/C3nr00709j.

R. Z. Khaliullin, J. Vandevondele, J. Hutter, Efficient Linear-Scaling Density Functional Theory for Molecular Systems, Journal of Chemical Theory and Computation, Doi 10.1021/Ct400595k.

M. Iannuzzi, I. Kalichava, H. F. Ma, S. J. Leake, H. T. Zhou, et al., Moire beatings in graphene on Ru(0001), Physical Review B, Doi 10.1103/Physrevb.88.125433.

K. R. Hahn, M. Iannuzzi, A. P. Seitsonen, J. Hutter, Coverage Effect of the CO2 Adsorption Mechanisms on CeO2(111) by First Principles Analysis, Journal of Physical Chemistry C, Doi 10.1021/Jp309565u.

D. Golze, M. Iannuzzi, M. T. Nguyen, D. Passerone, J. Hutter, Simulation of Adsorption Processes at Metallic Interfaces: An Image Charge Augmented QM/MM Approach, Journal of Chemical Theory and Computation, Doi 10.1021/Ct400698y.

J. G. Diaz, Y. Ding, R. Koitz, A. P. Seitsonen, M. Iannuzzi, et al., Hexagonal boron nitride on transition metal surfaces, Theoretical Chemistry Accounts, Doi 10.1007/S00214-013-1350-Z.

M. Del Ben, M. Schonherr, J. Hutter, J. Vandevondele, Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory, Journal of Physical Chemistry Letters, Doi 10.1021/Jz401931f.

M. Del Ben, J. Hutter, J. Vandevondele, Electron Correlation in the Condensed Phase from a Resolution of Identity Approach Based on the Gaussian and Plane Waves Scheme, Journal of Chemical Theory and Computation, Doi 10.1021/Ct4002202.

H. Y. Cun, M. Iannuzzi, A. Hemmi, S. Roth, J. Osterwalder, et al., Immobilizing Individual Atoms beneath a Corrugated Single Layer of Boron Nitride, Nano Letters, Doi 10.1021/Nl400449y.

Fortunat Joos, University of Bern

S. Zurcher, R. Spahni, F. Joos, M. Steinacher, H. Fischer, Impact of an abrupt cooling event on interglacial methane emissions in northern peatlands, Biogeosciences, Doi 10.5194/Bg-10-1963-2013.

W. Tinner, D. Colombaroli, O. Heiri, P. D. Henne, M. Steinacher, et al., The past ecology of Abies alba provides new perspectives on future responses of silver fir forests to global warming, Ecological Monographs, Doi 10.1890/12-2231.1.

P. Regnier, P. Friedlingstein, P. Ciais, F. T. Mackenzie, N. Gruber, et al., Anthropogenic perturbation of the carbon fluxes from land to ocean, Nature Geoscience, Doi 10.1038/Ngeo1830.

F. Joos, R. Roth, J. S. Fuglestvedt, G. P. Peters, I. G. Enting, et al., Carbon dioxide and climate impulse response functions for the computation of greenhouse gas metrics: a multi-model analysis, Atmospheric Chemistry and Physics, Doi 10.5194/Acp-13-2793-2013.

T. L. Frölicher, F. Joos, C. C. Raible, J. L. Sarmiento, Atmospheric CO2 response to volcanic eruptions: The role of ENSO, season, and variability, Global Biogeochemical Cycles, Doi 10.1002/Gbc.20028.

V. Cocco, F. Joos, M. Steinacher, T. L. Frölicher, L. Bopp, et al., Oxygen and indicators of stress for marine life in multi-model global warming projections, Biogeosciences, Doi 10.5194/Bg-10-1849-2013.

R. Bille, R. Kelly, A. Biastoch, E. Harrould-Kolieb, D. Herr, et al., Taking Action Against Ocean Acidification: A Review of Management and Policy Options, Environmental Management, Doi 10.1007/S00267-013-0132-7.

K. M. Keller, F. Joos, C. C. Raible, Time of Emergence of trends in ocean biogeochemistry, Biogeosciences Discuss., Doi 10.5194/bgd-10-18065-2013.

Leonhard Kleiser, ETH Zurich

S. Bühler, D. Obrist, L. Kleiser, Near-field and far-field acoustics of laminar and turbulent nozzle-jet flows in Proceedings of the 19th AIAA/CEAS Aeroacoustics Conference, Doi 10.2514/6.2013-2195.

Petros Koumoutsakos, ETH Zurich

J. H. Walther, K. Ritos, E. R. Cruz-Chu, C. M. Megaridis, P. Koumoutsakos, Barriers to Superfast Water Transport in Carbon Nanotube Membranes, Nano Letters, Doi 10.1021/Nl304000k.

W. M. Van Rees, M. Gazzola, P. Koumoutsakos, Optimal shapes for anguilliform swimmers at intermediate Reynolds numbers, Journal of Fluid Mechanics, Doi 10.1017/Jfm.2013.157.

G. Tauriello, P. Koumoutsakos, Coupling Remeshed Particle and Phase Field Methods for the Simulation of Reaction-Diffusion on the Surface and the Interior of Deforming Geometries, Siam Journal on Scientific Computing, Doi 10.1137/130906441.

F. Milde, S. Lauw, P. Koumoutsakos, M. L. Iruela-Arispe, The mouse retina in 3D: quantification of vascular growth and remodeling, Integrative Biology, Doi 10.1039/C3ib40085a.

P. Koumoutsakos, I. Pivkin, F. Milde, The Fluid Mechanics of Cancer and Its Therapy, Annual Review of Fluid Mechanics, Doi 10.1146/Annurev-Fluid-120710-101102.

P. Koumoutsakos, J. Feigelman, Multiscale stochastic simulations of chemical reactions with regulated scale separation, Journal of Computational Physics, Doi 10.1016/J.Jcp.2012.11.030.

M. V. Jensen, J. H. Walther, Numerical Analysis of Jet Impingement Heat Transfer at High Jet Reynolds Number and Large Temperature Difference, Heat Transfer Engineering, Doi 10.1080/01457632.2012.746153.

K. M. Ingvorsen, K. E. Meyer, J. H. Walther, S. Mayer, Turbulent swirling flow in a model of a uniflow-scavenged two-stroke engine, Experiments in Fluids, Doi 10.1007/S00348-013-1494-6.

M. M. Hejlesen, J. T. Rasmussen, P. Chatelain, J. H. Walther, A high order solver for the unbounded Poisson equation, Journal of Computational Physics, Doi 10.1016/J.Jcp.2013.05.050.

B. Hejazialhosseini, D. Rossinelli, P. Koumoutsakos, 3D shock-bubble interaction, Physics of Fluids, Doi 10.1063/1.4820017.

B. Hejazialhosseini, D. Rossinelli, P. Koumoutsakos, Vortex dynamics in 3D shock-bubble interaction, Physics of Fluids, Doi 10.1063/1.4819345.

S. Haider, T. Schnipper, A. Obeidat, K. E. Meyer, V. L. Okulov, et al., PIV study of the effect of piston position on the in-cylinder swirling flow during the scavenging process in large two-stroke marine diesel engines, Journal of Marine Science and Technology, Doi 10.1007/S00773-012-0192-Z.

D. Franco, F. Milde, M. Klingauf, F. Orsenigo, E. Dejana, et al., Accelerated endothelial wound healing on microstructured substrates under flow, Biomaterials, Doi 10.1016/J.Biomaterials.2012.10.007.

D. Franco, F. Milde, M. Klingauf, F. Orsenigo, E. Dejana, et al., Accelerated endothelial wound healing on microstructured substrates under flow, Biomaterials, Doi 10.1016/J.Biomaterials.2012.10.007.

P. Angelikopoulos, C. Papadimitriou, P. Koumoutsakos, Data Driven, Predictive Molecular Dynamics for Nanoscale Flow Simulations under Uncertainty, Journal of Physical Chemistry B, Doi 10.1021/Jp4084713.

Matthias Krack, Paul Scherrer Institute

J. Rabone, M. Krack, A procedure for bypassing metastable states in local basis set DFT+U calculations and its application to uranium dioxide surfaces, Computational Materials Science, Doi 10.1016/J.Commatsci.2013.01.023.

R. Ngayam-Happy, Investigation of the influence of off-stoichiometry on the radiation damage evolution in uranium dioxide, Progress in Nuclear Energy, Doi 10.1016/j.pnucene.2013.09.015.

Latévi Max Lawson Daku, University of Geneva

A. Vargas, I. Krivokapic, A. Hauser, L. M. L. Daku, Towards accurate estimates of the spin-state energetics of spin-crossover complexes within density functional theory: a comparative case study of cobalt(II) complexes, Physical Chemistry Chemical Physics, Doi 10.1039/C3cp44336a.

Q. C. Sun, S. Mosquera-Vazquez, L. M. L. Daku, L. Guenee, H. A. Goodwin, et al., Experimental Evidence of Ultrafast Quenching of the (MLCT)-M-3 Luminescence in Ruthenium(II) Tris-bipyridyl Complexes via a (3)dd State, Journal of the American Chemical Society, Doi 10.1021/Ja407225t.

Matthias Liebendörfer, University of Basel

Y. Suwa, T. Takiwaki, K. Kotake, T. Fischer, M. Liebendörfer, et al., On the Importance of the Equation of State for the Neutrino-Driven Supernova Explosion Mechanism, Astrophysical Journal, Doi 10.1088/0004-637x/764/1/99.

H. Berninger, E. Frenod, M. Gander, M. Liebendörfer, J. Michaud, Derivation of the Isotropic Diffusion Source Approximation (Idsa) for Supernova Neutrino Transport by Asymptotic Expansions, Siam Journal on Mathematical Analysis, Doi 10.1137/12089243x.

Vittorio Limongelli, University of Naples

V. Limongelli, S. De Tito, L. Cerofolini, M. Fragai, B. Pagano, et al., The G-Triplex DNA, Angewandte Chemie-International Edition, Doi 10.1002/Anie.201206522.

V. Limongelli, M. Bonomi, M. Parrinello, Funnel metadynamics as accurate binding free-energy method, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1303186110.

F. S. Di Leva, C. Festa, C. D'amore, S. De Marino, B. Renga, et al., Binding Mechanism of the Farnesoid X Receptor Marine Antagonist Suvanine Reveals a Strategy To Forestall Drug Modulation on Nuclear Receptors. Design, Synthesis, and Biological Evaluation of Novel Ligands, Journal of Medicinal Chemistry, Doi 10.1021/Jm400419e.

Ulrike Lohmann, ETH Zurich

A. Bichet, D. Folini, M. Wild, C. Schär, Enhanced Central European summer precipitation in the late 19th century: a link to the Tropics, Quarterly Journal of the Royal Meteorological Society, Doi 10.1002/qj.2111.

K. Emmanuel, S. Solomon, D. Folini, S. Davis, C. Cagnazzo, Influence of Tropical Tropopause Layer Cooling on Atlantic Hurricane Activity, Journal of Climate, Doi 10.1175/JCLI-D-12-00242.1.

Q. L. You, A. Sanchez-Lorenzo, M. Wild, D. Folini, K. Fraedrich, et al., Decadal variation of surface solar radiation in the Tibetan Plateau from observations, reanalysis and model simulations, Climate Dynamics, Doi 10.1007/S00382-012-1383-3.

Mathieu Luisier, ETH Zurich

A. Szabó, M. Luisier, Under-the-Barrier Model: An Extension of the Top-of-the-Barrier Model to Efficiently and Accurately Simulate Ultrascaled Nanowire Transistors, Ieee Transactions on Electron Devices, Doi 10.1109/Ted.2013.2263386.

R. Rhyner, M. Luisier, Phonon-limited low-field mobility in silicon: Quantum transport vs. linearized Boltzmann Transport Equation, Journal of Applied Physics, Doi 10.1063/1.4845515.

M. Luisier, A. Szabó, Paving the way for ultimate device scaling through nanoelectronic device simulations, 2013 14th International Conference on Ultimate Integration on Silicon (Ulis), WOS:000325214300013.

M. Luisier, O. Schenk, Gate-Stack Engineering in n-Type Ultrascaled Si Nanowire Field-Effect Transistors, Ieee Transactions on Electron Devices, Doi 10.1109/Ted.2013.2278573.

M. Luisier, T. B. Boykin, Z. Ye, A. Martini, G. Klimeck, et al., Investigation of ripple-limited low-field mobility in large-scale graphene nanoribbons, Applied Physics Letters, Doi 10.1063/1.4811761.

M. Luisier, Thermal transport and Matthiessen's rule in ultrascaled Si nanowires, Applied Physics Letters, Doi 10.1063/1.4821117.

R. Rhyner, M. Luisier, Phonon-limited low-field mobility in silicon: Quantum transport vs. linearized Boltzmann Transport Equation, Journal of Applied Physics, Doi 10.1063/1.4845515.

A. Kuzmin, M. Luisier, O. Schenk, Fast Methods for Computing Selected Elements of the Green's Function in Massively Parallel Nanoelectronic Device Simulations, Euro-Par 2013 Conference, Doi 10.1007/978-3-642-40047-6_54.

Lucio Mayer, University of Zurich

S. J. Shen, P. Madau, J. Guedes, L. Mayer, J. X. Prochaska, et al., The Circumgalactic Medium of Massive Galaxies at Z Similar to 3: A Test for Stellar Feedback, Galactic Outflows, and Cold Streams, Astrophysical Journal, Doi 10.1088/0004-637x/765/2/89.

V. Rashkov, A. Pillepich, A. J. Deason, P. Madau, C. M. Rockosi, et al., A "Light," Centrally Concentrated Milky Way Halo?, Astrophysical Journal Letters, Doi 10.1088/2041-8205/773/2/L32.

L. Mayer, Massive black hole binaries in gas-rich galaxy mergers; multiple regimes of orbital decay and interplay with gas inflows, Classical and Quantum Gravity, Doi 10.1088/0264-9381/30/24/244008.

M. Kuhlen, J. Guedes, A. Pillepich, P. Madau, L. Mayer, An Off-Center Density Peak in the Milky Way's Dark Matter Halo?, Astrophysical Journal, Doi 10.1088/0004-637x/765/1/10.

J. Guedes, L. Mayer, M. Carollo, P. Madau, Pseudobulge Formation as a Dynamical Rather Than a Secular Process, Astrophysical Journal, Doi 10.1088/0004-637x/772/1/36.

J. C. Bird, S. Kazantzidis, D. H. Weinberg, J. Guedes, S. Callegari, et al., Inside out and Upside Down: Tracing the Assembly of a Simulated Disk Galaxy Using Mono-Age Stellar Populations, Astrophysical Journal, Doi 10.1088/0004-637x/773/1/43.

Francesco Miniati, ETH Zurich

F. Miniati, A. Elyiv, Relaxation of Blazar-Induced Pair Beams in Cosmic Voids, Astrophysical Journal, Doi 10.1088/0004-637x/770/1/54.

MeteoSwiss

R. Gangstø, A. P. Weigel, M. A. Liniger, C. Appenzeller, Methodological aspects of the validation of decadal predictions, Climate Research, Doi 10.3354/cr01135.

F. A. Isotta, C. Frei, V. Weilguni, M. P. Tadi, P. Lassègues, et al., The climate of daily precipitation in the Alps: development and analysis of a high-resolution grid dataset from pan-Alpine rain-gauge data, International Journal of Climatology, Doi 10.1002/joc.3794.

R. Lorenz, E. L. Davin, D. M. Lawrence, R. Stöckli, S. I. Seneviratne, How important is vegetation phenology for euro- pean climate and heat waves?, Journal of Climate, Doi 10.1175/JCLI-D-13-00040.1.

O. Martius, H. Sodemann, H. Joos, S. Pfahl, A. Winschall, et al., The role of upper-level dynamics and surface processes for the Pakistan flood of July 2010, Quarterly Journal of the Royal Meteorological Society, Doi 10.1002/qj.2082.

A. Pauling, R. Gehrig, B. Clot, Towards optimized temperature sum parameterizations for forecasting the start of the pollen season, Aerobiologia, Doi 10.1007/s10453-013-9308-0.

B. Dürr, M. Schröder, R. Stöckli, R. Posselt, HelioFTH: combining cloud index principles and aggregated ratingfor cloud masking using infrared observations from geostationarysatellites, Atmospheric Measurement Techniques, Doi 10.5194/amt-6-1883-2013.

Marc Parlange, EPF Lausanne

M. Diebold, C. Higgins, J. N. Fang, A. Bechmann, M. B. Parlange, Flow over Hills: A Large-Eddy Simulation of the Bolund Case, Boundary-Layer Meteorology, Doi 10.1007/S10546-013-9807-0.

M. Hultmark, M. Calaf, M. B. Parlange, A New Wall Shear Stress Model for Atmospheric Boundary Layer Simulations, Journal of the Atmospheric Sciences, Doi 10.1175/Jas-D-12-0257.1.

Michele Parrinello, Università della Svizzera italiana

P. Tiwary, M. Parrinello, From Metadynamics to Dynamics, Physical Review Letters, Doi 10.1103/Physrevlett.111.230602.

M. Salvalaglio, T. Vetter, M. Mazzotti, M. Parrinello, Controlling and Predicting Crystal Shapes: The Case of Urea, Angewandte Chemie-International Edition, Doi 10.1002/Anie.201304562.

G. M. Pavan, A. Barducci, L. Albertazzi, M. Parrinello, Combining metadynamics simulation and experiments to characterize dendrimers in solution, Soft Matter, Doi 10.1039/C3sm27706b.

F. Palazzesi, A. Barducci, M. Tollinger, M. Parrinello, The allosteric communication pathways in KIX domain of CBP, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1313548110.

V. Limongelli, S. De Tito, L. Cerofolini, M. Fragai, B. Pagano, et al., The G-Triplex DNA, Angewandte Chemie-International Edition, Doi 10.1002/Anie.201206522.

V. Limongelli, M. Bonomi, M. Parrinello, Funnel metadynamics as accurate binding free-energy method, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1303186110.

A. Hassanali, F. Giberti, J. Cuny, T. D. Kuhne, M. Parrinello, Proton transfer through the water gossamer, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1306642110.

F. Giberti, G. A. Tribello, M. Parrinello, Transient Polymorphism in NaCl, Journal of Chemical Theory and Computation, Doi 10.1021/Ct4002027.

S. Caravati, G. C. Sosso, M. Bernasconi, M. Parrinello, Density functional simulations of hexagonal Ge2Sb2Te5 at high pressure, Physical Review B, Doi 10.1103/Physrevb.88.019903.

A. Barducci, M. Bonomi, M. K. Prakash, M. Parrinello, Free-energy landscape of protein oligomerization from atomistic simulations, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1320077110.

Alfredo Pasquarello, EPF Lausanne

G. Miceli, A. Pasquarello, First principles study of As 2p core-level shifts at GaAs/Al2O3 interfaces, Applied Physics Letters, Doi 10.1063/1.4807730.

G. Miceli, A. Pasquarello, Accurate determination of charge transition levels of the As-As dimer defect at GaAs/oxide interfaces through hybrid functionals, Applied Physics Letters, Doi 10.1063/1.4816661.

G. Miceli, A. Pasquarello, Defect energy levels of the As-As dimer at InGaAs/oxide interfaces: A first principles study, Microelectronic Engineering, Doi 10.1016/J.Mee.2013.03.053.

H. P. Komsa, A. Pasquarello, Finite-Size Supercell Correction for Charged Defects at Surfaces and Interfaces, Physical Review Letters, Doi 10.1103/Physrevlett.110.095505.

D. Colleoni, A. Pasquarello, Amphoteric defects in GaAs leading to Fermi-level pinning: A hybrid functional study, Microelectronic Engineering, Doi 10.1016/J.Mee.2013.03.068.

D. Colleoni, A. Pasquarello, Assignment of Fermi-level pinning and optical transitions to the (As-Ga)(2)-O-As center in oxygen-doped GaAs, Applied Physics Letters, Doi 10.1063/1.4824309.

W. Chen, A. Pasquarello, Correspondence of defect energy levels in hybrid density functional theory and many-body perturbation theory, Physical Review B, Doi 10.1103/Physrevb.88.115104.

Daniele Passerone, EMPA

L. Talirz, H. Sode, J. M. Cai, P. Ruffieux, S. Blankenburg, et al., Termini of Bottom-Up Fabricated Graphene Nanoribbons, Journal of the American Chemical Society, Doi 10.1021/Ja311099k.

A. Shchyrba, M. T. Nguyen, C. Wackerlin, S. Martens, S. Nowakowska, et al., Chirality Transfer in 1D Self-Assemblies: Influence of H-Bonding vs Metal Coordination between Dicyano[7] helicene Enantiomers, Journal of the American Chemical Society, Doi 10.1021/Ja407315f.

D. Golze, M. Iannuzzi, M. T. Nguyen, D. Passerone, J. Hutter, Simulation of Adsorption Processes at Metallic Interfaces: An Image Charge Augmented QM/MM Approach, Journal of Chemical Theory and Computation, Doi 10.1021/Ct400698y.

Igor Pivkin, Università della Svizzera italiana

Z. L. Peng, X. J. Li, I. V. Pivkin, M. Dao, G. E. Karniadakis, et al., Lipid bilayer and cytoskeletal interactions in a red blood cell, Proceedings of the National Academy of Sciences of the United States of America, Doi 10.1073/Pnas.1311827110.

X. J. Li, I. V. Pivkin, H. J. Liang, Hydrodynamic effects on flow-induced polymer translocation through a microfluidic channel, Polymer, Doi 10.1016/J.Polymer.2013.06.022.

Fernando Porté-Agel, EPF Lausanne

W. Zhang, C. D. Markfort, F. Porté-Agel, Wind-Turbine Wakes in a Convective Boundary Layer: A Wind-Tunnel Study, Boundary-Layer Meteorology, Doi 10.1007/S10546-012-9751-4.

W. Zhang, C. D. Markfort, F. Porté-Agel, Experimental study of the impact of large-scale wind farms on land-atmosphere exchanges, Environmental Research Letters, Doi 10.1088/1748-9326/8/1/015002.

Y. T. Wu, F. Porté-Agel, Simulation of Turbulent Flow Inside and Above Wind Farms: Model Validation and Layout Effects, Boundary-Layer Meteorology, Doi 10.1007/S10546-012-9757-Y.

F. Porté-Agel, Y. T. Wu, C. H. Chen, A Numerical Study of the Effects of Wind Direction on Turbine Wakes and Power Losses in a Large Wind Farm, Energies, Doi 10.3390/En6105297.

H. Lu, F. Porté-Agel, A modulated gradient model for scalar transport in large-eddy simulation of the atmospheric boundary layer, Physics of Fluids, Doi 10.1063/1.4774342.

G. V. Iungo, Y. T. Wu, F. Porté-Agel, Field Measurements of Wind Turbine Wakes with Lidars, Journal of Atmospheric and Oceanic Technology, Doi 10.1175/Jtech-D-12-00051.1.

G. V. Iungo, F. Viola, S. Camarri, F. Porté-Agel, F. Gallaire, Linear stability analysis of wind turbine wakes performed on wind tunnel measurements, Journal of Fluid Mechanics, Doi 10.1017/Jfm.2013.569.

W. C. Cheng, F. Porté-Agel, Evaluation of subgrid-scale models in large-eddy simulation of flow past a two-dimensional block, International Journal of Heat and Fluid Flow, Doi 10.1016/J.Ijheatfluidflow.2013.06.007.

M. Abkar, F. Porté-Agel, The Effect of Free-Atmosphere Stratification on Boundary-Layer Flow and Power Output from Very Large Wind Farms, Energies, Doi 10.3390/En6052338.

C. M. Smith, F. Porté-Agel, An intercomparison of subgrid models for large-eddy simulation of katabatic flows, Quarterly Journal of the Royal Meteorological Society, Doi 10.1002/qj.2212.

Alfio Quarteroni, EPF Lausanne

J. Bonnemain, A. C. I. Malossi, M. Lesinigo, S. Deparis, A. Quarteroni, et al., Numerical simulation of left ventricular assist device implantations: Comparing the ascending and the descending aorta cannulations, Medical Engineering & Physics, Doi 10.1016/J.Medengphy.2013.03.022.

Christoph C. Raible, University of Bern

U. Ulbrich, G. C. Leckebusch, J. Grieger, M. Schuster, M. Akperov, et al., Are Greenhouse Gas Signals of Northern Hemisphere winter extra-tropical cyclone activity dependent on the identification and tracking algorithm?, Meteorologische Zeitschrift, Doi 10.1127/0941-2948/2013/0420.

N. Merz, C. C. Raible, H. Fischer, V. Varma, M. Prange, et al., Greenland accumulation and its connection to the large-scale atmospheric circulation in ERA-Interim and paleoclimate simulations, Climate of the Past, Doi 10.5194/Cp-9-2433-2013.

F. Lehner, A. Born, C. C. Raible, T. F. Stocker, Amplified Inception of European Little Ice Age by Sea Ice-Ocean-Atmosphere Feedbacks, Journal of Climate, Doi 10.1175/Jcli-D-12-00690.1.

A. Laderach, C. C. Raible, Lower-tropospheric humidity: climatology, trends and the relation to the ITCZ, Tellus Series A-Dynamic Meteorology and Oceanography, Doi 10.3402/Tellusa.V65i0.20413.

T. L. Frölicher, F. Joos, C. C. Raible, J. L. Sarmiento, Atmospheric CO2 response to volcanic eruptions: The role of ENSO, season, and variability, Global Biogeochemical Cycles, Doi 10.1002/Gbc.20028.

J. Franke, D. Frank, C. C. Raible, J. Esper, S. Brönnimann, Spectral biases in tree-ring climate proxies, Nature Climate Change, Doi 10.1038/Nclimate1816.

L. Fernández-Donado, J. F. González-Rouco, C. C. Raible, C. M. Ammann, D. Barriopedro, et al., Large-scale temperature response to external forcing in simulations and reconstructions of the last millennium, Climate of the Past, Doi 10.5194/Cp-9-393-2013.

A. Born, T. F. Stocker, C. C. Raible, A. Levermann, Is the Atlantic subpolar gyre bistable in comprehensive coupled climate models?, Climate Dynamics, Doi 10.1007/S00382-012-1525-7.

Paolo Ricci, EPF Lausanne

A. Mosetto, F. D. Halpern, S. Jolliet, J. Loizu, P. Ricci, Turbulent regimes in the tokamak scrape-off layer, Physics of Plasmas, Doi 10.1063/1.4821597.

F. D. Halpern, P. Ricci, B. Labit, I. Furno, S. Jolliet, et al., Theory-based scaling of the SOL width in circular limited tokamak plasmas, Nuclear Fusion, Doi 10.1088/0029-5515/53/12/122001.

F. D. Halpern, S. Jolliet, J. Loizu, A. Mosetto, P. Ricci, Ideal ballooning modes in the tokamak scrape-off layer, Physics of Plasmas, Doi 10.1063/1.4807333.

Marc Robinson-Rechavi, University of Lausanne

S. Moretti, B. Laurenczy, W. H. Gharib, B. Castella, A. Kuzniar, et al., Selectome update: quality control and computational improvements to a database of positive selection, Nucleic Acids Research, Doi 10.1093/nar/gkt1065.

Ursula Röthlisberger, EPF Lausanne

A. Yella, R. Humphry-Baker, B. F. E. Curchod, N. A. Astani, J. Teuscher, et al., Molecular Engineering of a Fluorene Donor for Dye-Sensitized Solar Cells, Chemistry of Materials, Doi 10.1021/Cm401593b.

O. Valsson, P. Campomanes, I. Tavernelli, U. Röthlisberger, C. Filippi, Rhodopsin Absorption from First Principles: Bypassing Common Pitfalls, Journal of Chemical Theory and Computation, Doi 10.1021/Ct3010408.

M. Scarongella, A. Laktionov, U. Röthlisberger, N. Banerji, Charge transfer relaxation in donor-acceptor type conjugated materials, Journal of Materials Chemistry C, Doi 10.1039/C3tc00829k.

L. E. Polander, A. Yella, J. Teuscher, R. Humphry-Baker, B. F. E. Curchod, et al., Unravelling the Potential for Dithienopyrrole Sensitizers in Dye-Sensitized Solar Cells, Chemistry of Materials, Doi 10.1021/Cm401144j.

L. E. Polander, A. Yella, B. F. E. Curchod, N. A. Astani, J. Teuscher, et al., Towards Compatibility between Ruthenium Sensitizers and Cobalt Electrolytes in Dye-Sensitized Solar Cells, Angewandte Chemie-International Edition, Doi 10.1002/Anie.201304608.

M. Guglielmi, M. Dömer, I. Tavernelli, U. Röthlisberger, Photodynamics of Lys(+)-Trp protein motifs: Hydrogen bonds ensure photostability, Faraday Discussions, Doi 10.1039/C3fd00037k.

E. Brunk, B. Mollwitz, U. Röthlisberger, Mechanism to Trigger Unfolding in O6-Alkylguanine-DNA Alkyltransferase, Chembiochem, Doi 10.1002/Cbic.201200566.

Yohei Sato, Paul Scherrer Institute

Y. Sato, B. Niceno, A sharp-interface phase change model for a mass-conservative interface tracking method, Journal of Computational Physics, Doi 10.1016/J.Jcp.2013.04.035.

Christoph Schär, ETH Zurich

R. Vautard, A. Gobiet, D. Jacob, M. Belda, A. Colette, et al., The simulation of European heat waves from an ensemble of regional climate models within the EURO-CORDEX project, Climate Dynamics, Doi 10.1007/S00382-013-1714-Z.

C. Steger, S. Kotlarski, T. Jonas, C. Schär, Alpine snow cover in a changing climate: a regional climate model perspective, Climate Dynamics, Doi 10.1007/S00382-012-1545-3.

J. Schmidli, Daytime Heat Transfer Processes over Mountainous Terrain, Journal of the Atmospheric Sciences, Doi 10.1175/Jas-D-13-083.1.

J. Rajczak, P. Pall, C. Schär, Projections of extreme precipitation events in regional climate simulations for Europe and the Alpine Region, Journal of Geophysical Research-Atmospheres, Doi 10.1002/Jgrd.50297.

W. Langhans, J. Schmidli, O. Fuhrer, S. Bieri, C. Schär, Long-Term Simulations of Thermally Driven Flows and Orographic Convection at Convection-Parameterizing and Cloud-Resolving Resolutions, Journal of Applied Meteorology and Climatology, Doi 10.1175/Jamc-D-12-0167.1.

T. Bosshard, M. Carambia, K. Goergen, S. Kotlarski, P. Krahe, et al., Quantifying uncertainty sources in an ensemble of hydrological climate-impact projections, Water Resources Research, Doi 10.1029/2011wr011533.

O. Bellprat, S. Kotlarski, D. Lüthi, C. Schär, Physical constraints for temperature biases in climate models, Geophysical Research Letters, Doi 10.1002/Grl.50737.

Olaf Schenk, Università della Svizzera italiana

M. Luisier, O. Schenk, Gate-Stack Engineering in n-Type Ultrascaled Si Nanowire Field-Effect Transistors, Ieee Transactions on Electron Devices, Doi 10.1109/Ted.2013.2278573.

P. Basini, T. Nissen-Meyer, L. Boschi, E. Casarotti, J. Verbeke, et al., The influence of nonuniform ambient noise on crustal tomography in Europe, Geochemistry Geophysics Geosystems, Doi 10.1002/Ggge.20081.

A. Kuzmin, M. Luisier, O. Schenk, Fast Methods for Computing Selected Elements of the Green's Function in Massively Parallel Nanoelectronic Device Simulations, Euro-Par 2013 Conference, Doi 10.1007/978-3-642-40047-6_54.

Christoph Schwab, ETH Zurich

S. Mishra, C. Schwab, J. Sukys, Multi-level Monte Carlo finite volume methods for uncertainty quantification in nonlinear systems of balance laws, Lecture Notes in Computational Science and Engineerings, Doi 10.1007/978-3-319-00885-1_6.

Sonia Seneviratne, ETH Zurich

S. I. Seneviratne, M. Wilhelm, T. Stanelle, B. van den Hurk, S. Hagemann, et al., Impact of soil moisture-climate feedbacks on CMIP5 projections: First results from the GLACE-CMIP5 experiment, Geophysical Research Letters, Doi 10.1002/Grl.50956.

R. Lorenz, E. L. Davin, D. M. Lawrence, R. Stöckli, S. I. Seneviratne, How Important is Vegetation Phenology for European Climate and Heat Waves?, Journal of Climate, Doi 10.1175/Jcli-D-13-00040.1.

B. P. Guillod, E. L. Davin, C. Kundig, G. Smiatek, S. I. Seneviratne, Impact of soil map specifications for European climate simulations, Climate Dynamics, Doi 10.1007/S00382-012-1395-Z.

Nicola A. Spaldin, ETH Zurich

N. A. Spaldin, M. Fechner, E. Bousquet, A. Balatsky, L. Nordstrom, Monopole-based formalism for the diagonal magnetoelectric response, Physical Review B, Doi 10.1103/Physrevb.88.094429.

M. Setvin, U. Aschauer, P. Scheiber, Y. F. Li, W. Y. Hou, et al., Reaction of O-2 with Subsurface Oxygen Vacancies on TiO2 Anatase (101), Science, Doi 10.1126/Science.1239879.

D. Meier, M. Lilienblum, P. Becker, L. Bohaty, N. A. Spaldin, et al., Translation domains in multiferroics, Phase Transitions, Doi 10.1080/01411594.2012.696116.

I. Maclaren, L. Q. Wang, B. Schaffer, Q. M. Ramasse, A. J. Craven, et al., Novel Nanorod Precipitate Formation in Neodymium and Titanium Codoped Bismuth Ferrite, Advanced Functional Materials, Doi 10.1002/Adfm.201201835.

J. H. Lee, K. T. Delaney, E. Bousquet, N. A. Spaldin, K. M. Rabe, Strong coupling of Jahn-Teller distortion to oxygen-octahedron rotation and functional properties in epitaxially strained orthorhombic LaMnO3, Physical Review B, Doi 10.1103/Physrevb.88.174426.

L. Lahourcade, N. C. Coronel, K. T. Delaney, S. K. Shukla, N. A. Spaldin, et al., Structural and Optoelectronic Characterization of RF Sputtered ZnSnN2, Advanced Materials, Doi 10.1002/Adma.201204718.

Y. Kumagai, N. A. Spaldin, Structural domain walls in polar hexagonal manganites, Nature Communications, Doi 10.1038/Ncomms2545.

S. V. Kalinin, N. A. Spaldin, Functional Ion Defects in Transition Metal Oxides, Science, Doi 10.1126/Science.1243098.

R. L. Johnson-Wilke, D. Marincel, S. Zhu, M. P. Warusawithana, A. Hatt, et al., Quantification of octahedral rotations in strained LaAlO3 films via synchrotron x-ray diffraction, Physical Review B, Doi 10.1103/Physrevb.88.174101.

A. Grunebohm, P. Entel, C. Ederer, First-principles investigation of incipient ferroelectric trends of rutile TiO2 in bulk and at the (110) surface, Physical Review B, Doi 10.1103/Physrevb.87.054110.

N. M. Caffrey, D. Fritsch, T. Archer, S. Sanvito, C. Ederer, Spin-filtering efficiency of ferrimagnetic spinels CoFe2O4 and NiFe2O4, Physical Review B, Doi 10.1103/Physrevb.87.024419.

U. Aschauer, R. Pfenninger, S. M. Selbach, T. Grande, N. A. Spaldin, Strain-controlled oxygen vacancy formation and ordering in CaMnO3, Physical Review B, Doi 10.1103/Physrevb.88.054111.

Paul J. Tackley, ETH Zurich

N. Coltice, M. Seton, T. Rolf, R. D. Muller, P. J. Tackley, Convergence of tectonic reconstructions and mantle convection models for significant fluctuations in seafloor spreading, Earth and Planetary Science Letters, Doi 10.1016/J.Epsl.2013.09.032.

Romain Teyssier, University of Zurich

D. Martizzi, R. Teyssier, B. Moore, Cusp-core transformations induced by AGN feedback in the progenitors of cluster galaxies, Monthly Notices of the Royal Astronomical Society, Doi 10.1093/Mnras/Stt297.

J. Rosdahl, J. Blaizot, D. Aubert, T. Stranex, R. Teyssier, ramses-rt: radiation hydrodynamics in the cosmological context, Monthly Notices of the Royal Astronomical Society, Doi 10.1093/Mnras/Stt1722.

R. Teyssier, A. Pontzen, Y. Dubois, J. I. Read, Cusp-core transformations in dwarf galaxies: observational predictions, Monthly Notices of the Royal Astronomical Society, Doi 10.1093/Mnras/Sts563.

D. Martizzi, R. Teyssier, B. Moore, The role of Active Galactic Nuclei feedback in the formation of the brightest cluster galaxies, The Intriguing Life of Massive Galaxies, Proceedings of the International Astronomical Union, IAU Symposium, Doi 10.1017/S1743921313005371.

Matthias Troyer, ETH Zurich

L. Wang, M. Troyer, X. Dai, Topological Charge Pumping in a One-Dimensional Optical Lattice, Physical Review Letters, Doi 10.1103/Physrevlett.111.026802.

T. Uehlinger, D. Greif, G. Jotzu, L. Tarruell, T. Esslinger, et al., Double transfer through Dirac points in a tunable honeycomb optical lattice, European Physical Journal-Special Topics, Doi 10.1140/Epjst/E2013-01761-Y.

Joost VandeVondele, ETH Zurich

R. Z. Khaliullin, J. Vandevondele, J. Hutter, Efficient Linear-Scaling Density Functional Theory for Molecular Systems, Journal of Chemical Theory and Computation, Doi 10.1021/Ct400595k.

M. Del Ben, M. Schonherr, J. Hutter, J. Vandevondele, Bulk Liquid Water at Ambient Temperature and Pressure from MP2 Theory, Journal of Physical Chemistry Letters, Doi 10.1021/Jz401931f.

M. Del Ben, J. Hutter, J. Vandevondele, Electron Correlation in the Condensed Phase from a Resolution of Identity Approach Based on the Gaussian and Plane Waves Scheme, Journal of Chemical Theory and Computation, Doi 10.1021/Ct4002202.

Harry van Lenthe, ETH Zurich

F. A. Schulte, A. Zwahlen, F. M. Lambers, G. Kuhn, D. Ruffoni, et al., Strain-adaptive in silico modeling of bone adaptation - A computer simulation validated by in vivo micro-computed tomography data, Bone, Doi 10.1016/J.Bone.2012.09.008.

F. A. Schulte, D. Ruffoni, F. M. Lambers, D. Christen, D. J. Webster, et al., Local Mechanical Stimuli Regulate Bone Formation and Resorption in Mice at the Tissue Level, Plos One, Doi 10.1371/journal.pone.0062172.

D. Ruffoni, T. Kohler, R. Voide, A. J. Wirth, L. R. Donahue, et al., High-throughput quantification of the mechanical competence of murine femora - A highly automated approach for large-scale genetic studies, Bone, Doi 10.1016/J.Bone.2013.02.015.

A. Cohen, E. M. Stein, R. R. Recker, J. M. Lappe, D. W. Dempster, et al., Teriparatide for Idiopathic Osteoporosis in Premenopausal Women: A Pilot Study, Journal of Clinical Endocrinology & Metabolism, Doi 10.1210/Jc.2013-1172.

A. Cohen, D. W. Dempster, R. R. Recker, J. M. Lappe, H. Zhou, et al., Abdominal Fat Is Associated With Lower Bone Formation and Inferior Bone Quality in Healthy Premenopausal Women: A Transiliac Bone Biopsy Study, Journal of Clinical Endocrinology & Metabolism, Doi 10.1210/Jc.2013-1047.

D. Christen, L. J. Melton, A. Zwahlen, S. Amin, S. Khosla, et al., Improved Fracture Risk Assessment Based on Nonlinear Micro-Finite Element Simulations From HRpQCT Images at the Distal Radius, Journal of Bone and Mineral Research, Doi 10.1002/Jbmr.1996.

Laurent Villard, EPF Lausanne

L. Villard, P. Angelino, A. Bottino, S. Brunner, S. Jolliet, et al., Global gyrokinetic ion temperature gradient turbulence simulations of ITER, Plasma Physics and Controlled Fusion, Doi 10.1088/0741-3335/55/7/074017.

T. Vernay, S. Brunner, L. Villard, B. F. Mcmillan, S. Jolliet, et al., Global gyrokinetic simulations of TEM microturbulence, Plasma Physics and Controlled Fusion, Doi 10.1088/0741-3335/55/7/074016.

Viola Vogel, ETH Zurich

F. A. Herzog, V. Vogel, Multiple Steps to Activate FAK's Kinase Domain: Adaptation to Confined Environments?, Biophysical Journal, Doi 10.1016/J.Bpj.2013.04.021.

Lei Wang, ETH Zurich

L. Wang, M. Troyer, X. Dai, Topological Charge Pumping in a One-Dimensional Optical Lattice, Physical Review Letters, Doi 10.1103/Physrevlett.111.026802.

L. Wang, A. A. Soluyanov, M. Troyer, Proposal for Direct Measurement of Topological Invariants in Optical Lattices, Physical Review Letters, Doi 10.1103/Physrevlett.110.166802.

T. Uehlinger, D. Greif, G. Jotzu, L. Tarruell, T. Esslinger, et al., Double transfer through Dirac points in a tunable honeycomb optical lattice, European Physical Journal-Special Topics, Doi 10.1140/Epjst/E2013-01761-Y.

Oleg Yazyev, EPF Lausanne

C. Tournier-Colletta, L. Moreschini, G. Autes, S. Moser, A. Crepaldi, et al., Electronic Instability in a Zero-Gap Semiconductor: The Charge-DensityWave in (TaSe4)(2)I, Physical Review Letters, Doi 10.1103/Physrevlett.110.236401.

M. Ricco, M. Aramini, M. Mazzani, D. Pontiroli, M. Gaboardi, et al., Muons probe magnetism and hydrogen interaction in graphene, Physica Scripta, Doi 10.1088/0031-8949/88/06/068508.

F. Donati, Q. Dubout, G. Autes, F. Patthey, F. Calleja, et al., Magnetic Moment and Anisotropy of Individual Co Atoms on Graphene, Physical Review Letters, Doi 10.1103/Physrevlett.111.236801.

A. Crepaldi, C. Tournier-Colletta, M. Pivetta, G. Autes, F. Patthey, et al., Structural and electronic properties of the Bi/Au(110)-1x4 surface, Physical Review B, Doi 10.1103/Physrevb.88.195433.

G. Autes, O. V. Yazyev, Engineering quantum spin Hall effect in graphene nanoribbons via edge functionalization, Physical Review B, Doi 10.1103/Physrevb.87.241404.

Christoph Zollikofer, University of Zurich

S. Callegari, J. D. Weissmann, N. Tkachenko, W. P. Petersen, G. Lake, et al., An Agent-Based Model of Human Dispersals at a Global Scale, Advances in Complex Systems, Doi 10.1142/S0219525913500239.

Laura Zoppi, University of Zurich

L. Zoppi, J. S. Siegel, K. K. Baldridge, Electron transport and optical properties of curved aromatics, Wiley Interdisciplinary Reviews-Computational Molecular Science, Doi 10.1002/Wcms.1107.

L. Zoppi, A. Ferretti, K. K. Baldridge, Static and Field-Oriented Properties of Bowl-Shaped Polynuclear Aromatic Hydrocarbon Fragments, Journal of Chemical Theory and Computation, Doi 10.1021/Ct400575p.

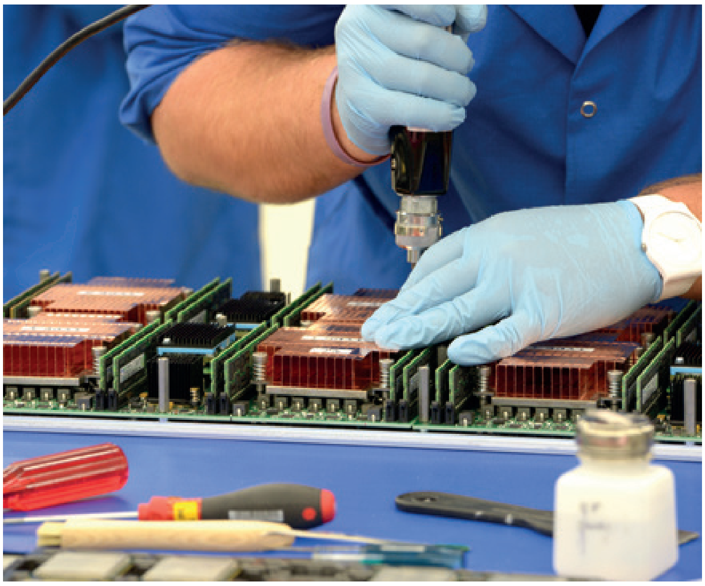
T. Bauert, L. Zoppi, G. Koller, J. S. Siegel, K. K. Baldridge, et al., Quadruple Anionic Buckybowls by Solid-State Chemistry of Corannulene and Cesium, Journal of the American Chemical Society, Doi 10.1021/Ja4063103.

IV

New Promising Hybrid Computer Architecture

With "Piz Daint" CSCS has a new supercomputer system in operation that provides the necessary compute performance while consuming less power. This was made possible by a novel hybrid computer system, which makes use of sophisticated graphics processors (GPUs).

The supercomputer "Piz Daint" in operation at CSCS since April 2013, has gone through a major upgrade in October 2013. The cabinets have more than doubled in size from 12 to 28 and the processors has been upgraded with graphic processing units (GPU) from processor manufacturer NVIDIA. With a total of 5'272 hybrid compute nodes as well as a powerful network, it will be possible for real simulations to sustain petaflops (10^{15} floating point operations per seconds) performance. With a peak performance of 7.788 petaflops "Piz Daint" has been listed during the Supercomputing Conference 13 in Denver, USA, the fastest supercomputer in Europe.



Assembling a hybrid blade of "Piz Daint".

First of its kind

In the extension, one of two conventional processors (CPU) located on a compute node was replaced by a GPU, which stem from the computer game and graphics industry. Compared to a conventional CPU, the GPU has reduced functionalities that are optimized for numerical calculations. In simple terms, this enables the GPU to compute much faster, while saving energy.

Furthermore, the new supercomputer gets much of its overall performance and efficiency from a novel interconnecting network between compute nodes that has been designed by computer manufacturer Cray. It is the first of its kind, and has been designed to help researchers solve more detailed, higher-resolution models – and this all while consuming less power.

CSCS-Director Thomas Schulthess is convinced that given the ever growing demands of computer models, energy consumption in supercomputing can only contain with a radical change in computer architecture. The new “Piz Daint” will enable researchers and scientists to study more detailed, higher-resolution models in less time. The benefit of the new system should go primarily to climate scientists, geoscientists, chemists, as well as materials and nano-scientist with their complex computations, but also physicists and biologist who run ever more compute-intensive applications at CSCS.

Up to seven times less energy

“Piz Daint” will be fully integrated into the CSCS user program in April 2014, with the start of the new allocation period. Initial tests revealed that a climate simulation on Piz Daint runs over three times faster and reaching the solution with seven times less energy consumed as compared to CSCS’ supercomputing system “Monte Rosa”, the former flagship supercomputer of CSCS. “Monte Rosa” runs with conventional CPUs that have been upgraded two years ago. Even compared to the exclusively CPU processors previously available in “Piz Daint”, the hybrid system with the GPU processors is expected to run almost three times more energy-efficiently than with CPUs only.

With the upgrade of “Piz Daint”, CSCS has successfully implemented the final step of the Swiss High Performance Computing and Networking (HPCN) initiative coordinated by ETH Board. The HPCN-strategy started in 2009 with the goal of providing the Swiss research community with a petaflop-scale supercomputer.

Back view of the Cray XC30 supercomputer “Piz Daint”.

V

Services for Third Parties

In addition to providing services as User Lab, CSCS makes the skills of its staff and flexible infrastructure available to academia, the public sector and national projects, by operating supercomputers on the basis of Service Level Agreements.

Academia

For some 10 years CSCS has been operating a cluster for **CHIPP**, the association of all Swiss particle physics laboratories, to analyze data from the Large Hadron Collider (LHC) experiments at CERN. This analysis is needed to elucidate the basic physics of particle collisions at very high energy. The CHIPP cluster utilized is called "Phoenix" and it is an integral part of the Worldwide LHC Computing Grid (WLCG) and, by extension, part of the infrastructure of the European Grid Initiative (EGI). The computing power and storage capacity of "Phoenix" is upgraded annually and currently (end of 2013) comprises a total of 2'464 computing cores from Intel and AMD as well as 1'880 TB storage.

Since August 2013 CSCS has hosted and operated the NEC cluster "Mönch" on behalf of a group of ETH Zurich professors. This supercomputer is dedicated to research in biomedicine, astronomy, geophysics, theoretical physics, materials science, and computational science. The cluster is a 9 rack NEC-provided Intel-based system with 4 login nodes, 312 standard compute nodes, 24 large-memory compute nodes and 8 servers to provide I/O to Lustre.

"Mönch", named after a mountain in the Bernese Alps.

Public Sector

MeteoSwiss runs its daily weather forecast simulations on computers operated by CSCS. Weather forecasts not only inform the public about the weather and possible natural hazards, they further provide essential data for security-relevant public services, such as air traffic control and disaster mitigation. In 2013 CSCS continued to operate two Cray XE6 systems, nicknamed "Albis" and "Monte Lema", which had been installed back in April 2012. MeteoSwiss currently operates a short-term forecast model at 2.2 km grid resolution in tandem with a standard long-term forecast model at 7 km resolution. These high-resolution models are run 8 times a day on the production system, "Albis", and form the numerical basis for the daily weather forecast. The second system, "Monte Lema", serves as backup for "Albis" and is otherwise used by MeteoSwiss for code and method development.

Every three hours a weather forecast for Switzerland is run on the Cray XE6 "Albis".

National Projects

One of the most ambitious computer simulation projects to date is the Blue Brain Project, which was launched by EPF Lausanne in 2005. Its declared goal is to reconstruct the brain piece by piece and to build a virtual brain in a supercomputer. The virtual brain will be an exceptional tool giving neuroscientists a new understanding of the brain and a better understanding of neurological diseases. The computing power needed is considerable. Each simulated neuron requires the equivalent of a laptop computer. A model of the whole brain would have billions of them. Supercomputing technology is rapidly approaching a level where simulating the whole brain becomes a concrete possibility.

The Blue Brain Project is the first ever attempt to reverse engineer the mammalian brain. In July, the “Blue Brain 4”, an IBM Blue Gene/Q, was acquired from the Blue Brain Project (EPF Lausanne) and installed at CSCS.

CSCS is also one of the numerous partners of the Human Brain Project led by Professor Henry Markram at EPF Lausanne. CSCS will coordinate the four supercomputer centers participating in the project, and will develop the simulation platform in collaboration with EPF Lausanne.

“Blue Brain 4”, the IBM Blue Gene/Q acquired from the Blue Brain Project (EPF Lausanne) and installed at CSCS.

A system engineer working on the CHIPP cluster “Phoenix”.

Finances

Expenditures

	CHF
Investments	**32 555 142.22**
Equipment and Furniture	**60 581.04**
Personnel	**7 249 675.71**
Payroll	5 698 564.40
Employer's Contributions	976 572.60
Further education, Travel, Recruitment	574 538.71
Other Material Expenses	**6 382 555.85**
Maintenance Building	608 581.03
Energy & Media	2 285 898.82
Administrative Expenses	41 307.52
Hardware, Software, Services	3 086 382.12
Remunerations, Marketing, Workshops Services, Technical Move	351 696.69
Other	8 689.67
Extraordinary Income / Expenditures	**-542 580.50**
Membership Fees / Overhead	7 245.15
Budget/Third Parties Fund Transfers	-549 825.65

Income

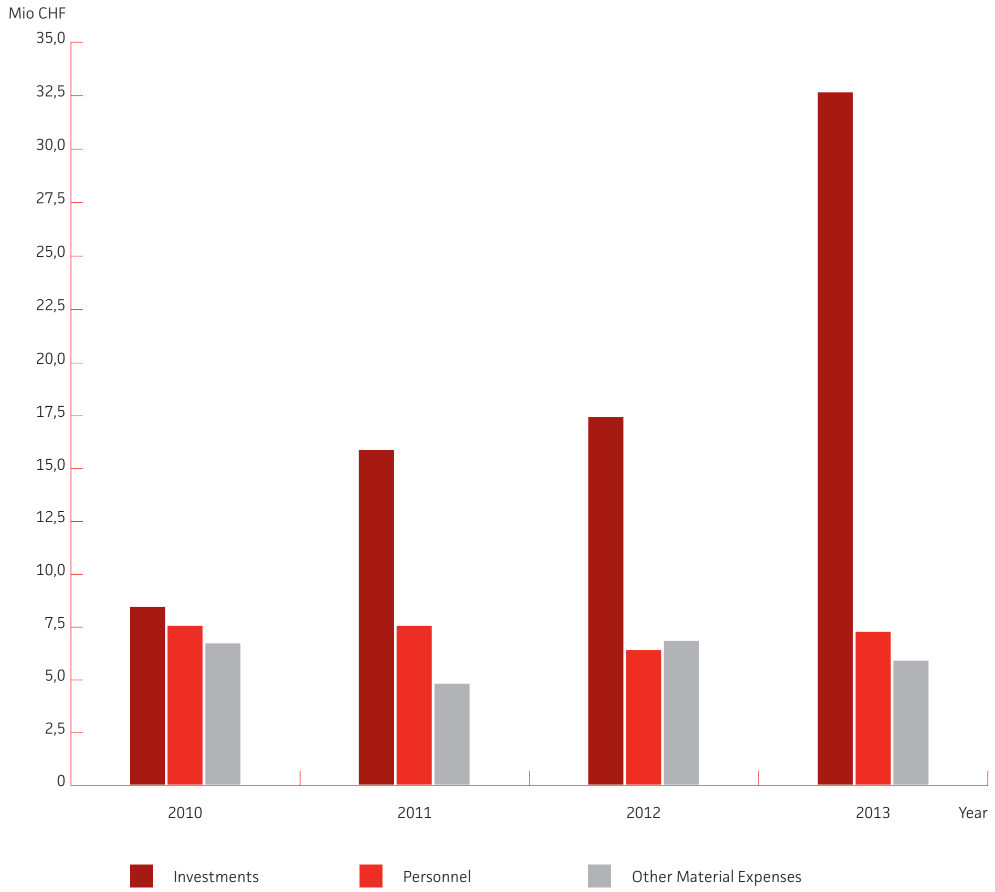
	CHF
Basic Budget	**50 580 694.07**
Contribution ETH Zurich	17 691 000.00
BM BFI-Botschaft HPCN	33 400 000.00
Salary Increase / Price Inflation / PK	78 570.00
Transfer of Project Funds - Personnel Costs	240 000.00
Building Costs Project Piz Daint	-828 875.93
Other Income	**54 248.60**
Services / Courses	28 401.32
Reimbursements	16 247.17
Credit for Accrued Interest	9 600.11

Total Expenses	**45 705 374.32**	**Total Income**	**50 634 942.67**
Balance			**4 929 568.35**

Third Parties Contributions	
Mönch Cluster	2 377 000.00
MeteoSwiss	1 178 000.00
CHIPP	924 030.00
Euler Cluster	550 000.00
USI	472 050.00
European Comission	358 340.91
Other	18 000.00

Development of Overall Expenses

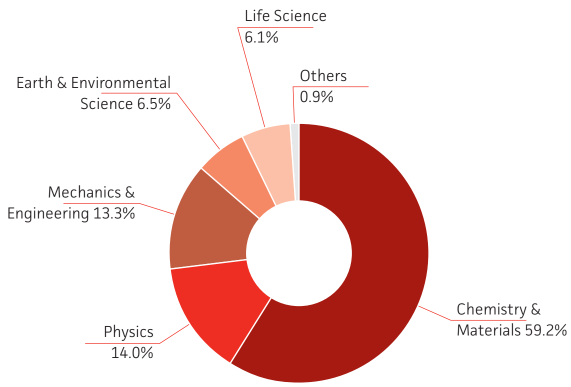
	2010	2011	2012	2013
Investments	8 417 349	15 777 324	17 320 218	32 555 142
Personnel	7 534 853	7 530 745	6 388 608	7 249 676
Other Material Expenses	6 706 740	4 818 411	6 825 156	5 900 556



Usage Statistics

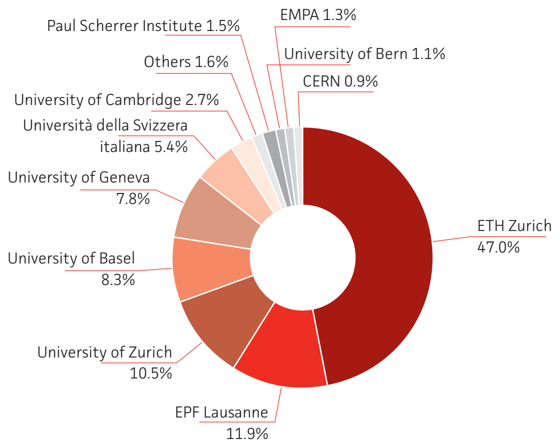
Usage by Research Field

Research Field	CPU h	%
Chemistry & Materials	271 678 665	59.2
Physics	64 572 626	14.0
Mechanics & Engineering	61 064 811	13.3
Earth & Environmental Science	29 798 267	6.5
Life Science	28 017 619	6.1
Others	4 201 576	0.9
Total Usage	**459 333 565**	**100.0**



Usage by Institution

Institution	CPU h	%
ETH Zurich	215 913 207	47.0
EPF Lausanne	54 724 572	11.9
University of Zurich	48 409 392	10.5
University of Basel	38 163 849	8.3
University of Geneva	35 801 371	7.8
Università della Svizzera italiana	24 693 893	5.4
University of Cambridge	12 421 880	2.7
Others	7 473 32	1.6
Paul Scherrer Institute	6 881 128	1.5
EMPA	5 754 15	1.3
University of Bern	4 929 446	1.1
CERN	4 167 355	0.9
Total Usage	**459 333 565**	**100.0**



Compute Infrastructure

HPC Systems for User Lab

Name	Supplier & Model	Installation / Upgrade	CPU Type
Piz Daint	Cray XC30	2012 / 2013	Intel Xeon E5-2670 & Nvidia Tesla K20X GPU
Monte Rosa	Cray XE6	2009 / 2011	AMD Opteron 6272 Interlagos 2.1 GHz
Tödi	Cray XK7	2009 / 2012	AMD Opteron 6272 Interlagos 2.1 GHz & Nvidia Tesla K20X GPU
Pilatus	DALCO Cluster	2012	Intel Xeon E5-2670 2.6 GHz
Rothorn	SGI UV 1000	2011	Intel Xeon E7-8837 2.67 GHz
Matterhorn	Cray XMT	2011	Threadstorm

Name	No. of Cores	Interconnect Type	Peak Performance (TFlops)
Piz Daint	42 176 + 5 272 GPUs	Cray Aries	7 787
Monte Rosa	47 872	Cray Gemini	402
Tödi	4 352 + 272 GPUs	Cray Gemini	393
Pilatus	704	Infiniband FDR PCI Gen 3	15
Rothorn	254	SGI Numalink	3
Matterhorn	8 192 hardware threads	Cray Gemini	NA

HPC Systems for Third Parties

Name	Supplier & Model	Installation / Upgrade	User	CPU Type
Blue Brain 4	IBM BG/Q	2013	EPF Lausanne	BGQ (PowerPC – 1.6 GHz) & Intel Xeon 2.6 GHz
Mönch	NEC Cluster	2013	ETH Zurich	Intel Xeon E5-2660 v2 2.2 GHz
Monte Lema	Cray XE6	2012	MeteoSwiss	AMD Opteron 6172 2.1 GHz
Phoenix	Cluster	2007 / 2012	CHIPP (LHC Grid)	AMD Opteron 6272 2.1 GHz & Intel Xeon CPU E5-2670 2.6 GHz
Albis	Cray XE6	2012	MeteoSwiss	AMD Opteron 6172 2.1 GHz

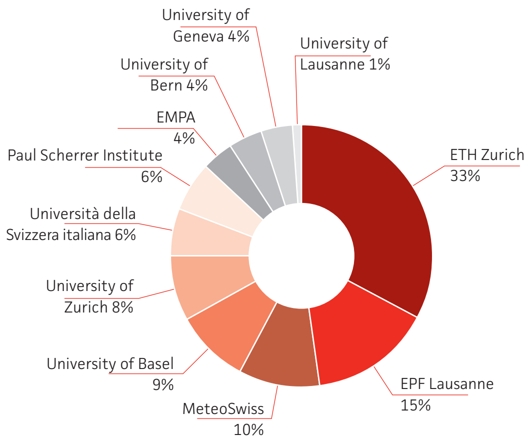
Name	No. of Cores	Interconnect Type	Peak Performance (TFlops)
Blue Brain 4	65 536 (BGQ) & 640 Intel Xeon	IBM BGQ 3D torus & Infiniband FDR	839 + 13
Mönch	6 720	Infiniband FDR PCI Gen 3	139
Monte Lema	4 032	Cray Gemini	34
Phoenix	2 208	Infiniband QDR PCI Gen 2	25
Albis	1 728	Cray Gemini	15

User Satisfaction

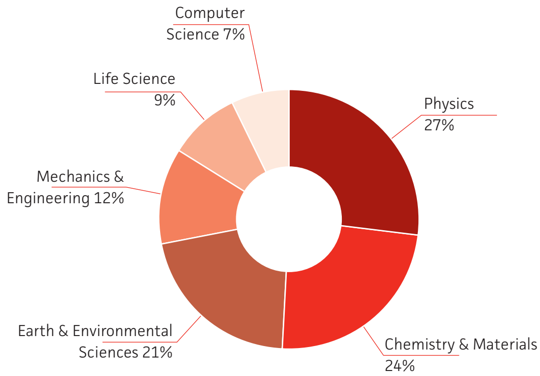
A user satisfaction survey was submitted to 696 users in January 2014. The response rate was of 31% (216 answers).

User Profile

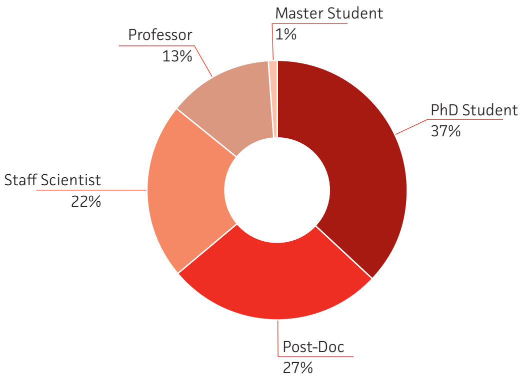
Your institution



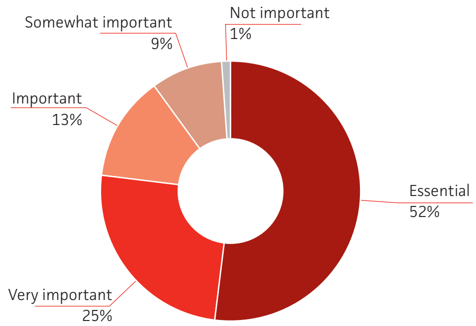
Your scientific field



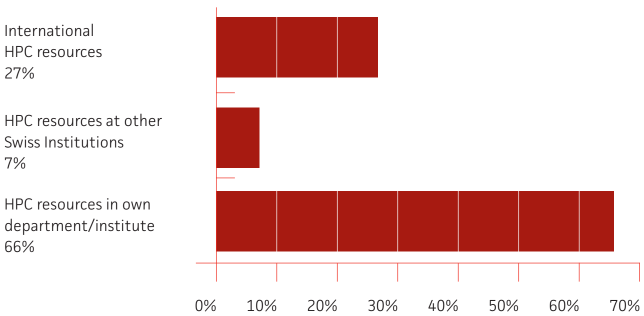
Your position



For my research, CSCS resources are



Which HPC resources are you using besides CSCS?



User Support

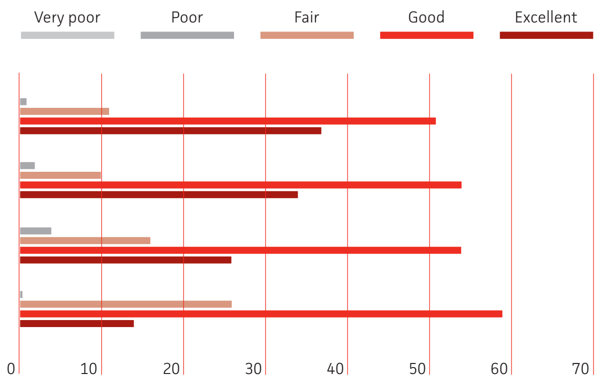
How do you rate the quality of...

Helpdesk support

System support

Application support

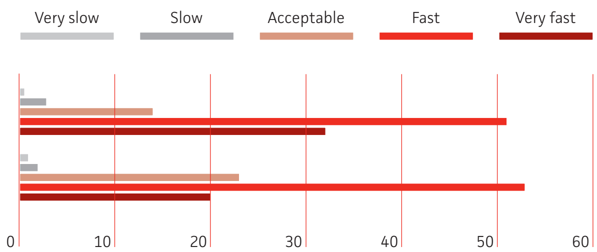
The offer of training courses and user events



How fast does support handle your request?

The reaction time of the helpdesk is

The time to solution for the support requests is



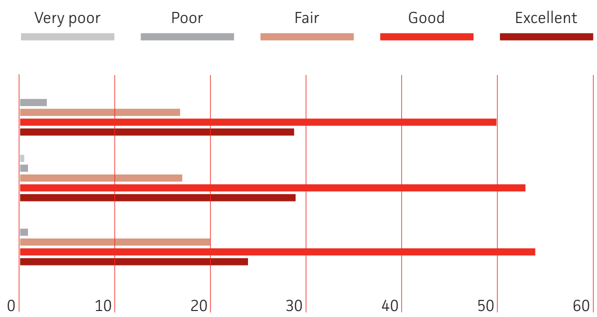
System Availability, Stability and Usability

How you perceive...

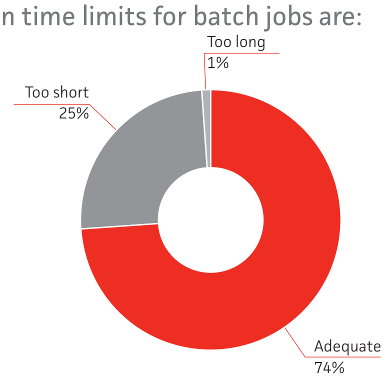
The availability of CSCS systems?

The stability of CSCS systems?

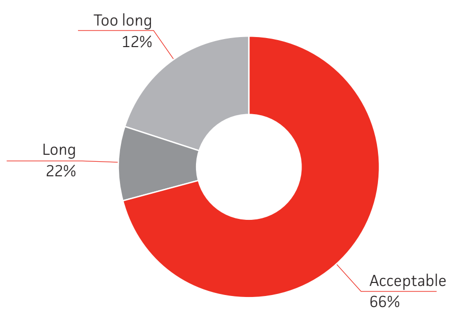
The ease of use of CSCS systems?



The run time limits for batch jobs are:

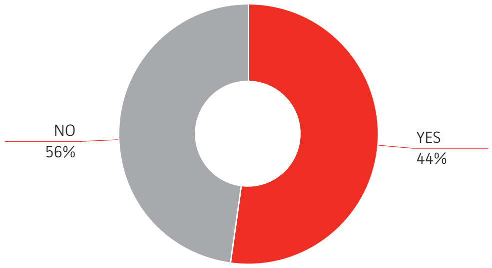


The job waiting time in the queue is:



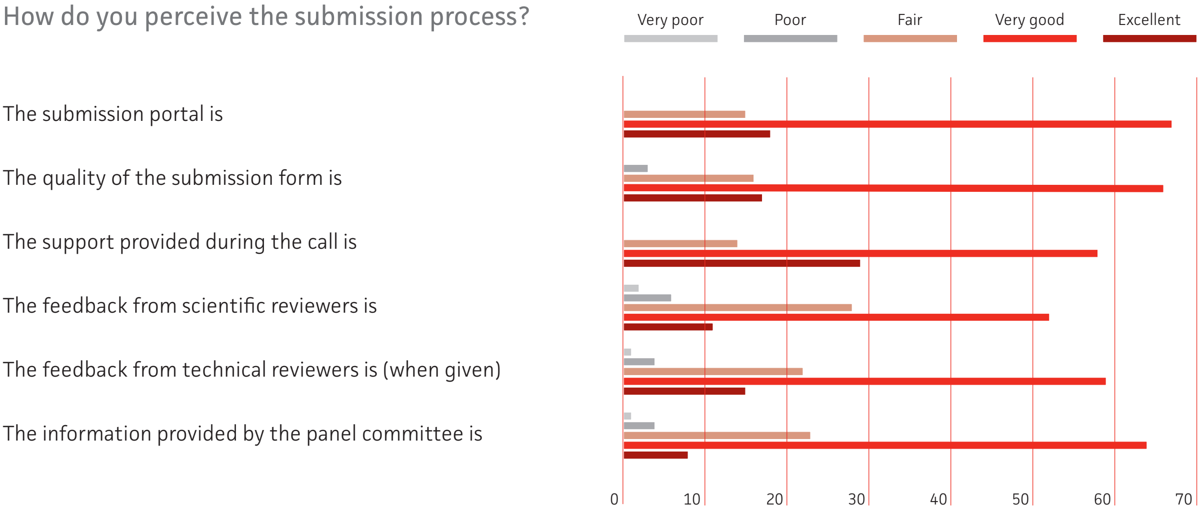
Project Proposal Process

Do you submit project proposals to CSCS (as PI or supporting the PI)?



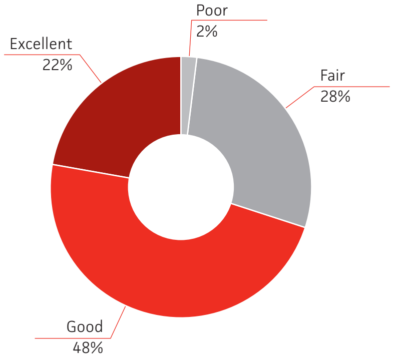
Is the reviewing process transparent?

How do you perceive the submission process?

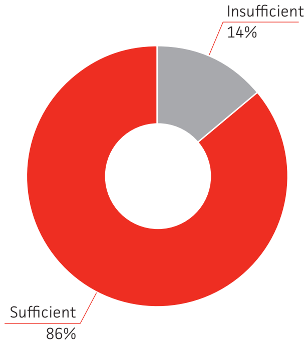


Adequacy of Allocated Resources

The resources assigned to my project are:

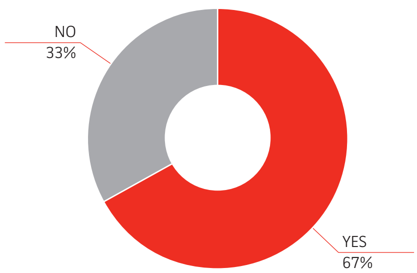


My storage allocation on /project is:

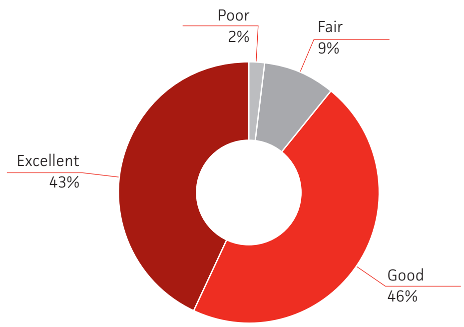


Application Development

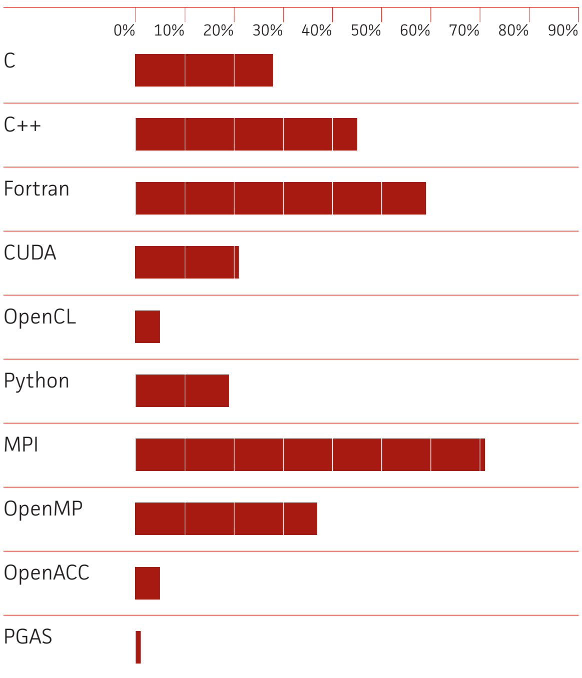
Do you develop and maintain application codes?



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



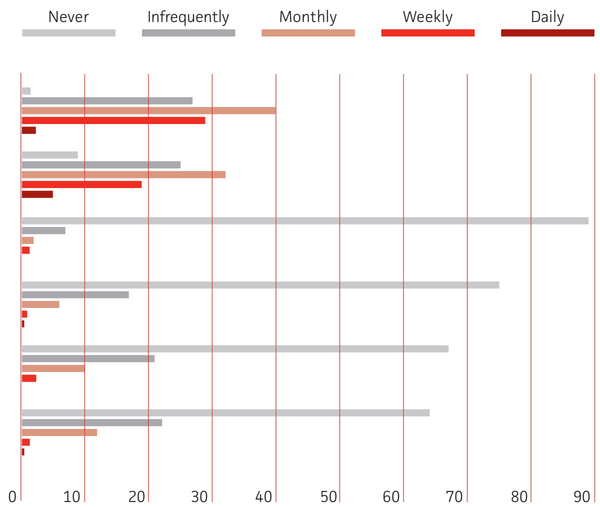
Which programming languages and parallelization paradigms are you using primarily?



Information & Communication

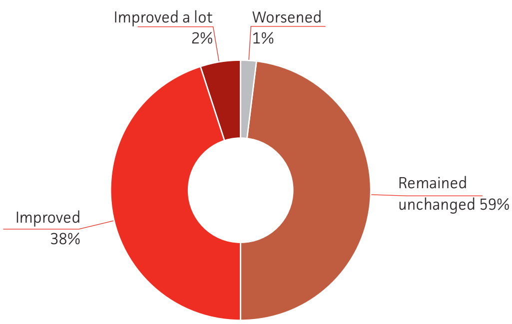
How do you feel informed about...

How often do you access the following communication channels:

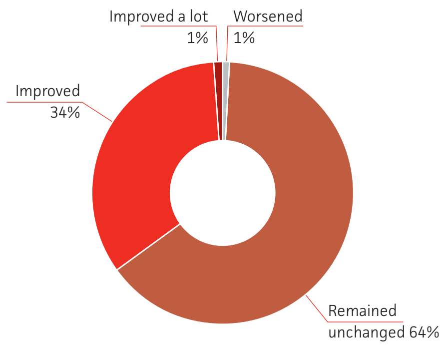


Perception of CSCS

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:



The cables interconnecting the compute nodes of the Cray XC30 supercomputer "Piz Daint".

Impressum

CSCS Swiss National Supercomputing Centre
Via Trevano 131
6900 Lugano
Switzerland

Phone +41 (0) 91 610 82 11
Fax +41 (0) 91 610 82 09
www.cscs.ch

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