CSCS

Annual Report
2015

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

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The photographer Igor Ponti has portrayed five young scientists of different scientific fields who use CSCS supercomputers for their research work: Michele Ceriotti (EPF Lausanne), Shyam Chikatamarla (ETH Zurich), Andreas Fichtner (ETH Zurich), Annette Milnik (University of Basel) and Igor Pivkin (Università della Svizzera italiana). The photos in this Annual Report presents the scientists and their work environment.

Welcome from the Director

Thomas Schulthess, Director of CSCS.

Welcome to the 2015 annual report of the Swiss National Supercomputing Centre (CSCS).

An important milestone this year has been the deployment of "Piz Kesch", an appliance for operational weather forecasting, which we built for MeteoSwiss and will operate on its behalf. "Piz Kesch" is the first supercomputer worldwide that uses hybrid, GPU-accelerated compute nodes for numerical weather forecasts. It uses about three times less energy compared to state-of-the art systems based on conventional processors; such are used by other weather services in Europe. "Piz Kesch" is the result of the refactoring activities of major simulation codes and of the co-design efforts addressed by the Swiss High-Performance Computing and Networking initiative under the auspices of CSCS and the Università della Svizzera italiana.

After seven years of operations, and having followed us from our old location in Manno to Lugano, "Monte Rosa" was shut down for the last time. "Monte Rosa", initially a Cray XT5, provided at once 10 times more computational resources than its predecessor when it came online. This system allowed us and our users to gain experience with massively parallel processor arrays at scale, a key competence that was essential for the introduction of "Piz Daint" and that will remain essential in the years to come.

In 2015 we continued investing in our building infrastructure to further improve the data centre's energy efficiency. At the Parco Ciani pumping station, we installed a micro hydro plant for the production of electrical energy from the water returned to Lake Lugano after cooling the supercomputers.

In response to an increased general interest in our centre and in recognition of continued strong support from the Canton of Ticino, we opened our doors to the local public for one day in October. The event attracted more than 1 000 visitors and features talks held by researchers at Swiss universities, visits to the machine room and the technical infrastructure as well as information booths with our staff explaining our various activities.

An important recognition by the Association for Computing Machinery's (ACM) allows us to look forward to 2016 with great expectations relating to the annual conference of the Platform for Advanced Scientific Computing (PASC) conference we are co-organizing. The PASC Conference is a leading event for researchers in computational science and high-performance computing. From 2016, the PASC Conference will be co-sponsored by ACM SIGHPC, the Special Interest Group on High Performance Computing. The support from the ACM SIGHPC serves as an acknowledgement of the conference's significance and sets well-defined quality standards. The ACM provides the computing field's premier digital library and serves its members and the computing profession with cutting-edge publications, conferences and career resources.

My deepest appreciation goes to the CSCS personnel for their commitment and everyday support. I also wish to thank ETH Zurich for supporting our activities, our user community for providing new scientific challenges related to HPC and our supplier who enables us to provide state-of-the-art services.

Prof. Thomas Schulthess
Director of CSCS

Content

Name
Michele Ceriotti

Position
Assistant Professor

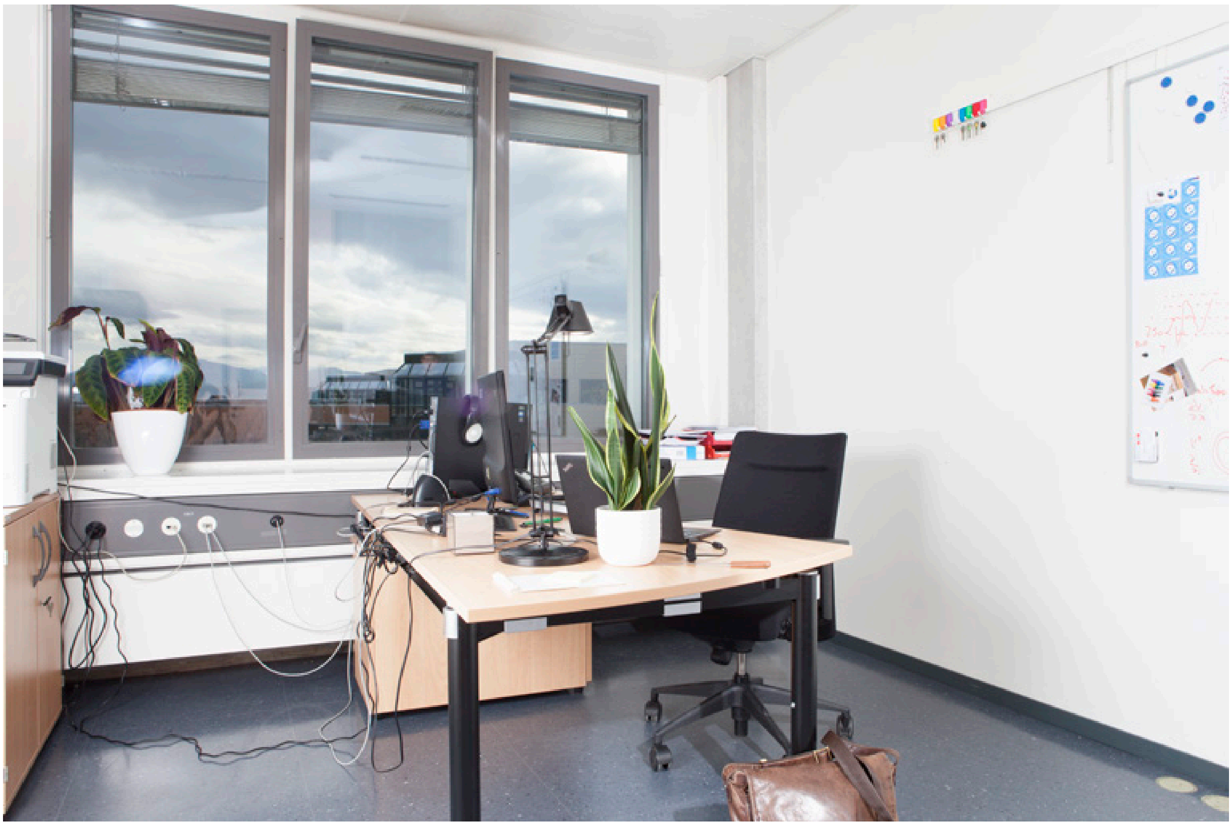
Institution
EPF Lausanne

Background
2001–2006 Studies in materials science, Milano Bicocca, Italy
2007–2010 PhD in physics, ETH Zurich
2011–2013 Post-doctoral researcher, University of Oxford, UK
Since 2013 Assistant professor, Laboratory of Computational Science and Modelling, EPF Lausanne

Area of Research
Computational materials science.

Specialised in
Molecular dynamics, enhanced sampling, machine learning, nuclear quantum effects.

HPC means for me
Enabling accurate, predictive simulations of complex systems by combining raw computational power and more efficient algorithms.



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
Piz Dora, Cray XC40, 1.2 PFlops

Computing Time for User Lab

2015: 1 201 734 615 CPU h
2014: 798 998 534 CPU h

User Community

2015: 105 Projects, 568 Users
2014: 85 Projects, 523 Users

Employees

2015: 70
2014: 64

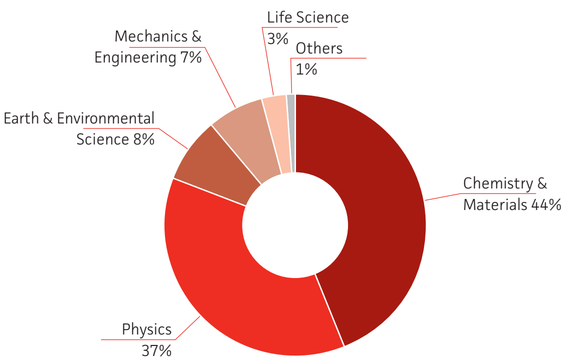
Investments

2015: 5.1 Mio CHF
2014: 8.1 Mio CHF

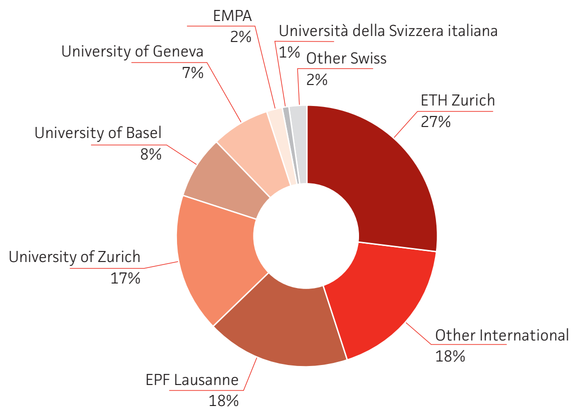
Operational Costs

2015: 15.1 Mio CHF
2014: 15.8 Mio CHF

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 / 13	User Lab	7 784
Piz Dora	Cray XC40	2014	User Lab	1 246
Pilatus	Intel Sandy Bridge Cluster	2012	User Lab	15

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
Piz Es-cha	Cray CS-Storm	2015	MeteoSwiss	305
Piz Kesch	Cray CS-Storm	2015	MeteoSwiss	305
Mönch	NEC Cluster	2013 / 14	ETH Zurich	132
Monte Lema	Cray XE6	2012	MeteoSwiss	34
Phoenix	Cluster	2007 / 15	CHIPP (LHC Grid)	43
Albis	Cray XE6	2012	MeteoSwiss	15

Name
Shyam Chikatamarla

Position
Senior Scientist

Institution
ETH Zurich

Background
2000–2005 Studies in mechanical engineering, Indian Institute of Technology Madras, India
2005–2008 PhD in mechanical engineering, ETH Zurich
2008–2011 Post-doctoral researcher, ETH Zurich
Since 2012 Senior Scientist, Institute of Energy Technology, ETH Zurich
Recipient of ETH Medal for outstanding PhD thesis in mechanical engineering.

Area of Research
Fluid dynamics, numerical methods, high performance computing

Specialised in
Lattice Boltzmann methods for wide range of applications including turbulence, multiphase, multiphysics and compressible flows.

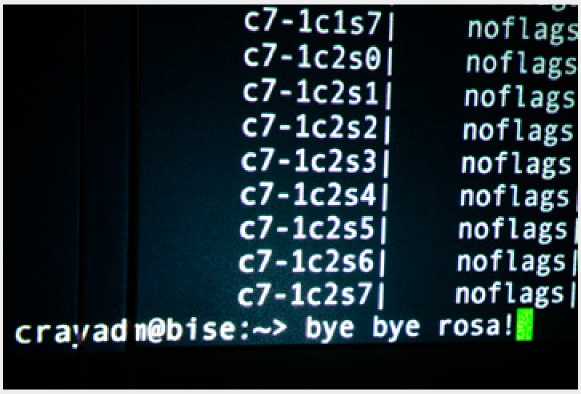
HPC means for me
HPC is the only means by which I can realize my aims and ambitions of exploring new physics.
In fluid dynamics, HPC gives us access to details and understanding that is beyond the reach of experimental observations.

February

25

"Monte Rosa" becomes historical artefact

Having been the main supercomputer of CSCS for six years, the Cray XE6 "Monte Rosa" has been shut down for the very last time. Some cabinets have been donated to the Bolo Museum in Lausanne.



March

02

Contribution to "Diamo i Numeri" exhibition

Ascona and Lugano hosted the interactive exhibition "Diamo i Numeri" introducing a young public to the fascinating world of numbers. CSCS as co-sponsor contributed with a video on visualisations of scientific simulations.

03/06

Peer review

Four experts in HPC, Prof. Richard Kenway, EPCC, University of Edinburgh, UK; Prof. Thomas Lippert, IAS/JSC, Research Centre Jülich, Germany (Chair); Prof. Daniel A. Reed, University of Iowa, USA; and Prof. Takayuki Aoki, Tokyo Institute of Technology, Japan, reviewed the activities of CSCS.

23/25

HPC Advisory Council Switzerland conference 2015

More than 130 professionals attended the sixth Swiss conference of the HPC Advisory Council. The conference, which is co-sponsored by CSCS, focused on HPC essentials, new developments and emerging technologies, best practices and hands-on training.

April

01

28 million node hours allocated in 2015 first call for proposals

A total of 28 million node hours was allocated to research projects on the "Piz Daint" flagship system and its add-on multi-core extension "Piz Dora". As usual, resources were granted to the proposals successfully passing the review process accessing the technical readiness as well as the scientific merit of the proposals submitted.

May

26

Extension of storage resources

The executive board of ETH Zurich approved the procurement of 8 Petabyte (PB) of disks to partly replace and extend the storage infrastructure. With this extension, the size of "project" could be extended to 6.2 PB and "store" up to 5 PB, reaching a total of 11.2 PB.

June

01/03

PASC15 Conference

The Platform for Advanced Scientific Computing (PASC) held its second annual conference on advanced scientific computing at ETH Zurich. The increase in the number of participants this year, 350 attendees compared to 250 last year, is testament to the rising demand for cross-disciplinary knowledge exchange in this field.

02

User meeting

As last year, the user meeting was integrated into the PASC Conference. This solution offered additional opportunities to discuss future developments at CSCS.

18/19

Introduction to GPU programming with CUDA and OpenACC

Two-day workshop intended to offer an introduction to GPU computing using two different programming models: CUDA and OpenACC.

25

Datamover service

A new service to easily move large data sets between the centre and users based on GridFTP technology was introduced and presented during a webinar.

July

06/10

First OpenACC EuroHack

There was plenty of "hacking" going on in Lugano, but it was all completely legal, as CSCS hosted a workshop for developing efficient supercomputer codes with over 60 computer specialists from all over the world.

12/15

HPC in Switzerland at ISC15

CSCS and hpc-ch presented the latest developments in HPC in Switzerland at a booth at the ISC15 in Frankfurt.

20/30

Summer school

In collaboration with the Institute of Computational Science at the Università della Svizzera italiana, CSCS organized a summer school dedicated to HPC with about 30 students.

21

Producing electricity with cooling water

To further improve its energy efficiency, two turbines were installed at Parco Ciani pumping station to produce electricity using the water returning to Lake Lugano after cooling the supercomputers.

September

03/04

User meeting at EPF Lausanne and University of Basel

In addition to the user meeting organised during the PASC15 Conference, CSCS invited its user community to EPF Lausanne and University of Basel to discuss key issues related to proposal submission.

15

Paving the way for more detailed weather forecasts

The new "super weather computer" of the Swiss Federal Office of Meteorology and Climatology (MeteoSwiss) came onstream. This new GPU-based computer architecture will be able to calculate weather models with twice as high a resolution, while ensuring greater efficiency and speed than in the past. Read more on page 50.

October

01

14 million node hours allocated in 2015 second call for proposals

The second allocation period granted a total of 14 million node hours to renewals, new projects and small projects. The high quality of the research carried out on the CSCS HPC systems is demonstrated by the 251 publications, of which 24 are in journals with an impact factor higher than 10.

17

Open doors

"I cervelli che contano" was the slogan of the open-house event. More than 1 000 visitors had the possibility to see the infrastructure and speak with the staff and scientists from different Swiss universities. Read more on page 52.

26

Adecco Solidarity Day

CSCS participated in Global Solidarity Day 2015, an Adecco's fund-raising event, in order to provide support refugees. Thanks to a sunny day and the willingness of all employees who decided to participate, the centre was the most active company in all of Ticino, clocking up a total of 514 kilometres (equal to CHF 514 in donations).

29

ACM becomes co-sponsor of the PASC Conference

The Association for Computing Machinery's (ACM) and CSCS announced that the PASC Conference will be co-sponsored by ACM' Special Interest Group on High Performance Computing (SIGHPC) from 2016. The support from the ACM SIGHPC serves as an acknowledgement of the conference's importance and sets well-defined quality standards.

Association for Computing Machinery

sighpc

November

16/19

HPC in Switzerland at Supercomputing 2015

CSCS and the Swiss HPC community hpc-ch presented the latest developments in HPC in Switzerland at SC15, the world's largest supercomputing conference held in Austin, Texas .

December

14/15

Workshop on advanced C++ for HPC

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

Name
Andreas Fichtner

Position
Assistant professor

Institution
ETH Zurich

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

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

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

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

Farewell to “Monte Rosa”, “Piz Daint” is the new driving force

One of the events that marked the beginning of 2015 at CSCS was the official ceremony to finally shut down “Monte Rosa”. This was the flagship Cray XE6 system that successfully supported users in their research for six long years. “Monte Rosa” will always hold a special place in the history of CSCS. It was the system with which CSCS entered the international HPC scene to become one of the world’s leading computer centres.

“Piz Daint”, the heterogeneous Cray XC30 system, slowly but steadily took over tasks from “Monte Rosa”, and eventually became the User Lab flagship system to serve the Swiss and international scientific community, definitively consolidating the position of CSCS in the HPC domain. After two years, “Piz Daint” is still among the most powerful supercomputers in the world. At the same time it is one of the most energy-efficient systems in the petaflop class thanks to its hybrid composition of 5 272 compute notes, each equipped with one Intel Xeon E5 CPU and one NVIDIA Tesla K20x GPU. “Piz Daint” is also the first system at CSCS that is ideally meant to “do everything”. This is the path that supercomputer centres will try to pursue in the future – in other words, to have a supercomputer that can not only carry out computations, but also process generated data, analyse, structure, visualise and store it.

Resources allocated in 2015

Analysis of usage statistics reveals a number of interesting trends: First, Chemistry & Materials still remains by far the most compute-intensive research field at CSCS, using 44 % of the total allocation (56 % in 2014). However, there seems to be a steady trend in Physics, which is embarking on more and more compute-intensive projects as well, increasing its share from a mere 14 % in 2013 to 31 % in 2014 and 37 % in 2015. This increase primarily reflects projects in plasma physics and quantum chromodynamics. The remaining disciplines have consumed less than 10 % each, including Earth & Environmental Sciences, Life Sciences, and Mechanics & Engineering. Their relative share of HPC resources has proven to remain fairly constant over the last few years.

Statistics of usage by institution show some trends: Although ETH Zurich is still the biggest user by far, its percentile share (27 %) has seen a decrease compared to 2014 (35 %), mostly in favour of international proposals, which have increased from 12 % in 2014 to 18 % in 2015. The share of the other two major users, EPF Lausanne and the University of Zurich, has remained almost unchanged at 18 % and 17 % respectively. The numbers demonstrate that CSCS is a high-profile computing resource for excellent research in all of Switzerland that has additionally consolidated its position on the international scene, attracting very interesting and challenging projects from all over the world.

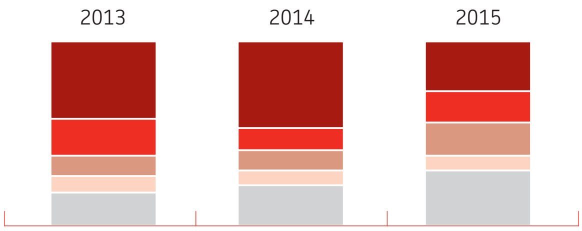
List of CHRONOS Projects

Principal Investigator	Organisation	Research Field	Project Title	Granted Allocation in Mio CPU h
Joost VandeVondele	ETH Zurich	Chemistry & Materials	Exploring frontiers in nanoscale simulation: new models and improved accuracy	100.00
Lucio Mayer	University of Zurich	Physics	SuperARGO: a galaxy population at ERIS resolution to unfold galaxy evolution across different mass scales	75.00
Constantia Alexandrou	University of Cyprus	Physics	The neutron electric dipole moment and proton charge radius using lattice QCD simulations at physical pion mass	60.00
Andreas Fichtner	ETH Zurich	Earth & Environmental Science	Global waveform inversion across the scales	50.00
Nicola Marzari	EPF Lausanne	Chemistry & Materials	Computational materials science in the cloud: an open-access database of materials’ data and computational workflows	40.00
Christoph Schär	ETH Zurich	Earth & Environmental Science	Continental-scale cloud-resolving climate simulations for Europe	40.00

Usage Statistics

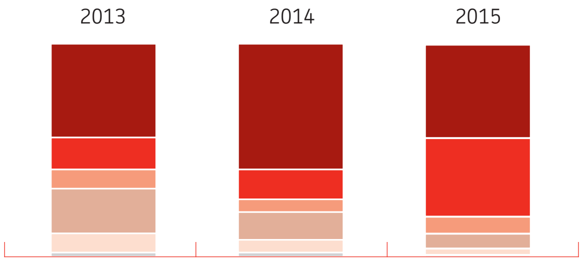
Usage by Institution (%)

Institution	2013	2014	2015
ETH Zurich	47	35	27
University of Zurich	12	20	17
EPF Lausanne	11	20	18
University of Basel	8	4	8
Others	22	21	30
Total Usage	**100**	**100**	**100**



Usage by Research Field (%)

Research Field	2013	2014	2015
Chemistry & Materials	59	56	44
Physics	14	31	37
Earth & Environ. Science	6	7	8
Mechanics & Engineering	13	4	7
Life Science	6	2	3
Others	2	0	1
Total Usage	**100**	**100**	**100**



16 Largest Projects

Principal Investigator	Organisation	Research Field	Project Title	Granted Allocation in Mio CPU h
Stefan Brunner	EPF Lausanne	Physics	TCV-relevant GENE simulations	72.00
Alfio Quarteroni	EPF Lausanne	Life Science	Cardiac and vascular numerical simulations	43.10
Franco Vazza	Hamburg Observatory	Physics	On the seeding of large-scale magnetic fields in the Universe: cosmological radiative simulations with Enzo-MHD on the GPU	36.56
Thierry Giamarchi	University of Geneva	Chemistry & Materials	Understanding the 2D Hubbard model: studying unconventional superconductivity through simulation of coupled Hubbard ladders using massively parallel DMRG	35.07
Lucio Mayer	University of Zurich	Physics	Planet formation via disk instability entering the domain of massively parallel radiation hydrodynamics simulations	30.00
Richard Sandberg	University of Melbourne	Mechanics & Engineering	GPU-accelerated high-fidelity simulations of full turbine stages	28.76
Wanda Andreoni	EPF Lausanne	Chemistry & Materials	Mechanical and vibrational properties of perovskite photovoltaics: the effects of water from first principles calculations	27.26
Nicola Spaldin	ETH Zurich	Chemistry & Materials	Coupled and competing instabilities in complex oxides	27.15
Satish Rao	EPF Lausanne	Chemistry & Materials	Large-scale 3D dislocation dynamics simulations of flow, strain hardening and strain-burst characteristics in multimicron-scale Ni and Al micropillars	24.00
Andrew Jackson	ETH Zurich	Earth & Environ. Science	Beyond conventional planetary dynamo models	24.00
Harry van Lenthe	ETH Zurich	Life Science	The role of mechanics in fracture healing and bone turnover	21.70
Mathieu Luisier	ETH Zurich	Chemistry & Materials	Ab initio simulation of the source and drain contact resistances in ultra-scaled nano-transistors	19.80
Shyam Chikatamarla	ETH Zurich	Mechanics & Engineering	Entropic lattice Boltzmann method for compressible flows	17.47
William Curtin	EPF Lausanne	Mechanics & Engineering	Large scale atomic simulations of dislocation plasticity and fracture in magnesium and alloys	15.00
Nicola Marzari	EPF Lausanne	Chemistry & Materials	THEOS NANO: thermal, electrical, and optical properties of nanoscale materials	15.00
Stefan Goedecker	University of Basel	Chemistry & Materials	Developmentof charge equilibration force fields based on machien learning	15.00

List of Projects by Institution

EMPA

CarboCount CH: quantifying greenhouse gas fluxes and their sensitivity to climate variations, Dominik Brunner (Earth & Environmental Science, 1.80 Mio CPU h)

EPF Lausanne

Mechanical and vibrational properties of perovskite photovoltaics: the effects of water from first principles calculations, Wanda Andreoni (Chemistry & Materials, 27.26 Mio CPU h)

TCV-relevant GENE simulations, Stefan Brunner (Physics, 72.00 Mio CPU h)

Understanding the impact of nuclear quantum effects on the stability of molecular crystals, Michele Ceriotti (Chemistry & Materials, 9.60 Mio CPU h)

Long Range ordering of water in aqueous solutions: insights from atomistic simulations of second harmonic scattering, Michele Ceriotti (Chemistry & Materials, 5.76 Mio CPU h)

Large scale atomic simulations of dislocation plasticity and fracture in magnesium and alloys, William Curtin (Mechanics & Engineering, 15.00 Mio CPU h)

Large eddy simulation of very-large-scale motions in atmospheric boundary layer flows: the influences of the Coriolis force and thermal stability, Jiannong Fang (Earth & Environmental Science, 7.80 Mio CPU h)

Study of land-atmosphere interaction over Antarctic snow-ice formations by large eddy simulation, Michael Lehning (Earth & Environmental Science, 6.00 Mio CPU h)

Study on snow precipitation and accumulation over complex alpine terrain, Michael Lehning (Earth & Environmental Science, 7.20 Mio CPU h)

THEOS NANO: thermal, electrical, and optical properties of nanoscale materials, Nicola Marzari (Chemistry & Materials, 15.00 Mio CPU h)

Defect and band-edge levels through GW and hybrid functionals, Alfredo Pasquarello (Chemistry & Materials, 6.75 Mio CPU h)

Cardiac and vascular numerical simulations, Alfio Quarteroni (Life Science, 43.10 Mio CPU h)

Large-scale 3D dislocation dynamics simulations of flow, strain hardening and strain-burst characteristics in multimicron-scale Ni and Al micropillars, Satish Rao (Chemistry & Materials, 24.00 Mio CPU h)

Simulation of plasma turbulence in the edge of tokamak devices, Paolo Ricci (Physics, 8.98 Mio CPU h)

Large energetic particle physics in magnetically confined configurations, Jonathan Graves (Physics, 3.24 Mio CPU h)

Dissipative particle dynamics simulations of amphiphilic polymer systems, Nicholas Miller (Chemistry & Materials, 2.79 Mio CPU h)

ETH Zurich

Evaluating aerosol cloud interactions at the regional scale, Isabelle Bey (Earth & Environmental Science, 3.00 Mio CPU h)

Hydrogenation of carbon dioxide using immobilized molecular catalysts anchored on mesoporous silica, Praveen Chandramathy (Chemistry & Materials, 6.00 Mio CPU h)

Entropic lattice Boltzmann method for compressible flows, Shyam Chikatamarla (Mechanics & Engineering, 17.47 Mio CPU h)

DNS of turbulent hetero-/homogeneous combustion with detailed chemistry, Christos Frouzakis (Mechanics & Engineering, 3.30 Mio CPU h)

Beyond conventional planetary dynamo models, Andrew Jackson (Earth & Environmental Science, 24.00 Mio CPU h)

Simulation of microfluidics for mechanical cell separation: building the in-silico lab-on-a-chip, Petros Koumoutsakos (Life Science, 9.00 Mio CPU h)

Ab-initio simulation of the source and drain contact resistances in ultra-scaled nano-transistors, Mathieu Luisier (Chemistry & Materials, 19.80 Mio CPU h)

European regional climate simulations of stable water isotopes in the atmospheric water cycle with COSMOiso (EURECIS), Stephan Pfhal (Earth & Environmental Science, 5.47 Mio CPU h)

Coupled and competing instabilities in complex oxides, Nicola Spaldin (Chemistry & Materials, 27.15 Mio CPU h)

The role of mechanics in fracture healing and bone turnover, Harry van Lenthe (Life Science, 21.70 Mio CPU h)

Simulating the transduction of mechanical forces into biological signals, Viola Vogel (Life Science, 5.55 Mio CPU h)

Full-annular simulation of a real supersonic multi-stage steam turbine, Reza Abhari (Mechanics & Engineering, 1.94 Mio CPU h)

Computational nanometrology for technology nodes beyond 16 nm, Mauro Ciappa (Physics, 2.32 Mio CPU h)

High-frequency reference seismograms for the Mars insight mission, Amir Khan (Earth & Environmental Science, 2.11 Mio CPU h)

Impacts of lower crustal flow on regional and global scale geodynamics, Dave May (Earth & Environmental Science, 1.34 Mio CPU h)

Computing measure valued and statistical solutions of the equations of fluid dynamics, Siddharta Mishra (Computer Science, 1.05 Mio CPU h)

Dynamic percolation theory for immiscible multiphase flow with the lattice Boltzmann method and its implications for magma chamber dynamics, Andrea Parmigiani (Earth & Environmental Science, 0.98 Mio CPU h)

Lithium-ion batteries: an ab-initio study of their static and kinetic electrode properties, Andreas Pedersen (Chemistry & Materials, 1.92 Mio CPU h)

High resolution glacier modelling with PISM, Julien Seguinot (Earth & Environmental Science, 3.12 Mio CPU h)

Institute for Research in Biomedicine

STAT3 structure and dynamics explored by molecular simulations with an eye to drug induced aggregation, Andrea Cavalli (Life Science, 1.89 Mio CPU h)

IRSOL

Magnetohydrodynamic models of the solar atmosphere, Oskar Steiner (Physics, 1.73 Mio CPU h)

Paul Scherrer Institute

Study of negative-thermal expansion in ScF3, Dmitrijs Bocarovs (Chemistry & Materials, 2.10 Mio CPU h)

Detailed understanding of metal adsorption on clay minerals obtained by combining atomistic simulations and X-ray spectroscopy, Sergey Churakov (Earth & Environmental Science, 3.45 Mio CPU h)

Study of the molecular mechanism of activation of the angiotensin II type 1 receptor by natural and biased ligands using enhanced molecular dynamics simulations, Xavier Deupi (Life Science, 6.00 Mio CPU h)

Study of chromia-doped uranium dioxide, Matthias Krack (Chemistry & Materials 2.01 Mio CPU h)

SUPSI

insiGth into Ataxin 3 aggregation by coMputational modEling (GAME), Marco Agostino Deriu (Life Science, 1.83 Mio CPU h)

Università della Svizzera italiana

Mechanical sensing of red blood cells by the human spleen: implications for hereditary spherocytosis and red blood cell aging, Igor Pivkin (Life Science, 5.29 Mio CPU h)

All atom characterization of all-vanadium flow batteries with carbon based electrodes, Daniela Polino (Chemistry & Materials, 4.50 Mio CPU h)

Improving diagnosis of atrial fibrillation, Mark Potse (Life Science, 1.61 Mio CPU h)

Unraveling the dynamical nature of the L44-alpha4 region in the L30e protein system with molecular simulations, Omar Valsson (Life Science, 1.76 Mio CPU h)

University of Basel

Development of charge equilibration force fields based on machine learning, Stefan Goedecker (Chemistry & Materials, 15.00 Mio CPU h)

Genome-wide assessment of epistatic associations in the epigenome of European and African populations, Andreas Papassotiropoulos (Life Science, 5.01 Mio CPU h)

Activation and inactivation of voltage gated K channels, Simon Bernèche (Life Science, 1.98 Mio CPU h)

University of Bern

ISOTOPE (modelling ISOTOPEs in the Earth system), Fortunat Joos (Earth & Environmental Science, 1.86 Mio CPU h)

Extreme events and underlying mechanisms in the last millennium and implications for the future, Christoph Raible (Earth & Environmental Science, 11.24 Mio CPU h)

Study of the structure-function relationship in potassium channels, Niklaus Johner (Life Science, 1.88 Mio CPU h)

Properties of amino acid-derived materials from accurate electron density determination, Mauro Macchi (Chemistry & Materials, 1.20 Mio CPU h)

University of Geneva

Quantum systems with strong correlations: materials and novel computational approach, Antoine Georges (Chemistry & Materials, 13.00 Mio CPU h)

Understanding the 2D Hubbard model: studying unconventional superconductivity through simulation of coupled Hubbard ladders using massively parallel DMRG, Thierry Giamarchi (Chemistry & Materials, 35.07 Mio CPU h)

University of Zurich

Formation and properties of 2-nm Voids @h-BN/Rh, Marcella Iannuzzi (Chemistry & Materials, 9.90 Mio CPU h)

Planet formation via disk instability entering the domain of massively parallel radiation hydrodynamics simulations, Lucio Mayer (Physics, 30.00 Mio CPU h)

Radiation hydrodynamics in simulations of high redshift galaxies, Valentin Perret (Physics, 3.00 Mio CPU h)

Solving high-dimensional dynamic stochastic economic models with adaptive sparse grids, Simon Scheidegger (Computer Science, 10.50 Mio CPU h)

Simulating the Euclid Universe and correcting for baryons, Aurel Schneider (Physics, 13.20 Mio CPU h)

Applications of a scalable algorithm to improve sampling efficiency in molecular dynamics simulations of biological systems, Andreas Vitalis (Life Science, 4.50 Mio CPU h)

CEFCA

The HexaHalo project: simulating dark matter structures in the continuous limit, Raul Angulo (Physics, 12.00 Mio CPU h)

EMBL

Investigating the activation mechanism of SHP-1 through enhanced sampling simulations, Teresa Carlomagno (Life Science, 1.26 Mio CPU h)

Hamburg Observatory

On the seeding of large-scale magnetic fields in the Universe: cosmological radiative simulations with Enzo-MHD on the GPU, Franco Vazza (Physics, 36.56 Mio CPU h)

Hungarian Academy of Science

Description of changes of hydration structures of proteins during complex formation, Csaba Hetényi (Life Science, 1.89 Mio CPU h)

ITT - Rome

Protein post-translational modification detection via graphene nanopores, Mauro Chinappi (Life Science, 1.92 Mio CPU h)

Observatoire de Côte d'Azur

Gas and galaxies in simulations of massive clusters of galaxies, Oliver Hahn (Physics, 3.00 Mio CPU h)

Rice University

High temperature electronic structure by a novel Monte Carlo method for the warm dense electron gas and plasmonic catalysis, James Shepherd (Chemistry & Materials, 10.00 Mio CPU h)

University College London

Towards an understanding of ice formation in clouds, Gabriele Sosso (Chemistry & Materials, 4.45 Mio CPU h)

University of Melbourne

GPU-accelerated high-fidelity simulations of full turbine stages, Richard Sandberg (Mechanics & Engineering, 28.76 Mio CPU h)

Renewals

University of Basel

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

EPF Lausanne

Application of large-eddy simulation to atmospheric boundary layer flows and transports of scalars above urban surfaces, Wai Chi Cheng (Mechanics & Engineering, 5.76 Mio CPU h)

Large eddy simulation of diurnal cycles of alpine slope winds, Marc Parlange (Earth & Environmental Science, 1.70 Mio CPU h)

Multiscale simulations of biological systems and bioinspired, Ursula Röthlisberger (Chemistry & Materials, 9.08 Mio CPU h)

Light-matter interaction from first principles: new developments in nonadiabatic dynamics with applications in energy production, saving, and storage, Ivano Tavernelli (Chemistry & Materials, 1.09 Mio CPU h)

ORB5-GENE turbulence, Laurent Villard (Physics, 10.08 Mio CPU h)

Computational exploration of emerging electronic materials, Oleg Yazyev (Chemistry & Materials, 3.60 Mio CPU h)

ETH Zurich

Entropic lattice Boltzmann method for fluid dynamics, Shyam Chikatamarla (Mechanics & Engineering, 2.39 Mio CPU h)

Direct numerical simulation of formation and propagation of turbulent spherical premixed syngas/air flames, Christos Frouzakis (Mechanics & Engineering, 4.50 Mio CPU h)

Optimization of shape, motion and formation patterns of single and multiple swimmers, Petros Koumoutsakos (Mechanics & Engineering, 12.05 Mio CPU h)

Uncertainty quantification and propagation for large scale molecular dynamics simulations of nano-fluidics, Petros Koumoutsakos (Chemistry & Materials, 3.75 Mio CPU h)

Cloud cavitation collapse, Petros Koumoutsakos (Mechanics & Engineering, 6.48 Mio CPU h)

The role of aerosols in the climate system: a global Earth system perspective, Ulrike Lohmann (Earth & Environmental Science, 5.82 Mio CPU h)

Land-climate feedbacks in a changing climate, Sonia Seneviratne (Earth & Environmental Science, 1.62 Mio CPU h)

Topological quantum computation and the fractional quantum Hall effect, Matthias Troyer (Chemistry & Materials, 6.63 Mio CPU h)

University of Basel

Structure prediction of clusters and solids, Stefan Goedekcer (Chemistry & Materials, 45.00 Mio CPU h)

Elephant: a three-dimensional supernova model for efficient parameter studies with spectral neutrino transport, Matthias Liebendörfer (Physics, 4.68 Mio CPU h)

University of Zurich

CP2K program development, Jürg Hutter (Chemistry & Materials, 2.88 Mio CPU h)

Atomistic simulation of molecules at interfaces, Jürg Hutter (Chemistry & Materials, 27.00 Mio CPU h)

Investigation and design of Co(II)-based cubane water-oxidation catalysts, Sandra Luber (Chemistry & Materials, 11.75 Mio CPU h)

University of Lausanne

Mechanisms controlling acid-sensing ion channel (ASIC) activity, StephanKellenberger (Life Science, 4.08 Mio CPU h)

University of Geneva

Photoinduced spin crossover in iron(II) complexes in solution: 1. Spin-state dependence of the solution structures, Max Lawson Daku (Chemistry & Materials, 27.00 Mio CPU h)

Realistic 3D modelling of stellar winds, Aline Vidotto (Physics, 0.45 Mio CPU h)

EMPA

Toward novel nanomaterials and functional surfaces: from spectroscopy to chirality, Carlo Pignedoli (Chemistry & Materials, 7.92 Mio CPU h)

Institute of Meteorology and Water Management-National Research Institute, Warsaw

COSMO - EULAG verification and tuning for Alpine weather prediction, Zbigniew Piotrowski (Earth & Environmental Science, 0.21 Mio CPU h)

University of Leiden

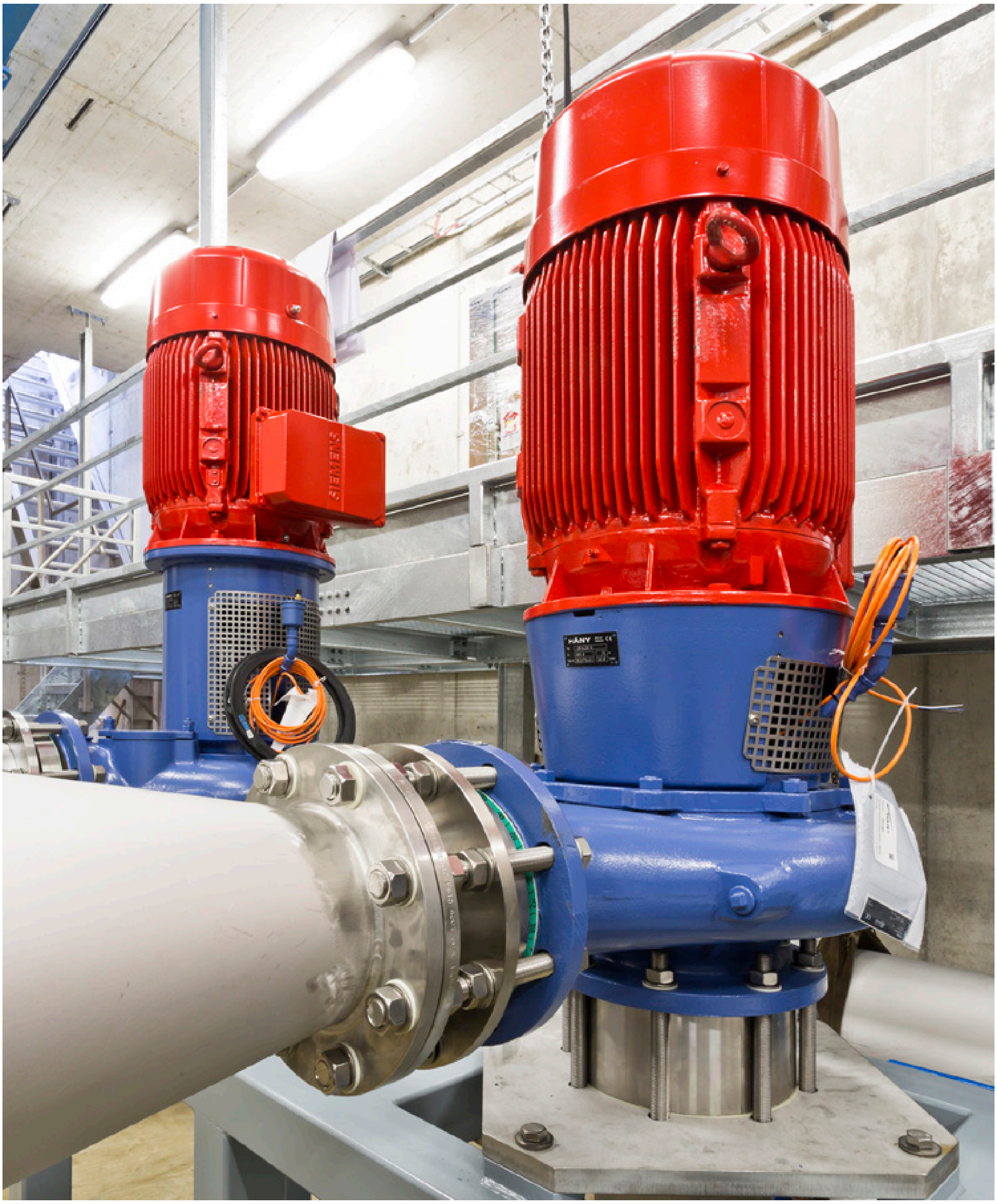
The fine structure of the Milky Way galaxy, Simon Portegies Zwart (Physics, 26.00 Mio CPU h)

University of Bern

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

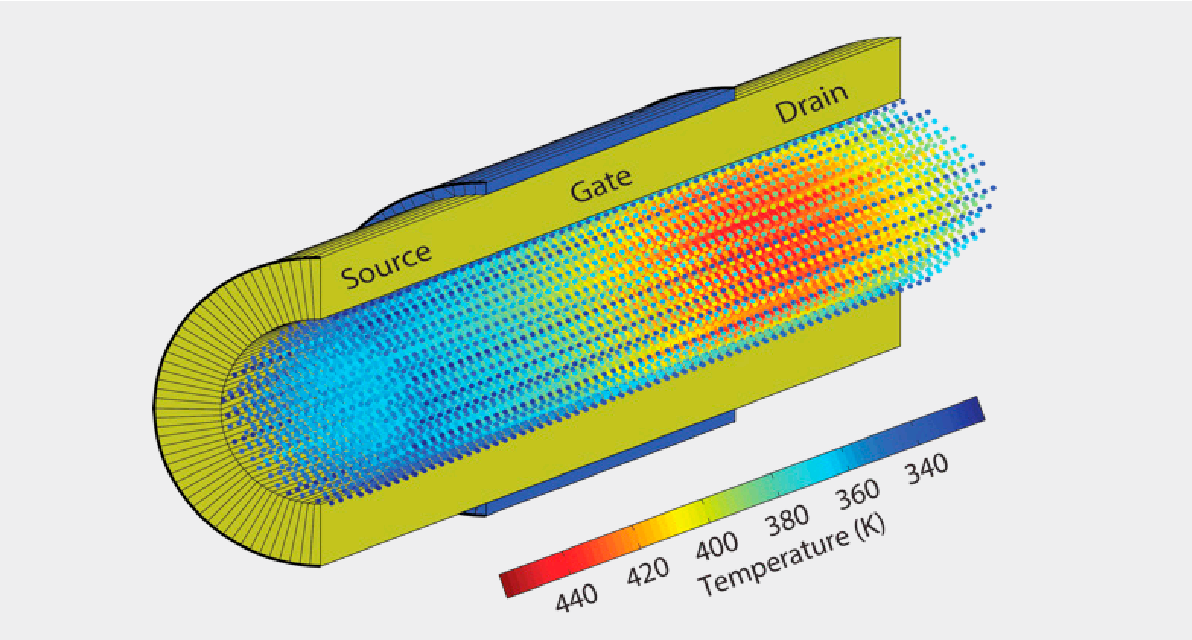
Hellenic National Meteorological Service

Objective calibration of weather prediction models, Antigoni Voudouri (Earth & Environmental Science, 31.98 Mio CPU h)



The new turbines installed at the Parco Ciani pumping station to produce electricity from the water returned to Lake Lugano after cooling the supercomputers.

Nanoelectronic components on the “computer test bench”



Schematic view of the interior of a gate-all-around Si nanowire transistor with an atomistic resolution. The color of each atom corresponds to its effective temperature, showing self-heating effects close to the drain side of the device. (Mathieu Luisier, ETH Zurich)

Thanks to a special computer programme, researchers from ETH Zurich are able to simulate electronic nanocomponents and help materials science and industry in the development and production process.

Electronic components are often only a few nanometres (billionths of a metre) in size. According to Moore’s Law, a transistor halves in size every two years, for example, which is the only possibility to place two billion transistors in a nanoformat on a Smartphone chip. The tiny devices ensure that the Smartphone can keep up with the constantly changing demands – to be a telephone and camera, as well as a quality video camera, search engine, personal health monitor and entertainer. And in doing so, the components need to work energy-efficiently and be producible at low costs.

The tinier electronic components become, however, the harder they are to manufacture. By way of comparison: a red blood cell is 7 000 nanometres in diameter, a human hair 80 000. Consequently, producing a transistor that is 20 nanometres in size and smaller from semiconductors such as the element silicon is not just a technical challenge.

Physical effects, so-called quantum mechanical patterns, alter the materials’ properties on a nanometre scale, which complicates life for designers and engineers in the development and construction of nanodevices. ETH Zurich professor Mathieu Luisier from the Integrated Systems Laboratory has now come to the rescue.

Computer predictions

Luisier has spent over ten years honing a software programme that simulates transistors of the future, which are only a few nanometres in size. He is supported by the CSCS supercomputer “Piz Daint”, which helps to predict what happens when the composition, form and size of materials change in the nanoworld. As far as Luisier is concerned, “Piz Daint” is currently the best and most efficient simulation machine in the search for new, ideal material combinations. The ETH Zurich professor’s work has been met with great interest in industry as the simulations save experimentation time and costs in the development of new, efficient electronic components.

One problem when billions of conventional transistors are placed on one chip is that they generate a huge amount of heat and easily overheat. This is because the electrons release energy on their way through the transistor. Luisier and his team use their software OMEN – a so-called quantum simulator – to simulate the electron transport at atomic level in order to study exactly what happens. The simulated transistor consists of a nanowire made of silicon crystals. “When the electrons flow through the wire, they initially possess a constant, high amount of energy, which gradually decreases and is absorbed by the silicon’s crystal lattice in the form of so-called phonons,” explains Luisier. The interaction between the electrons and phonons heats the crystal and the overall energy remains intact – evidence for the researchers that their model reproduces the process correctly. The goal now is to construct the transistor based on the results obtained via the simulations in such a way that the electrons lose as little energy as possible along the way.

Playing with crystals

On the one hand, the researchers are able to “play” with the order of different crystal levels in the crystal and alter the crystal structure or replace silicon with another semiconductor material in their simulations. On the other hand, they can check the functionalities and different properties of the crystals simulated. For instance, the researchers simulated a nanowire, where the channel is encased in an oxide and a metallic contact (gate). The phonons emitted by the electrons are effectively “captured” in the channel and can only leave the structure at certain points – the beginning and end of the nanowire. “Replacing the shell around the wire with a structure that resembles the letter omega yields a larger area for the phonons to escape from,” says Luisier. If the area is also directly in contact with a cooling segment, the transistor heats up to a lesser extent. The semiconductors would also generate less heat if they were constructed from materials such as indium gallium arsenide or germanium because these materials enable the electrons to move through faster. However, they are much more expensive than silicon.

During the simulations, the researchers produce the structures designed atom by atom. Like in the conventional so-called “ab initio” method, which is used intensively to analyse the properties of materials, the Schrödinger Equation is also solved in the simulations conducted by Luisier’s team. This enables them to study how electrons and phonons interact.

However, there are two main differences: while the *ab initio* method solves the electrons’ wave movement in a closed or periodically repetitive system, Luisier’s group supplements the method with open boundary conditions, which enables transport to be simulated. The scientists can then observe both the electron flows and the thermal currents, and describe the interconnection with the surroundings, the interplay of the electron flow with the thermal currents. Another difference is that the calculations using OMEN are currently conducted based on empirical models as they are still too complex and more computer-intensive *ab initio*.

High-performance computing

However, new algorithms are being developed in a collaborative PASC project with scientists from the Università della Svizzera italiana and EPF Lausanne to render the calculations more efficient. “In the medium term, we want to replace all empirical models with *ab initio* ones so that we can calculate structures made of different materials more easily and accurately,” says Luisier. “This is why we need optimised algorithms and machines like Piz Daint.”

Nonetheless, Luisier stresses that, to the best of his knowledge, his team’s empirical approach is more state of the art than ever before in the development of electronic nanocomponents. Another of his group’s research focuses is the simulation of lithium ion batteries. “If we understand heat development in transistors or batteries more precisely, we will be able to propose better designs,” says Luisier. “OMEN is a component simulator of the new generation, where engineers use concepts that have never been used before in materials science, chemistry or physics.”

Improving the theory of phase transitions with supercomputers

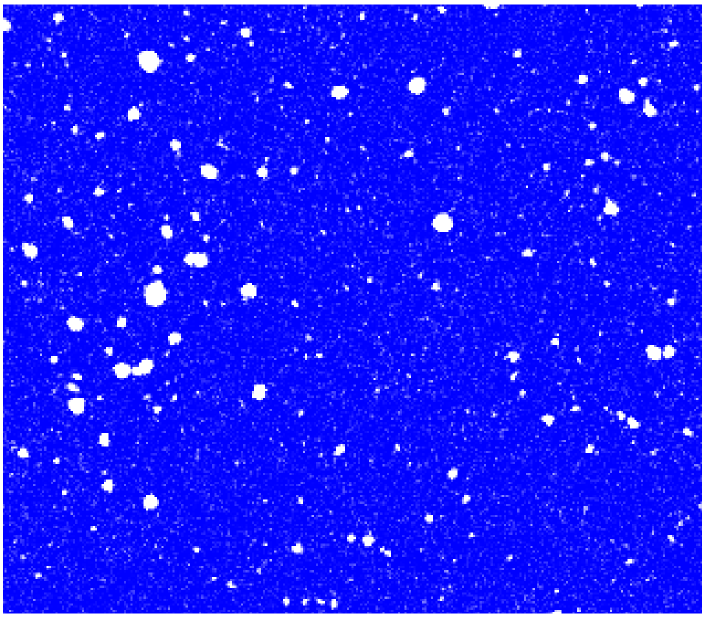
Supercomputers help researchers where experimentation and observation reach their limits. Physicists Jürg Diemand and Raymond Angélil from the University of Zurich use them to detect flaws in theoretical models of phase transitions, for instance.

When water molecules evaporate from a liquid phase into a gaseous phase, they alter their aggregate state. The mathematical description of such a phase transition harbours pitfalls as nucleation is needed for the change to take place. The theory behind this, classical nucleation theory (CNT), however, is deemed highly inaccurate. Earlier studies suggest that the rate of the bubble nucleation determined with the CNT is underestimated. The research team headed by physicist Jürg Diemand, a professor at the University of Zurich, enlisted the aid of the CSCS supercomputers to scrutinise the process in which liquid vaporises. They revealed that, to some extent, the theory actually reflects the reality. The nucleation theory only underestimates the formation rate of the gas bubbles at very low temperatures. The simulations also gave the researchers an insight into possible causes of the deviations.

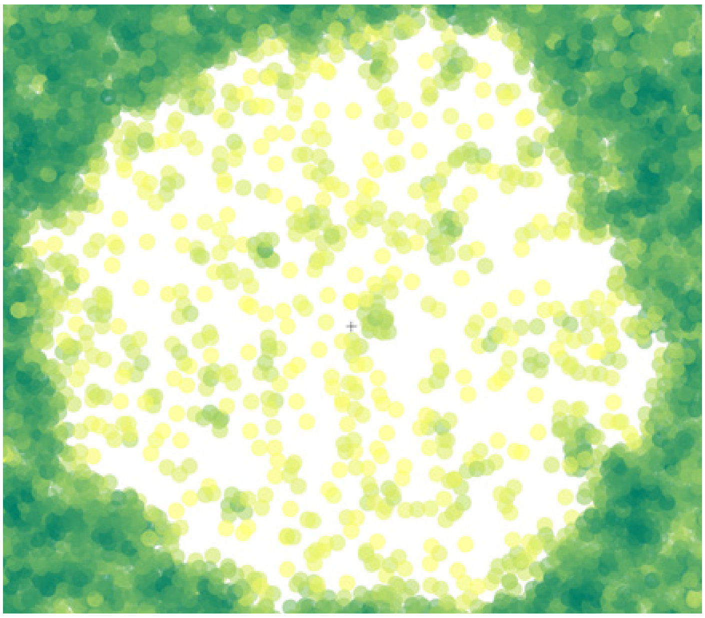
A "black box" in science

Shedding light into the darkness of the "black box" of phase transition, where a previously stable substance becomes metastable in order to transform into a new stable form, is relevant for many research fields. This is because similar things occur when clouds form or dust particles condense out of gas develop in the cosmos. Although, according to Diemand, theoretical physics describes the states of equilibrium and the macroscopic objects very well with thermodynamics, the central processes in a phase transition take place on a much smaller nanometre scale. One nanometre is one billionth of a metre. On account of their size, nanoparticles can possess completely different properties and functionalities to their macroscopic siblings.

In their study, the scientists under Diemand examined the issue of why the CNT is often inaccurate and how the assumptions in the model differ from the actual properties of the gas bubbles. In their study, the scientists succeeded in simulating such molecularly dynamic processes directly for the first time – "brute force" – rather than approximately. In order to illustrate the conditions realistically, the simulated volume selected was as large as possible, with half a billion particles.



A projection through the complete simulation is displayed: the liquid in which the white bubbles form is shown in blue. (Jürg Diemand, University of Zurich)



A single bubble develops: every circle is an atom. The different green tones correspond to the local potential energy. (Raymond Angélil, University of Zurich)

"This is only possible if you have an enormous computer capacity and efficiently programmed codes at your disposal, which can share the work among individual calculation cores virtually loss-free," says Diemand. Under these conditions, several stable gas bubbles formed during the simulation, without the temperature or pressure in the simulated system changing significantly as a result. The researchers were also able to determine the gas bubbles' formation rate.

No congruence at low temperatures
By comparing their simulations with the CNT, the researchers are not only able to verify the theory, but also detect any flaws and ultimately initiate improvements. Many researchers have spent years working on improving the CNT. For Diemand and his team, the new study indicates that the surface tension of the tiny, young gas bubbles behaves very differently to that of macroscopic bubbles. As the surface tension evidently depends on the radius and temperature, and the critical nucleus sizes already amount to 20 to 30 in atomic diameter at high temperatures, clear deviations from the model can only be observed at very low temperatures with tiny nucleus sizes. Presumably, different values for the surface tension for different bubble radii would need to be taken into account in the theoretical model. Furthermore, the researchers were able to show that the critical size of the gas bubble at which it remains stable tallies well with the CNT prediction. Another important result of the study for the researchers is the fact that no temperature hotspots could be observed in the areas where the condensation nuclei form, as was posited by another study. In the simulations by Diemand and his team, nucleation took place at average temperatures.

The simulations bring the researchers closer to the reality of phase transition than observations or experiments. Using the computer experiment and the visualisations of the calculations, it is possible to follow and study the rapid processes. Surprisingly, the depiction of Diemand's group's simulations reveals that the bubbles depicted are not sharply defined or perfectly round, as was commonly assumed. And a broad "ribbon" is apparent during the phase transition from liquid to gas instead of a sharp divide, Diemand notes.

Tracking down dark matter
Diemand and his team are currently researching the behaviour of metastable liquids that are used as dark matter detectors. Dark matter, which was posited based on astronomical observations, is an omnipresent mass of an unknown composition in the universe. According to current estimates, it makes up 85 per cent of the universe's matter. Using a special method, it should be possible to detect dark matter as soon as it hits a nucleus of a metastable liquid enclosed in a detector. The collision should produce a gas bubble that can be registered with measuring devices. Similar detectors, so-called bubble chambers, were used successfully at Cern and other particle accelerators in the 1960s and 1970s. The method is currently making a comeback in the search for dark matter. While the theoretical model to calculate the phase transition in the detectors stems from the 1960s and is based on the CNT, it has never been tested with simulations. As a result, nobody knows how well it describes the reality and what really happens microscopically, says Diemand. He and his team are now clarifying this using new simulations in collaboration with researchers from the European SIMPLE experiment (Superheated Instrument for Massive ParticLe Experiments), which is seeking evidence of the existence of dark matter.

Papers with Highest Journal Impact Factor[1)]

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Impact Factor: 45.66

E. Brunk, U. Röthlisberger, Mixed quantum mechanical/molecular mechanical molecular dynamics simulations of biological systems in ground and electronically excited states, Chemical Reviews, DOI 10.1021/cr500628b.

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Impact Factor: 42.35

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Impact Factor: 33.26

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Energy & Environmental Science

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Impact Factor: 12.03

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Plos Biology
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G. Gógl, K. D. Schneider, B. J. Yeh, N. Alam, A. N. Nguyen, A. M. Moses, C. Hetényi, A. Reményi, E. L. Weiss, The structure of an NDR/LATS Kinase – Mob complex reveals a novel Kinase-coactivator system and substrate docking mechanism, Plos Biology, DOI 10.1371/journal.pbio.1002146.

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Y. Lee, Z. Q. Liu, J. T. Heron, J. D. Clarkson, J. Hong, C. Ko, M. D. Biegalski, U. Aschauer, S. L. Hsu, M. E. Nowakowski, J. Wu, H. M. Christen, S. Salahuddin, J. B. Bokor, N. A. Spaldin, D. G. Schlom, R. Ramesh, Large resistivity modulation in mixed-phase metallic systems, Nature Communications, DOI 10.1038/ncomms6959.

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Advanced Functional Materials
Impact Factor: 10.44

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Impact Factor: 10.40

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There was plenty of "hacking" going on during the first EuroHack hosted by CSCS in Lugano.

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Constantia Alexandrou, University of Cyprus

A. Abdel-Rehim, C. Alexandrou, M. Constantinou, P. Dimopoulos, R. Frezzotti, K. Hadjiyiannakou, K. Jansen, Ch. Kallidonis, B. Kostrzewa, G. Koutsou, M. Mangin-Brinet, M. Oehm, G. C. Rossi, C. Urbach, and U. Wenger, Nucleon and pion structure with lattice QCD simulations at physical value of the pion mas, Physical Review D, DOI 10.1103/PhysRevD.92.114513.

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Name
Annette Milnik

Position
Post-doctoral researcher

Institution
University of Basel

Background
1999–2005 Studies of psychology, University of Würzburg, Germany
2001–2008 Studies of human medicine, University of Würzburg, Germany
2006–2013 MD in cognitive neuroscience, Universities of Frankfurt and Magdeburg, Germany
2009–2012 Assistant Doctor at the Department of Neurology, University of Magdeburg, Germany
2010–2012 Guest scientist at the Division of Molecular Neuroscience, University of Basel
2014–2016 PhD in molecular neuroscience, University of Basel
Since 2013 Post-doctoral researcher, University of Basel

Area of Research
Molecular and cognitive neuroscience, life science.

Specialised in
Applied statistics, data management, data mining.

HPC means for me
The unique chance to dig deep into the treasure chest of our data.

MeteoSwiss and CSCS pave the way for more detailed weather forecasts

"Piz Kesch" and "Piz Es-cha", the dedicated supercomputers of MeteoSwiss.

The new "super weather computer" of the Swiss Federal Office of Meteorology and Climatology (MeteoSwiss) has started at CSCS its operation in September 2015. MeteoSwiss is the first meteorological service which has switched to a new GPU based computer architecture. Thus, the new supercomputer is able to calculate weather models with a resolution twice as high more efficiently and quicker than before.

Expectations in the Swiss national meteorological service continuously increase. To ensure air traffic safety, for warnings against severe weather, or in case of a nuclear or chemical accident, the weather simulations by MeteoSwiss are essential. Also individuals expect reliable weather forecasts for instance for mountain climbing, water sports or other activities where extreme weather conditions could pose a risk. Until September 2015 the weather models used by MeteoSwiss were only able to predict local weather events such as storms or the Foehn effect across the Alpine region with limited accuracy. The granularity of the previous 2.2-kilometre grid was insufficient to produce precise models of storm clouds as they are forming. To generate a more realistic simulation of this phenomenon, new higher-resolution weather models with a grid of 1.1 kilometres were required.

Only a supercomputer that is 40 times more powerful than the current MeteoSwiss system running at CSCS could provide the required processing power.

Better spotting extreme events

MeteoSwiss worked closely with CSCS, the Center for Climate Systems Modeling (C2SM), the development partner Supercomputing Systems AG, the computer manufacturer Cray and the accelerated computing specialist NVIDIA to develop a powerful, yet cost-effective, compact and energy-efficient supercomputer. Due to a new system architecture and completely revised application software of the so-called COSMO model, it is now possible to produce the kind of state-of-the-art weather forecasts required. To guarantee more detailed weather forecasts, the simulation are based on a grid spacing of 1.1 kilometres which runs recurrently every three hours. "This grid spacing makes it possible to predict with more detail the precipitation distribution, the risk of storms or valley wind systems in the Swiss mountains. It is an additional step to increase the utility of the weather forecasts" said Peter Binder, Director General of MeteoSwiss.

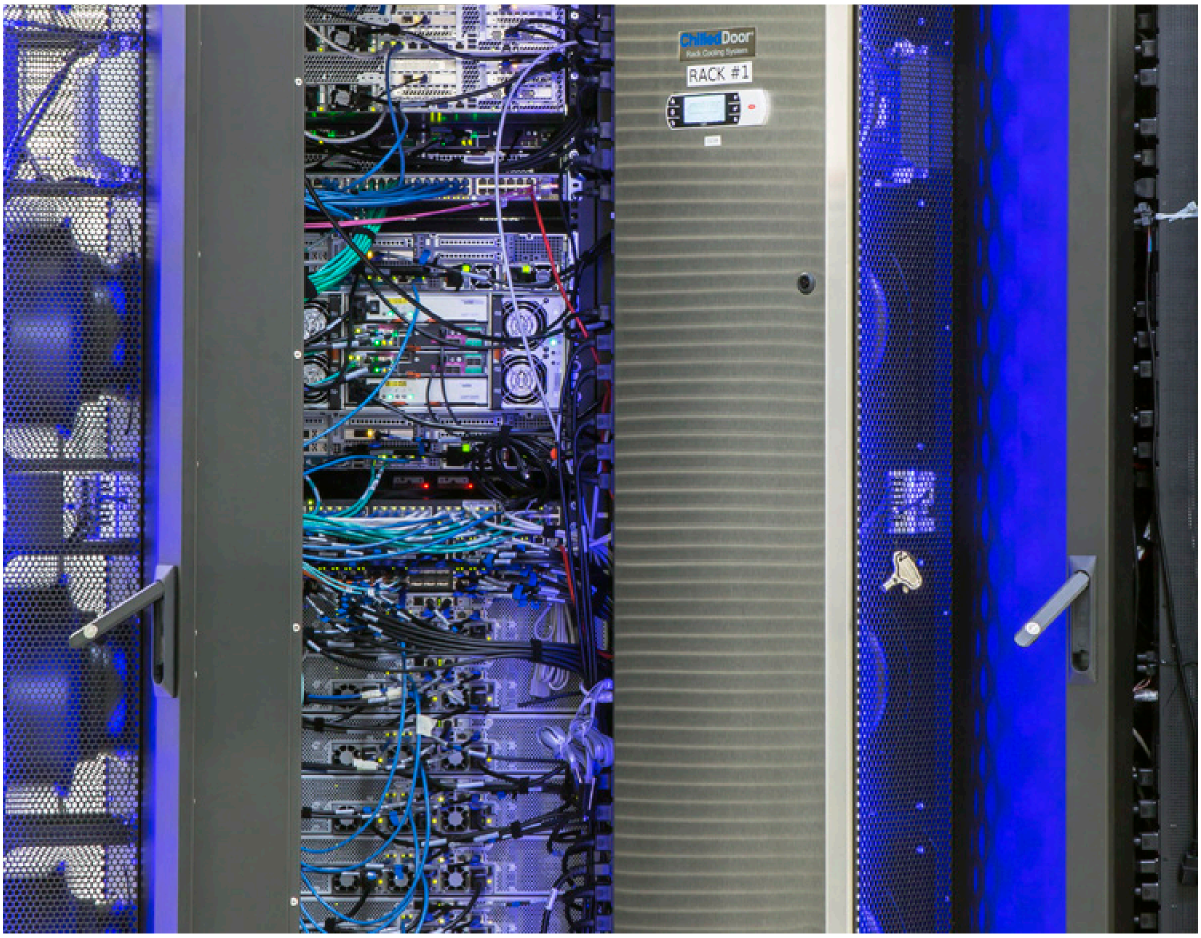
In addition to these simulations, MeteoSwiss runs now 21 twice-daily forecasts, each with a grid spacing of 2.2 kilometres but with slight variations in terms of basic conditions (ensembles).

These 21 forecasts are compared with each other to better estimate the most likely weather conditions and possible meteorological developments up to five days into the future, thus allowing for a more detailed prediction of extreme weather events.

MeteoSwiss opts for innovative technology

The two cabinets of the Cray CS-Storm supercomputer at CSCS are tightly packed. Each cabinet consists of 12 hybrid computing nodes for a total of 96 NVIDIA Tesla K80 GPU accelerators and 24 Intel Haswell CPUs. The GPUs are one of the key elements of the new computer system. They allow simulations which are three times more energy-efficient and twice as fast as conventional CPUs. "High-quality weather forecasts always depend upon processing power," said CSCS Director Thomas Schulthess. "With the GPUs and the revised model, we can compute weather simulations more quickly and accurately than with conventional systems – and more energy and cost-efficient."

MeteoSwiss is the first national meteorological service which has chosen a computer architecture based on GPUs for operational numerical weather prediction. The Cray CS-Storm computer architecture, developed by Cray and CSCS for meteorological applications, further contributed to enhance the efficiency. After a transitional period, the new system replaces the current one by spring/summer 2016. Until then both systems will run in parallel for weather prediction in Switzerland.



The cables interconnecting the compute nodes of "Piz Kesch" and "Piz Es-cha".

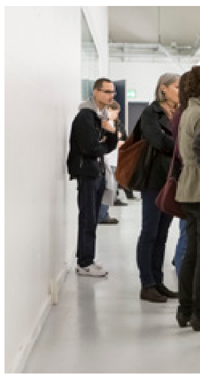
A glimpse behind the scenes at CSCS in Lugano

"I cervelli che contano": the motto of the Swiss National Supercomputing Centre's open day, which attracted more than 1 000 visitors.

For the second time at its new location in Lugano, CSCS opened its doors to the interested public on Saturday, 17 October. The open day was organised against the backdrop of "Ricerca live", Italian-speaking Switzerland's regional contribution to the celebrations marking the 200th anniversary of the Academy of Sciences (SCNAT).

Like in 2012, when the new building in Lugano was inaugurated, people of all ages flocked to Via Trevano 131 to experience CSCS at first hand. More than 1 000 visitors enjoyed a versatile programme. On a tour of the building, the guests gained an insight into high-performance computing (HPC), the supercomputer and building's technology, the history of computer-based research, and the various research fields. Scientists from all over the country showcased their research in packed-out lecture theatres, relating how they use CSCS's computer infrastructure and benefit from its supercomputers.

CSCS staff stationed at various information islands highlighted the research fields where supercomputers are used, which they explained on posters or monitors with the aid of visualisations of the supercomputers' capabilities. The visitors showed a keen interest in climate research, for instance. Experts explained to them how climate models are created and used to extrapolate forecasts for the future. The entire staff were on hand to answer any questions and the visitors were able to learn about the work conducted at CSCS and ETH Zurich.

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Name
Igor Pivkin

Position
Senior assistant professor

Institution
Università della Svizzera italiana

Background
1993-1999 BSc and MSc in mathematics, Novosibirsk State University, Russia
2000-2006 MSc in computer science, Brown University, USA
2000-2006 MSc and PhD in applied mathematics, Brown University, USA
2006-2008 Post-doctoral researcher, Brown University, USA
2008-2011 Post-doctoral researcher, Massachusetts Institute of Technology, USA.
2011-2013 Assistant professor, Institute of Computational Science, Università della Svizzera italiana
Since 2013 Senior assistant professor, Institute of Computational Science, Università della Svizzera italiana

Area of Research
Multiscale/multiphysics modeling, corresponding numerical methods and parallel large-scale simulations of biological and physical systems.

Specialised in
biophysics, cellular and molecular biomechanics, stochastic multiscale modeling, and coarse-grained molecular simulations.

HPC means for me
HPC is an essential component in solving challenging problems in biological and physical systems. We are extremely grateful to CSCS for an exceptional support and for providing excellent HPC environment in Switzerland.

Finances

Expenditures

	CHF
Investments	**5 042 501.01**
Equipment and Furniture	**16 880.19**
Personnel	**7 842 930.29**
Payroll	6 248 464.30
Employer's Contributions	1 070 458.25
Further Education, Travel, Recruitment	524 007.74
Other Material Expenses	**6 994 698.07**
Maintenance Building & Technical Infrastructure	563 143.11
Energy & Media	2 151 892.91
Administrative Expenses	17 807.80
Hardware, Software, Services	3 691 474.08
Remunerations, Marketing, Workshops, Services	560 585.31
Other	9 794.86
Extraordinary Income / Expenditures	**259 525.60**
Membership Fees	44 525.60
EM/DM Transfers	215 000.00
Total Expenses	**20 156 535.16**

Income

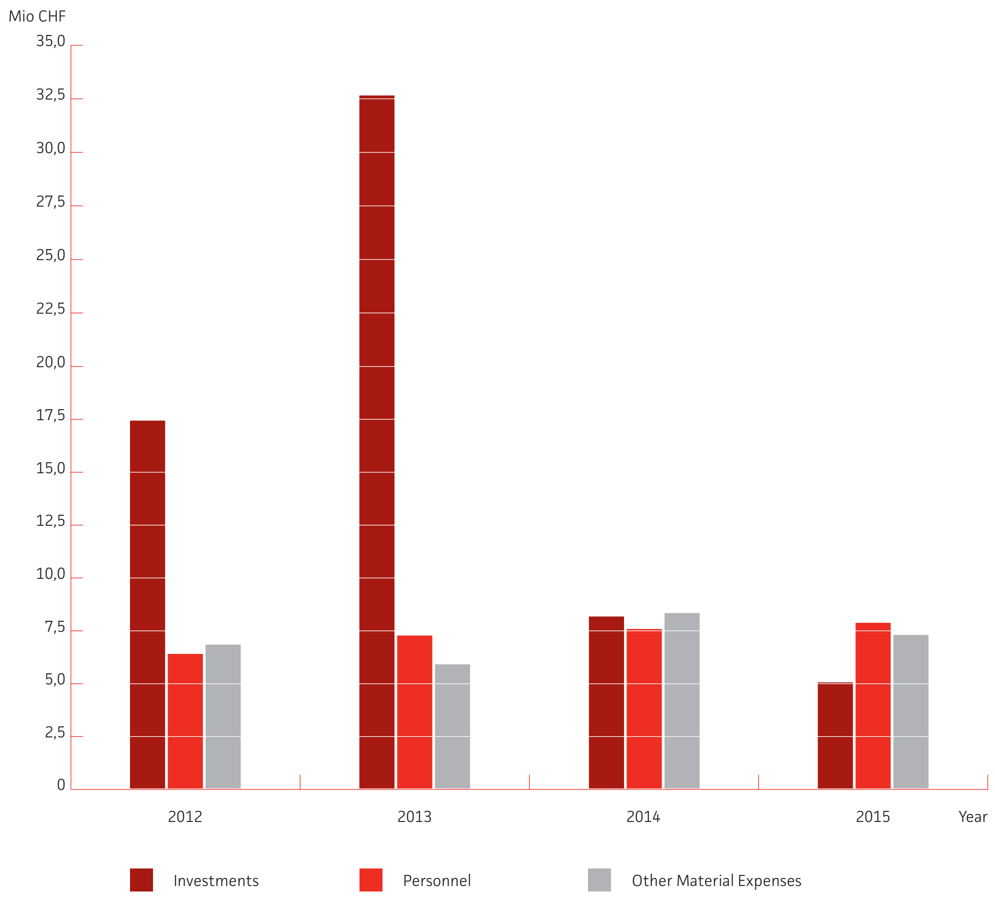
	CHF
Basic Budget	**20 999 370.71**
Contribution ETH Zurich	20 879 560.71
Salary Increase / Price Inflation	119 810.00
Other Income	**138 829.32**
Services / Courses	54 176.22
Reimbursements	7 350.89
Other Income	77 302.21
Total Income	**21 138 200.03**

Balance current Year	**981 664.87**
Rollover Project Fund Investments 2015	2 179 038.14
Total Balance User Lab 2015	**3 160 703.01**
./. Rollover Project Fund Investments 2016	2 879 930.61
Balance operational Funds CSCS - Rollover to ETH Zurich 2015	280 772.40

Third-Party Contributions	
MeteoSwiss	1 434 650.00
EU Projects	967 355.50
Blue Brain	867 523.45
CHIPP	880 515.59
Marvel	705 000.00
Euler Cluster	560 648.11
University of Zurich	542 500.00
Università della Svizzera italiana	450 000.00
Monch Cluster	307 250.00
C2SM	224 000.00

Development of Overall Expenses

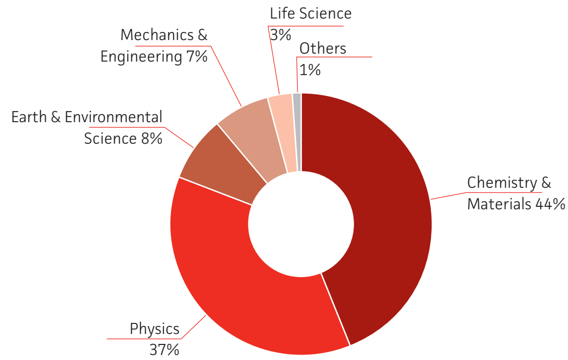
	2012	2013	2014	2015
Investments	17 320 218	32 555 142	8 118 445	5 042 501
Personnel	6 388 608	7 249 675	7 538 405	7 842 930
Other Material Expenses	6 825 156	5 900 556	8 268 005	7 271 103



Usage Statistics

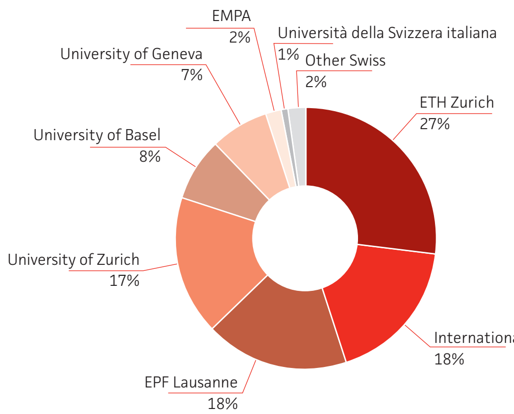
Usage by Research Field

Research Field	CPU h	%
Chemistry & Materials	510 340 666	44
Physics	428 829 284	37
Earth & Environmental Science	90 743 215	8
Mechanics & Engineering	75 461 708	7
Life Science	36 034 789	3
Others	9 189 769	1
Total Usage	**1 150 599 431**	**100**



Usage by Institution

Institution	CPU h	%
ETH Zurich	311 825 916	27
International	206 624 364	18
EPF Lausanne	203 344 684	18
University of Zurich	197 658 102	17
University of Basel	95 996 558	8
University of Geneva	78 319 376	7
EMPA	22 911 492	2
Università della Svizzera italiana	12 715 576	1
Other Swiss	19 905 242	2
Total Usage	**1 149 301 310**	**100**



Compute Infrastructure

HPC Systems for User Lab

Name	Supplier & Model	Installation / Upgrade	CPU Type
Piz Daint	Cray XC30	2012 / 13	Intel Xeon E5-2670 & Nvidia Tesla K20x GPU
Piz Dora	Cray XC40	2014	Intel Xeon E5-2690 v3
Pilatus	Intel Sandy Bridge Cluster	2012	Intel Xeon E5-2670 2.6 GHz

Name	No. of Cores	Interconnect Type	Peak Performance (TFlops)
Piz Daint	42 176 + 5 272 GPUs	Cray Aries	7 784
Piz Dora	29 952	Cray Aries	1 246
Pilatus	608	Infiniband FDR PCI Gen 3	12.6

HPC Systems for Third Parties

Name	Supplier & Model	Installation / Upgrade	User	CPU Type
Blue Brain 4	IBM BG/Q	2013	EPF Lausanne	IBM BGQ (PowerPC – 1.6 GHz) + Intel Xeon 2.6 GHz
Piz Es-cha	Cray CS-Storm	2015	MeteoSwiss	Intel E5-2690v3 + Nvidia K80x
Piz Kesch	Cray CS-Storm	2015	MeteoSwiss	Intel E5-2690v3 + Nvidia K80x
Mönch	NEC Cluster	2013 / 14	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 / 15	CHIPP (LHC Grid)	Intel Xeon CPU E5-2670 2.6 GHz + Intel Xeon E5-2680 v2 2.8 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
Piz Es-cha	408 + 96 GPUs	Infiniband FDR PCI Gen 3	305
Piz Kesch	408 + 96 GPUs	Infiniband FDR PCI Gen 3	305
Mönch	7 520	Infiniband FDR PCI Gen 3	132
Monte Lema	4 032	Cray Gemini	34
Phoenix	2 000	Infiniband FDR PCI Gen 2	43
Albis	1 728	Cray Gemini	15

Communication Statistics

Website

cscs.ch

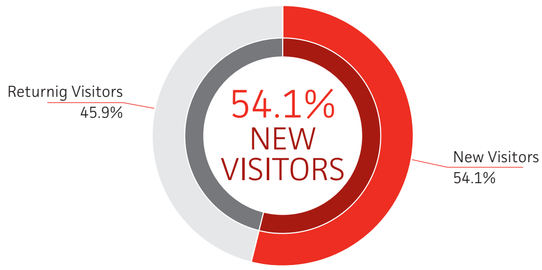
	2014	2015	
Total Website Visitors	66 275.00	72 991.00	+ 10% ↑
Average Website Visits (Minutes)	2.73	2.43	- 12% ↓

user.cscs.ch

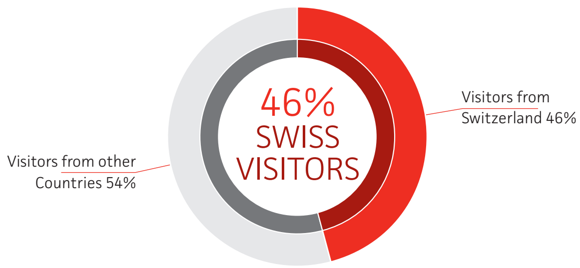
	2014	2015	
Total Website Visitors	21 419.00	21 271.00	- 0.7% ↓
Average Website Visits (Minutes)	3.21	3.35	+ 4% ↑

Website cscs.ch

New visitors



Visitors origin



Top 5 most visited website pages

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

Twitter

	2014	2015	
Followers	241	375	+ 156% ↑

LinkedIn

	2014	2015	
Followers	874	3 830	+ 338% ↑

YouTube
Published videos

	2014	2015	
Watch Time (Minutes)	354 282.00	402 370.00	+ 14%
Average View Duration (Minutes)	4.33	4.45	+ 3%
Number of Views	77 710.00	84 438.00	+ 9%

Facebook
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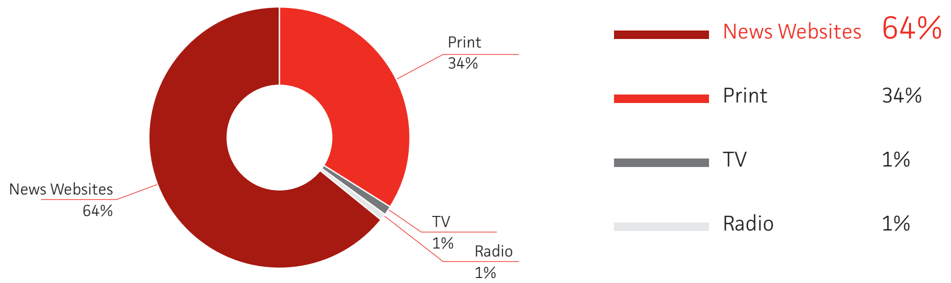
November 2015 creation of the CSCS page

CSCS in the News



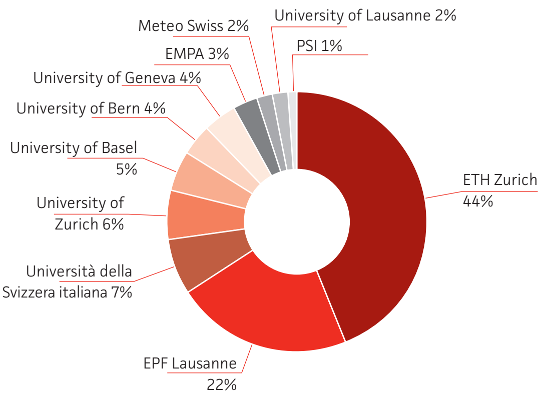
Word Cloud of News Related to CSCS

User Satisfaction

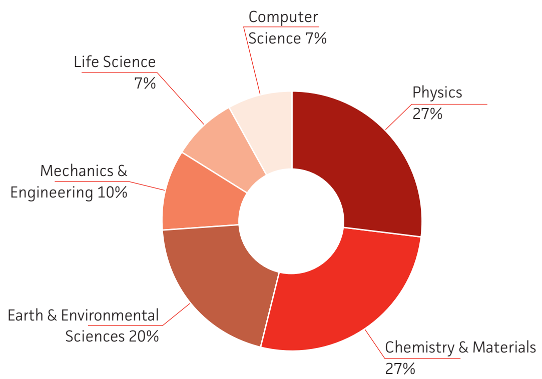
A user satisfaction survey was submitted to 568 users in January 2016. The response rate was of 25% (149 answers).

User Profile

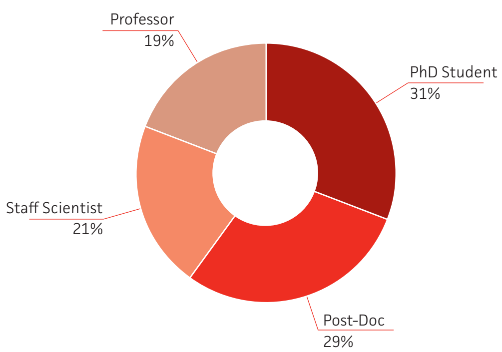
Your institution



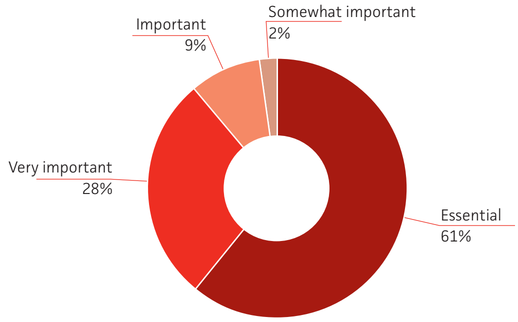
Your scientific field



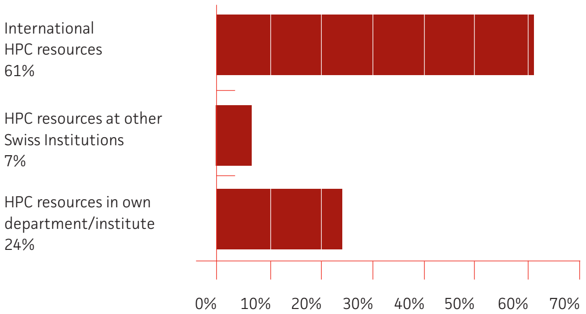
Your position



For my research, CSCS resources are:



Which HPC resources are you using besides CSCS?



User Support

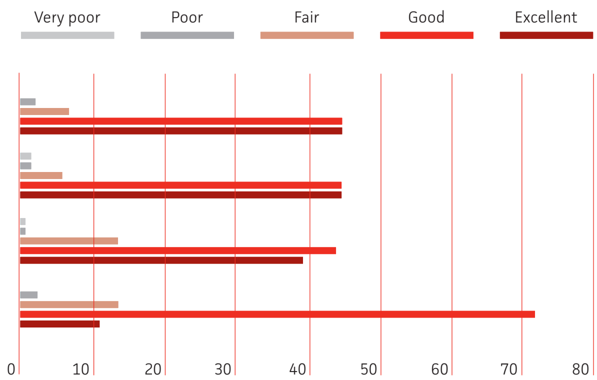
How do you rate the quality of...

Helpdesk support

System support

Application support

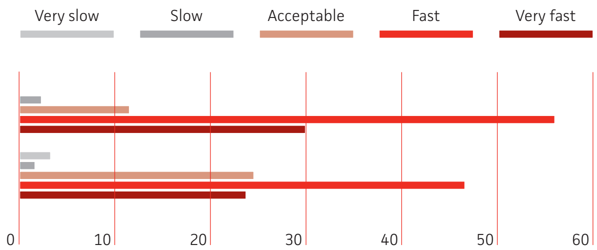
The offer of training courses and user events



How fast does support handle your request?

The reaction time of the helpdesk is

The time to solution for the support requests is



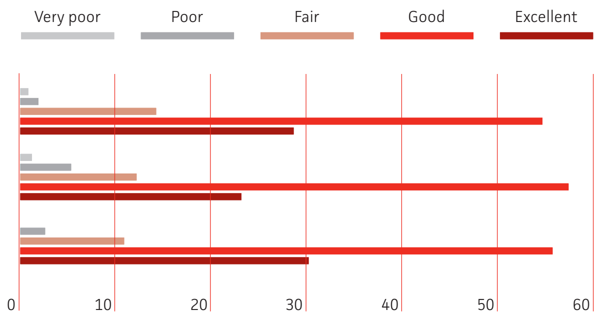
System Availability, Stability and Usability

How you perceive...

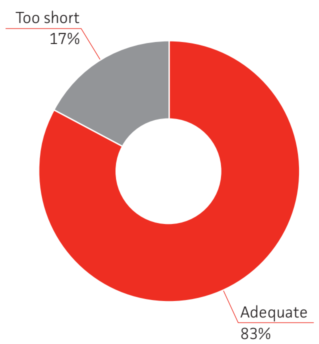
The availability of CSCS systems?

The stability of CSCS systems?

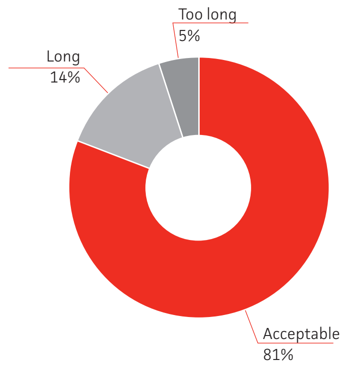
The ease of use of CSCS systems?



The run time limits for batch jobs are:

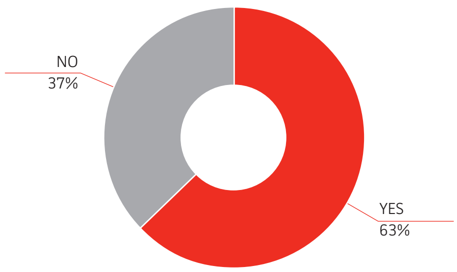


The job waiting time in the queue is:

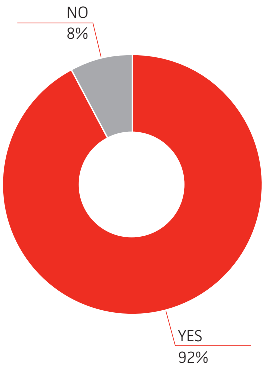


Project Proposal Process

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



Is the reviewing process transparent?



How do you perceive the submission process?

The submission portal is

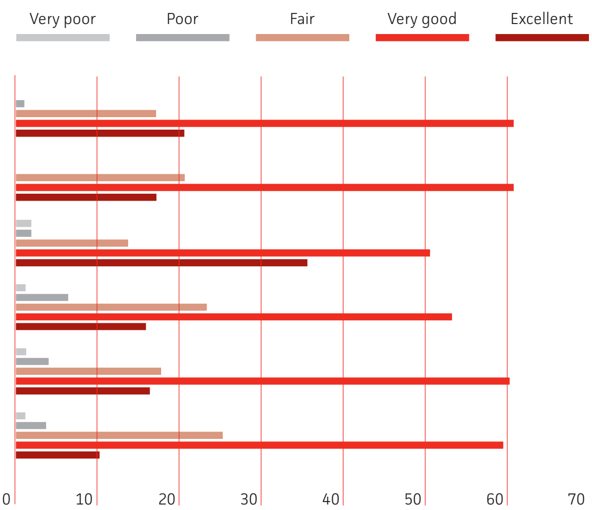
The quality of the submission form is

The support provided during the call is

The feedback from scientific reviewers is

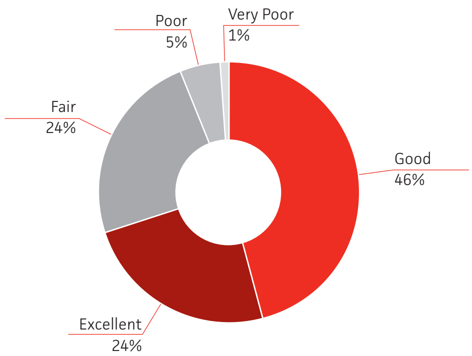
The feedback from technical reviewers is (when given)

The information provided by the panel committee is

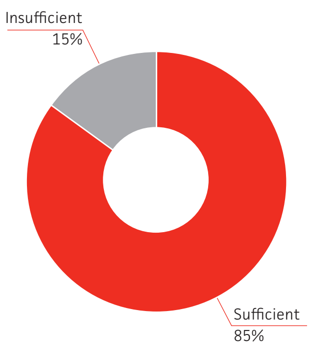


Adequacy of Allocated Resources

The resources assigned to my project are:

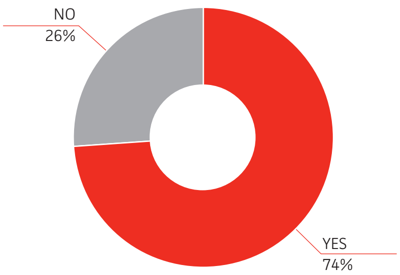


My storage allocation on “project” is:

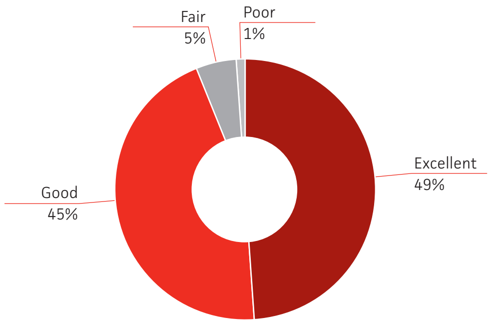


Application Development

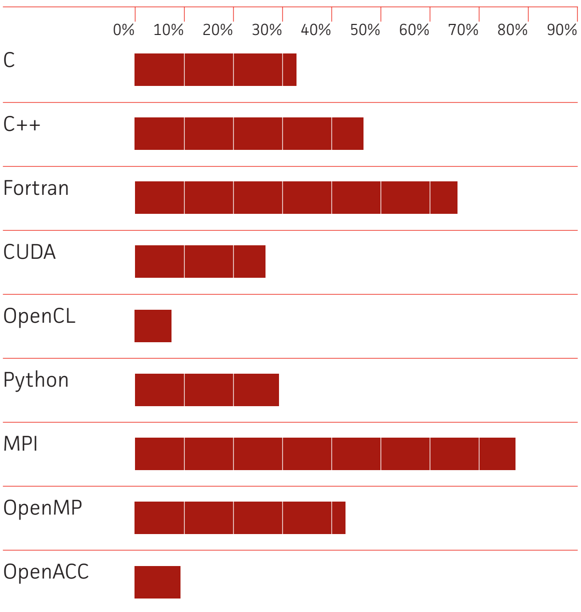
Do you develop and maintain application codes?



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



Which programming languages and parallelization paradigms are you using primarily?



Information & Communication

How do you feel informed about...

Status of the systems

Software and applications

Hardware configuration

Available computing resources

Own allocations

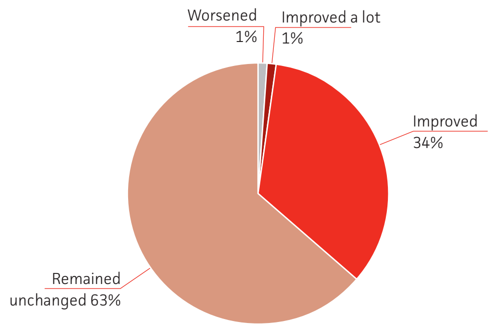
Your consumption of your allocation

Upcoming events and courses

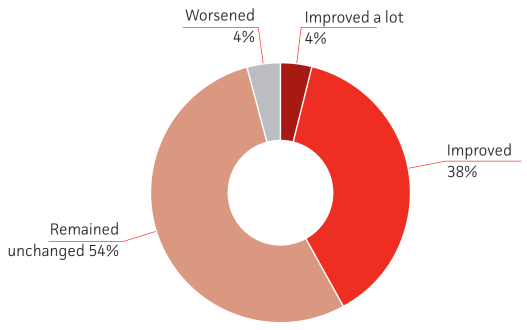
Future developments at CSCS

Perception of CSCS

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



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



The four experts that reviewed the activities of CSCS posing together with the director of CSCS. From left to right: Prof. Daniel A. Reed, University of Iowa, USA; Prof. Thomas Lippert, IAS/JSC, Research Centre Jülich, Germany (Chair); Prof. Takayuki Aoki, Tokyo Institute of Technology, Japan; Prof. Thomas Schulthess, CSCS; and Prof. Richard Kenway, EPCC, University of Edinburgh, UK.

Impressum

CSCS Swiss National Supercomputing Centre
Via Trevano 131
6900 Lugano
Switzerland

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

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Matteo Aroldi
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