







# Annual Report 2014

# CSCS

Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre

# Welcome from the Director



Thomas Schulthess, Director of CSCS.

Welcome to the 2014 annual review of the Swiss National Supercomputing Centre (CSCS). We are proud to report that this has been a year where the rubber hit the road for peta-scale computing in Switzerland.

"Piz Daint", the world's most energy-efficient, peta-scale supercomputing system, was accepted just before New Year 2013 and started production in the Early Science Program in January. The system was co-designed along with climate and chemistry applications and thus was ready to run simulations on a successful scale right from the start. The first results of the Early Science Program were already presented at the inauguration of the new system in March 2014. One of the research projects succeeded in validating a method that aims at solving the key problems of simulating chemical reactions that involve liquid water. Another early science project successfully verified a cloud-resolving climate model.

From an operational point of view, "Piz Daint" was an entirely new experience for the centre. Running a 5000-node system poses new challenges to the scalability of system level operations that the centre has never before had to face. This led to the conclusion that CSCS had to redesign all auxiliary systems, since both the building infrastructure and the new peta-scale system were built for an operation that would be able to grow many orders of magnitude above what the centre was used to dealing with so far. This resulted in turn in a consolidation of all our pre- and postprocessing systems, including visualisation, into a heterogeneous Cray XC platform. We extended this 28 cabinet system in 2014 with seven additional Cray XC40 cabinets that would allow us to replace the services we ran on "Monte Rosa", add a cluster service on behalf of the University of Zurich, and allow users to do pre- and post-processing of data from the same supercomputing platform on which they run their main simulations.

One of the most exciting developments in this context was the capability to use the GPUs on "Piz Daint" to render the results of simulations that were running simultaneously on the same machine. We had a fascinating demonstration of this insitu data analysis in the booth of NVIDA at Supercomputing 2014 in New Orleans. Here we were able to present a visualisation of data from a 1000+ node astrophysics simulation that was running in real time on "Piz Daint" in Lugano while the picture frames were displayed in New Orleans.

During discussions of the new in-situ visualisation capability, Simon Portegies Zwart, the head of the research project behind these simulations and senior author of one of the Gordon Bell finalist papers at the conference, suddenly noticed the development of a ring galaxy, something that was previously conjectured theoretically and was now demonstrated numerically. A scientist analysed the data of this large simulation without it leaving the memory of the machine. This is an important step towards improvement of workflow efficiency and high productivity.

It is thanks to the joint efforts with our national and global partners that we have been able to build another milestone in the history of computational science and open new horizons for society at large. I am grateful to all these invaluable partners, amongst whom I would like to mention ETH Zurich, the University of Zurich, NVIDIA and Cray. My deepest appreciation also goes to the CSCS personnel for their everyday support of our mission.

Prof. Thomas Schulthess Director of CSCS

# Content

I Key Information	6
II Activity Report	8
III User Lab	14
IV Insights	44
V Facts & Figures	50

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

### User Community

2014: 85 Projects, 523 Users 2013: 90 Projects, 372 Users

Investments 2014: 8.1 Mio CHF 2013: 32.5 Mio CHF Computing Time for User Lab 2014: 874 791 472 CPU hrs 2013: 459 333 565 CPU hrs

Employees 2014: 64 2013: 65

Operational Costs 2014: 15.8 Mio CHF 2013: 13.1 Mio CHF



## Usage by Institution



### Computing Systems for User Lab

	-	Installation /		Peak Performance
Name	Supplier & Model	Upgrade	User	(TFlops)
Piz Daint	Cray XC30	2012 / 2013	User Lab	7 784
Piz Dora	Cray XC40	2014	User Lab	1 246
Monte Rosa	Cray XE6	2009/2011	User Lab	402
Tödi	Cray XK7	2009 / 2012	R&D	429
Pilatus	Intel Sandy Bridge 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

		Installation /		Peak Performance
Name	Supplier & Model	Upgrade	User	(TFlops)
Blue Brain 4	IBM BG/Q	2013	EPF Lausanne	839 + 13
Mönch	NEC Cluster	2013 / 2014	ETH Zurich	132
Monte Lema	Cray XE6	2012	MeteoSwiss	34
Phoenix	Cluster	2007 / 2012 / 2014	CHIPP (LHC Grid)	32
Albis	Cray XE6	2012	MeteoSwiss	15

#### January

#### Visualisation and graphics tutorial

On 20-21 January, CSCS organised a 2-day tutorial on visualisation and graphics. The course attracted a large and varied audience interested in python-driven 2D plots and information visualisation techniques for non-spatial data, run on the desktop and in large-scale, parallel, 3D scientific visualisation techniques, run on powerful CSCS production machines.

#### March

#### Richard Walker talks to the public about the Human Brain Project

On 11 March, CSCS hosted a public lecture on "Understanding the brain through the simulation" that was presented by Richard Walker of EPFL. The event was organised as part of the "Settimana del Cervello 2014", a series of public lectures held all over the canton of Ticino. Richard Walker, responsible for the editorial services of the Human Brain Project and the official spokesman of the project, explained to a large public how simulations done on supercomputers could help improve understanding the human brain.



8 Richard Walker talking to the public about the Human Brain Project.

# SOS18 conference: "Supercomputers as scientific instruments"

SOS (Sandia, Oak Ridge, Switzerland) is a series of highly interactive workshops on distributed supercomputing organised by Sandia National Laboratories, Oak Ridge National Laboratories and CSCS. Participation is by invitation only. CSCS hosted this year's meeting in St. Moritz on 17-20 March, focussing on the general topic "Supercomputers as scientific instruments".



St.Moritz, in the Engadin Valley, hosted the SOS18 conference.

#### Inauguration of "Piz Daint"

On 21 March, President of the ETH Board Fritz Schiesser, President of ETH Zurich Ralph Eichler, and guests from research, politics and industry convened in Lugano to inaugurate "Piz Daint", the new flagship supercomputer of CSCS and most powerful computer in Switzerland. Read the special feature for the full story (page 48).

#### Introduction course for CSCS hybrid Cray XC30

On 24-27 March, CSCS organised a 4-day training course to familiarise participants with the new Cray XC30 hybrid system "Piz Daint". Experts from Cray and NVIDIA along with CSCS staff explained to the participants how to make best use of the new architecture.

### April

#### HPC Advisory Council Switzerland conference 2014

On occasion of its 5th anniversary, the HPC Advisory Council and CSCS organised the HPC Advisory Council Switzerland conference as a 4-day event (31 March – 3 April). The first day was

dedicated to tutorials and the ensuing conference covered a whole range of topics, including HPC education, progress made toward exascale computing, accelerators, high-speed interconnects, Big Data, HPC Cloud, OpenStack, advances in storage and server development, new topologies, middleware and communication libraries. This year's social event was an evening boat trip on Lake Lugano with dinner on board.

# Start of "Piz Daint" production projects, and initial CHRONOS projects

1 April marked the beginning of a new phase of supercomputing at CSCS: the upgraded "Piz Daint", now featuring a fully hybrid architecture with one GPU on each of its 5,272 nodes, was made available to all CSCS users. The date coincided with the start of a new allocation period for production projects and for the newly launched big-scale CHRONOS (Computationally-Intensive, High-Impact Research on Novel Outstanding Science) projects. A total of 534,572 node-hours/year were allocated on "Piz Daint" to new production projects, and a total of 736,111 node-hours/year to CHRONOS projects.

#### May CUG 2014

CSCS hosted the CUG 2014 meeting on 4-8 May. The Cray User Group (CUG) is an independent, international cooperation of member organisations that own Cray computer systems. CUG was established to facilitate collaboration and information exchange in the HPC community. This annual event took place in Lugano and participants had the opportunity to discuss and debate openly the immediate future of supercomputing, in which the architectures for exascale computing are beginning to emerge.



The 2014 edition of the Cray User Group conference was hosted by CSCS in Lugano.

#### Node-level performance engineering course

The 2-day training course (15-16 May) taught performance engineering approaches on the compute node level and focussed on a comprehensive understanding of interactions between software and hardware. The instructors were Prof. Gerhard Wellein and Dr Georg Hager, both from Regionales Rechenzentrum Erlangen (RRZE) in Germany.

#### June PASC14 conference

Almost 250 researchers flocked to the first PASC conference at ETH Zurich (2-3 June) co-organized by CSCS in the scope of the PASC initiative to join an interdisciplinary meeting on the use of high-performance computing (HPC) in computational science. The success of the conference and the large number of participants demonstrated the strong demand for such a platform of knowledge exchange in Europe.



At the PASC conference: ETH Zurich professor Petros Koumoutsakos gives a public lecture on the "Arrow of Computational Science".

#### User meeting 2014

In recent years, CSCS has organised the annual User Day to update its user community on CSCS roadmaps, projects and developments, and at the same time to provide a platform to users to showcase their work in poster sessions and talks. This year CSCS decided to integrate the user meeting into the newly launched PASC conference, thus offering additional opportunities to discuss science and HPC, either formally through presentations and poster sessions or informally during the various breaks and social events. Prof. Thomas Schulthess opened the user meeting with an update on services provided by CSCS, and



Prof. Thomas Schulthess at the user meeting during PASC14.

staff members Drs Sadaf Alam, Maria Grazia Giuffreda, Claudio Gheller and Themis Athanassiadou reported on CSCS systems, the CSCS User Lab, the new CSCS service "HPC Data & Visualization" and upcoming CSCS training events respectively.



30 students attended the Summer School in Serpiano.

#### July CSCS-USI Summer School

Together with Università della Svizzera italiana, CSCS organised a 10-day Summer School on parallel programming with MPI, OpenMP, CUDA and OpenACC (30 June – 10 July). The Summer School addressed students who were new to the world of highperformance computing and hybrid systems and who wished to learn the basic skills required to write, develop and maintain parallel applications in scientific computing. A large portion of the available time was dedicated to practical exercises. The Summer School was held at a hotel in beautiful and secluded Serpiano, over the lake of Lugano.

#### August

#### PRACE 2IP workpackage 8 lead by CSCS

Prace-2IP WP8 was designed to support science by enabling numerical applications and simulation codes for future generations of HPC architectures. This was accomplished by involving a number of scientific communities in a close synergy between scientists, code developers and HPC experts, the first two contributing their deep understanding of the research subjects and algorithms, the last providing the necessary skills and competencies on novel HPC solutions. Sixteen codes were at the end successfully ported to innovative HPC systems. Besides the outstanding technical results, the establishment of durable synergies between scientists and HPC resource providers represented an additional valuable achievement of WP8.

#### Swiss ambassadors and senior officials of the Federal Department of Foreign Affairs visit CSCS

On 18-21 August, the city of Lugano hosted the Swiss ambassadors' conference 2014, organised by the Federal Department of Foreign Affairs (FDFA). During the event the ambassadors had the chance to participate in various workshops, visits and meetings, discussing diverse topics of relevance to diplomacy and economic promotion. Some 35 ambassadors visited CSCS, where they took the opportunity to learn about the centre and its activities.



Group photo with Swiss ambassadors in front of "Piz Daint".

### September

#### SLURM user group meeting

CSCS hosted the 2014 SLURM user group meeting, held on 23 and 24 September at the Lugano convention centre. The meeting discussed experiences with and improvements for the open-source job scheduler SLURM (Simple Linux Utility for Resource Management), which was implemented on all CSCS supercomputers some time ago.

#### October

#### Practical performance analysis of parallel applications course

CSCS organised a 2-day training course on the practical performance analysis of parallel applications, which took place at CSCS on 6-7 October 2014. The course was part of a series of presentations with associated hands-on sessions on the "Piz Daint" system. The training started with basic application instrumentation and measurement tools to generate execution profiles, then moved on to discussing custom-tailored profiling as well as the interactive and automated analysis of execution traces.

#### OpenACC hackathon at Oak Ridge

In partnership with the Oak Ridge Leadership Computing Facility (OLCF), CSCS delegated two instructors to the supercomputer centre in Tennessee (USA) as coaches for the OpenACC hackathon, held on 27-31 October. This event was the first ever hackathon at OLCF and attracted teams of developers to a 5-day hands-on workshop to port their scalable application to GPU accelerated systems.

# The State Secretariat for Education, Research and Innovation visits CSCS

On 24 October, Prof. Thomas Schulthess welcomed 40 members of the Swiss State Secretariat for Education, Research and Innovation (SERI) to CSCS. This is a government agency handling matters of research and education, both nationally and internationally. Some of the visitors represented the Swissnex Network, which is run by SERI and is responsible for international research partnerships. The visitors were introduced to the centre and its services by the director, Prof. Schulthess, and were then offered a guided tour through the machine room.



Prof. Thomas Schulthess with members of SERI and Swissnex in front of the "Blue Brain 4" supercomputer.

### November

#### "Piz Dora", a Cray XC40 complementing services of "Piz Daint"

In early 2014, CSCS decided to expand its existing facilities through the acquisition of a new multi-core Cray XC40, to be known as "Piz Dora". The system was configured to satisfy a variety of high-end computing needs, from extreme-scale computing to data analytics, as well as general pre- and post-processing and visualisation. "Piz Dora" is expected to improve the science workflow of the User Lab. This new heterogeneous system was installed in early November 2014, was made available to a larger group of users in January 2015, and is scheduled to go into full production mode as of 1 April 2015.

#### TecDay at Liceo Locarno

42 experts active in research and technical institutes, universities and industry came to present their activities to young students at the TecDay of the Liceo di Locarno on 14 November. Mario Valle of CSCS explained to 20 students "Why supercomputers are super". He showed what supercomputers are used for and why they are needed today, and gave a hands-on demonstration of concepts that CSCS deals with on a daily basis.



The new booth for CSCS and hpc-ch at SC14.

#### SC14: a brand new booth for "HPC in Switzerland"

CSCS and hpc-ch – the Swiss HPC Service Provider community – participated in Supercomputing 2014 (SC14, 16-21 November) in New Orleans, Louisiana (USA), and decided to underline their dedication toward sustainable supercomputing by making their booth entirely from environmentally friendly cardboard. The idea was to create a "Swiss House of HPC" where visitors could meet Swiss HPC specialists and scientists and get to know the latest about HPC and science in Switzerland. A schedule with hourly talks was set up that demonstrated excellence in Swiss HPC and research. Visitors received coffee and Swiss chocolate in addition to a cardboard tablet holder.



Visitors at the CSCS and hpc-ch booth at SC14 and participants to one of the numerous talks offered.

#### December

# High-end connection for rapid, large-volume data transfer

On 3 December, CSCS became Switzerland's first service provider for the scientific community to offer a high-performance, 100 gigabit-per-second network connection. Up to five times as much data as before can be transmitted in any given period of time, thus significantly speeding up the transfer of data between the institutions of the users and the computing centre.



100 gigabit of data per second can be transmitted over the SWITCH network on up to 88 channels.

# Collaboration contracts with University of Zurich and NCCR Project MARVEL

The University of Zurich has entered into a research partnership with ETH Zurich and CSCS to make a share of "Piz Dora" available to its researchers. The CSCS supercomputer will replace the University of Zurich's Schrödinger supercomputer in order to meet researchers' demands for high-performance computing. Likewise, EPF Lausanne has entered into a partnership that opens a share of Piz Dora to projects within its National Centre of Competence: MARVEL – Materials' Revolution: Computational Design and Discovery of Novel Materials.



Close up view of a Cray XC chassis showing the centre latches of the left and right modules in a "Piz Daint" cabinet.

### Consolidation of the User Lab

After a busy 2012, in which CSCS moved to its new building in Lugano, and a no less fast-paced 2013 that saw the flagship computer system "Monte Rosa" (Cray XE6) being replaced by the new "Piz Daint" (Cray XC30), CSCS returned to a quieter mode in 2014 and started a consolidation phase that will reach well into 2015.

"Piz Daint" has been upgraded from 12 to 28 cabinets and now features a hybrid system of 5,272 compute notes, each with one Intel Xeon E5 CPU and one NVIDIA Tesla K20x GPU. The system was inaugurated on 21 March 2014 and opened up to full production the following month. CSCS then decided to extension "Piz Daint" with a second system, "Piz Dora", about one guarter the size of the former, and based on a CPU-only architecture that is dedicated to smaller projects. The duo of "Piz Daint" and "Piz Dora" not only serves to replace the former flagship computer "Monte Rosa", but addresses most peripheral computing needs as well. With its strong hybrid architecture, "Piz Daint" will take over visualisation tasks previously performed on "Eiger", and "Piz Dora" will replace "Julier" and "Pilatus" for pre- and post-processing. "Eiger" was switched off in 2014 and "Julier" and "Pilatus" are going to be decommissioned in 2015. The duo of Daint and Dora thus serves to concentrate computing tasks on two main systems and streamlines and consolidates CSCS's computing infrastructure.

Following an established tradition, the names of "Piz Daint" and "Piz Dora" were selected from the names of well-known mountains in Switzerland. Both are located in the Swiss canton of Grisons, rising between the valleys of Müstair and Mora. In the local language, Romansh, "Piz Daint" ("Piz d'Aint") means interior peak, and "Piz Dora" ("Piz d'Ora") exterior peak, which aptly suits the purpose of the "Daint-Dora" duo.

### Resources allocated in 2014

Analysis of usage statistics reveals a number of interesting trends. First, Chemistry & Materials remains by far the most computer-intensive research field at CSCS, using 56% of the total allocation (59% in 2013). This undoubtedly reflects the emerging possibility of studying even fairly large material and chemical models with more accurate and more versatile (though also quite expensive) first-principle models that move empirical models further into the background. Secondly, the percentile allocation to Physics projects has increased significantly from 14% to 31%. Scrutinising the data identifies several new types of very compute-intensive projects, among them nuclear physics and chemical physics. Thirdly, the remaining disciplines consumed less than 10% each, including Earth & Environmental Sciences, Life Sciences, and Mechanics & Engineering. Their importance initially appears to have lessened compared to 2013; however, taking into account the roughly double compute capacity of CSCS, absolute numbers are reasonably consistent with last year's statistics.

Statistics for usage by institution show a pleasing trend. Although ETH Zurich is still the biggest user by far, its percentile share (35%) has seen a significant decrease compared to 2013 (47%), giving way mostly to EPF Lausanne (20% vs 11% in 2013) and to the University of Zurich (19% vs 12% in 2013). This demonstrates that CSCS is a high-profile computing resource for excellent research in all of Switzerland.

### List of CHORNOS Projects

Principal Investigator	Organisation	Research Field	Project Title	Granted Allocation in core hrs (Mi	o CPU h)
Joost VandeVondele	ETH Zurich	Chemistry & Materials	Exploring frontiers in nanoscale simulation: new models and improved accuracy		100.00
Constantia Alexandrou	University of Cyprus	Physics	Precision nucleon structure using t	wisted mass lattice QCD	87.00
Andreas Fichtner	ETH Zurich	Earth & Environmental Science	e 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	ence Continental-scale cloud-resolving climate simulations for Europe		40.00
Franco Vazza	Hamburg Observatory	Physics	Investigating the origin of cosmic magnetism in large-scale struct cosmological simulations with Enzo on the GPU		35.00

# **Usage Statistics**

# Usage by Institution (%)

Institution	2012	2013	2014
ETH Zurich	42	47	35
University of Zurich	20	12	20
EPF Lausanne	11	11	20
University of Basel	9	8	4
Others	18	22	21
Total Usage	100	100	100



# Usage by Research Field (%)

Research Field	2012	2013	2014
Chemistry & Materials	44	59	56
Physics	15	14	31
Earth & Environ. Science	9	6	7
Mechanics & Engineering	21	13	4
Life Science	9	6	2
Others	2	2	0
Total Usage	100	100	100



# 16 Largest Projects

Principal Investigator	Organisation	Research Field	Project Title	Granted Allocation in core hrs (M	io CPU h)
Jürgen Diemand	University of Zurich	Physics	Petascale molecular dynamics simulations o	f water nucleation	51.20
Antigoni Voudouri	Hellenic National	Earth & Environ. Science	Objective calibration of weather prediction	models	31.98
	Meteorological Service				
Romain Teyssier	University of Zurich	Physics	Euclid simulations		31.00
Simon Portegies Zwart	University of Leiden	Physics	The fine structure of the milky way galaxy		26.00
Stefan Goedecker	University of Basel	Chemistry & Materials	Structure prediction of clusters and solids		25.00
Max Lawson Daku	University of Geneva	Chemistry & Materials	Photoinduced spin crossover in iron(II) comp	lexes in solution:	25.00
			1. Spin-state dependence of the solution str	uctures	
Jürg Hutter	University of Zurich	Chemistry & Materials	Atomistic simulation of molecules at interfa	ces	19.20
Mathieu Luisier	ETH Zurich	Chemistry & Materials	Reducing heat dissipation in nanoelectronic	devices	16.40
			through quantum transport simulations		
Petros Koumoutsakos	ETH Zurich	Mechanics & Engineering	Optimization of shape, motion and formatio	n patterns	15.00
			of single and multiple swimmers		
Matthias Troyer	ETH Zurich	Chemistry & Materials	High-order series expansions for strongly co	rrelated electron systems	15.00
Lucio Mayer	University of Zurich	Physics	Formation and evolution of dwarf galaxy sat	ellites with ErisSAT, a massively	15.00
			parallel high resolution cosmological hydrod	ynamical simulation with ChaNGa	
Rubén Cabezón	University of Basel	Physics	Matter accretion on compact objects: the ro	le of neutrinos,	12.48
			magnetic field and equations of state		
Matthias Troyer	ETH Zurich	Chemistry & Materials	Development of a highly parallel DMRG code	2	12.00
			for quantum chemistry problems		
Leonardo Scapozza	University of Geneva	Life Science	Insights into phosphoinositide 3-kinase (PI3	<) regulation	12.00
			using molecular dynamics simulations		
Antoine Georges	University of Geneva	Chemistry & Materials	Static and dynamic control of materials with	strong electron correlations	11.86
Oliver Hahn	ETH Zurich	Physics	Galaxy clusters as cosmological probes		10.00

# List of Projects by Institution

#### **EMPA**

Toward novel nanomaterials and functional surfaces: from spectroscopy to chirality, Carlo Pignedoli (Chemistry & Materials, 5.50 Mio CPU h)

#### **EPF** Lausanne

Top-down formation of carbon nanotubes from graphene: learning and designing with large-scale ab initio simulations, Wanda Andreoni (Chemistry & Materials, 9.22 Mio CPU h)

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

Nuclear quantum dynamics of water and its constituent ions from first principles, Michele Ceriotti (Chemistry & Materials, 2.00 Mio CPU h)

Application of large-eddy simulation to atmospheric boundary layer flows and transports of scalars above urban surfaces, Wai Chi Cheng (Mechanics & Engineering, 6.00 Mio CPU h)

Energetic particle physics in magnetically confined configurations, Anthony Cooper (Physics, 6.48 Mio CPU h)

Atomistic simulation of internal protein dynamics and proteinprotein interactions under cell-like conditions, Matteo Dal Peraro (Life Science, 2.00 Mio CPU h)

Large eddy simulation of very-large-scale motions in atmospheric boundary layer flows, Jiannong Fang (Earth & Environmental Science, 3.00 Mio CPU h)

Kinetic simulations of plasma biasing, Federico Halpern (Physics, 2.40 Mio CPU h)

Computational materials science in the cloud: an open-access database of materials' data and computational workflows, Nicola Marzari (Chemistry & Materials, 40.00 Mio CPU h)

Large eddy simulation of diurnal cycles of alpine slope winds, Marc Parlange (Earth & Environmental Science, 1.00 Mio CPU h)

Numerical simulations of vascular districts, Alfo Quarteroni (Mechanics & Engineering, 6.00 Mio CPU h) Simulation of plasma turbulence in the edge of tokamak devices, Paolo Ricci (Physics, 5.44 Mio CPU h)

**ORB5-GENE turbulence**, Laurent Villard (Physics, 6.00 Mio CPU h)

Development of a GPU-accelearted large-eddy simulation code using a hybrid mpi-openmp-openacc algorithm, Yu-Ting Wu (Mechanics & Engineering, 1.02 Mio CPU h)

Computational exploration of emerging electronic materials, Oleg Yazyev (Chemistry & Materials, 3.00 Mio CPU h)

#### **ETH Zurich**

CUDA accelerated classical MD simulations, Dirk Bakowies (Chemistry & Materials, 7.00 Mio CPU h)

Aerosol-cloud interaction studies using COSMO-ART-M7, Isabelle Bey (Earth & Environmental Science, 1.50 Mio CPU h)

Knotted vortices: entropic lattice Boltzmann method for simulation of vortex dynamics, Shyam Chikatamarla (Mechanics & Engineering, 3.70 Mio CPU h)

Entropic lattice Boltzmann method for fluid dynamics, Shyam Chikatamarla (Mechanics & Engineering, 2.50 Mio CPU h)

**Global waveform Inversion across the scales,** Andreas Fichtner (Earth & Environmental Science, 50.00 Mio CPU h)

Direct numerical simulation of formation and propagation of turbulent spherical premixed syngas/air flames, Christos Frouzakis (Mechanics & Engineering, 2.50 Mio CPU h)

Cloud cavitation collapse, Petros Koumoutsakos (Mechanics & Engineering, 6.00 Mio CPU h)

Reducing heat dissipation in nanoelectronic devices through quantum transport simulations, Mathieu Luisier (Chemistry & Materials, 16.40 Mio CPU h)

Impacts of lower crustal flow on regional and global scale geodynamics, David May (Earth & Environmental Science, 1.31 Mio CPU h)

Transonic MHD turbulence in cosmic structure, Francesco Miniati (Physics, 4.00 Mio CPU h) Pore-scale investigation of volatiles behavior in magmaticsystems with the lattice Boltzmann method, Andrea Parmigiani (Earth & Environmental Science, 0.46 Mio CPU h)

Continental-scale cloud-resolving climate simulations for Europe, Christoph Schär (Earth & Environmental Science, 40.00 Mio CPU h)

Development of a highly parallel DMRG code for quantum chemistry problems, Matthias Troyer (Chemistry & Materials, 12.00 Mio CPU h)

High-order series expansions for strongly correlated electron systems, Matthias Troyer (Chemistry & Materials, 15.00 Mio CPU h)

**Topological quantum computation and the fractional quantum Hall effect,** Matthias Troyer (Chemistry & Materials, 7.47 Mio CPU h)

Exploring frontiers in nanoscale simulation: new models and improved accuracy, Joost VandeVondele (Chemistry & Materials, 100.00 Mio CPU h)

Simulating the transduction of mechanical forces into biological signals, Viola Vogel (Life Science, 1.10 Mio CPU h)

#### Hamburg Observatory

Investigating the origin of cosmic magnetism in large-scale structures: cosmological simulations with Enzo on the GPU, Franco Vazza (Physics, 35.00 Mio CPU h)

#### Hellenic National Meteorological Service

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

#### Hydrocean

Numerical study of physics, scaling and hydroelasticity during liquid impacts with SPH-flow solver, Pierre-Michel Guilcher (Mechanics & Engineering, 1.50 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, 0.20 Mio CPU h)

#### Paul Scherrer Institute

Large eddy simulation of particle-laden flow in the steam generator bundle, Roman Mukin (Mechanics & Engineering, 2.00 Mio CPU h)

#### Università della Svizzera italiana

**Broadly neutralizing influenza antibodies,** Albert Ardèvol (Life Science, 1.10 Mio CPU h)

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

Towards a molecular description of fat bloom in chocolate, Matteo Salvalaglio (Chemistry & Materials, 1.60 Mio CPU h)

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

Large scale simulations of heterogeneous crystallization of the phase change material GeTe, Gabriele Sosso (Chemistry & Materials, 1.82 Mio CPU h)

A thermodynamic and kinetic description of the B2-A2 loop landscape in prion proteins, Pratyush Tiwary (Life Science, 2.28 Mio CPU h)

#### Università di Napoli

Unravelling the functional conformational transitions of human serine racemase: a new target for the treatment of CNS disorders, Vittorio Limongelli (Life Science, 0.42 Mio CPU h)

#### University of Cyprus

Precision nucleon structure using twisted mass lattice QCD, Constantia Alexandrou (Physics, 87.00 Mio CPU h)

#### University fo Geneva

Cosmic strings simulations: probing abelian Higgs parameter, Martin Kunz (Physics, 8.76 Mio CPU h)

Insights into phosphoinositide 3-kinase (PI3K) regulation using molecular dynamics simulations, Leonardo Scapozza (Life Science, 12.00 Mio CPU h)

Realistic 3D modelling of stellar winds, Aline Vidotto (Physics, 0.38 Mio CPU h)

#### University of Basel

Gating mechanisms of the ASIC acid-sensing ion channel, Simon Bernèche (Life Science, 3.20 Mio CPU h)

Structure prediction of clusters and solids, Stefan Goedecker (Chemistry & Materials, 25.00 Mio CPU h)

#### University of Bern

High-resolution simulation of hailstorms over Switzerland in current and changing climate conditions (HRHail), Andrey Martynov (Earth & Environmental Science, 3.00 Mio CPU h)

#### University of Geneva

Static and dynamic control of materials with strong electron correlations, Antoine Georges (Chemistry & Materials, 11.86 Mio CPU h)

Study of coupled organic chains by parallelized DMRG, Thierry Giamarchi (Chemistry & Materials, 8.10 Mio CPU h)

Photoinduced spin crossover in iron(II) complexes in solution: 1. Spin-state dependence of the solution structures, Max Lawson Daku (Chemistry & Materials, 25.00 Mio CPU h)

#### University of Lausanne

Mechanisms controlling acid-sensing ion channel (ASIC) activity, Stephan Kellenberger (Life Science, 4.02 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 Milan

Atomistic simulations of the heterogeneous crystallization of phase change GeSbTe alloys, Marco Bernasconi (Chemistry & Materials, 3.60 Mio CPU h)

#### University of Zurich

Petascale molecular dynamics simulations of water nucleation, Jürgen Diemand (Physics, 51.20 Mio CPU h)

Investigation and design of Co(II)-based cubane water-oxidation catalysts, Sandra Luber (Chemistry & Materials, 9.04 Mio CPU h)

Formation and evolution of dwarf galaxy satellites with ErisSAT, a massively parallel high resolution cosmological hydrodynamical simulation with ChaNGa, Lucio Mayer (Physics, 15.00 Mio CPU h)

High-dimensional dynamic stochastic economic modeling using adaptive sparse grids, Simon Scheidegger (Computer Science, 9.00 Mio CPU h)

Euclid simulations, Romain Teyssier (Physics, 31.00 Mio CPU h)

Charge transfer excitations for organic photovoltaics applications, Laura Zoppi (Chemistry & Materials, 1.00 Mio CPU h)

### Renewals

#### EMPA

CarboCount CH, Dominik Brunner (Earth & Environmental Science, 1.00 Mio CPU h)

#### **EPF** Lausanne

First-principle design and engineering of electronic and thermal transport from nanoelectronics devices to novel thermo-electrics, Nicola Marzari (Chemistry & Materials, 4.80 Mio CPU h)

Defect levels at interfaces of high-mobility semiconductors through hybrid density functionals, Alfredo Pasquarello (Chemistry & Materials, 1.60 Mio CPU h)

Multiscale simulations of biological systems and bioinspired devices, Ursula Röthlisberger (Chemistry & Materials, 6.44 Mio CPU h)

Large eddy simulation of diurnal cycles of alpine slope winds, Marc Parlange (Earth & Environmental Science, 1.00 Mio CPU h)

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

#### **ETH Zurich**

Computational science for the metrology of nanostructures, Mauro Ciappa (Computer Science, 0.36 Mio CPU h)

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

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

Numerical simulation of particle-laden multi-phase flows, Leonhard Kleiser (Mechanics & Engineering, 3.40 Mio CPU h)

SILENS - Subcritically bifurcating instability of the leadingedge boundary layer investigated by numerical simulations, Leonhard Kleiser (Mechanics & Engineering, 1.75 Mio CPU h)

Precessionally driven turbulence and dynamos in spheroidal and cylindrical enclosures, Stijn Vantieghem (Earth & Environmental Science, 4.00 Mio CPU h)

Massively parallel multilevel Monte-Carlo finite volume simulations for uncertainty quantification in nonlinear wave propagation, Chritsoph Schwab (Computer Science, 2.20 Mio CPU h)

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

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

Optimization of shape, motion and formation patterns of single and multiple swimmers, Petros Koumoutsakos (Mechanics & Engineering, 14.00 Mio CPU h)

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

Development of a database of physics-based synthetic earthquakes for ground motion prediction, Luis Dalguer (Earth & Environmental Science, 3.44 Mio CPU h)

Coupled and competing instabilities in complex oxides, Nicola Spaldin (Chemistry & Materials, 8.00 Mio CPU h)

#### Università della Svizzera italiana

Improving diagnosis of atrial fibrillation, Mark Potse (Life Science, 4.40 Mio CPU h)

#### University of Basel

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

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

#### University of Bern

ISOCARB, Fortunat Joos (Earth & Environmental Science, 0.88 Mio CPU h)

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

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

#### University of Zurich

CP2K program development, Jürg Hutter (Chemistry & Materials, 2.40 Mio CPU h)

Atomistic simulation of molecules at interfaces, Jürg Hutter (Chemistry & Materials, 12.00 Mio CPU h)

# Continents set the pace



According to new simulations the continental crust influences the formation of the oceanic crust, such as here in the Atlantic Ocean. (Source: Google Earth)

The origins of plate tectonics and the stimuli behind them have been simulated with the aid of high-performance computers. A new study sheds light on the role continents play in the formation of oceanic crust.

The seafloor opens up at the mid-ocean ridges (MOR), which stretch through the world's oceans for 10,000 kilometres. Here, hot magma material generated by the convection of the Earth's mantle reaches the surface and creates new oceanic crust. How these processes were triggered in Earth's early history, however, is the subject of ongoing debate. Researchers from ETH Zurich and the University of Lyon have now reignited the discussion with new computer simulations.

#### Continental mass formed early on

According to the scientists, the simulations reveal that the continental crust influences the rate at which the oceanic crust is formed and thus influences the dynamics of the entire Earth. Moreover, the scientists' calculations indicate that while the continents were growing to their present size, the thermal output of the Earth's mantle varied greatly. Their results also support the theory that around 90 percent of the continental crust that exists today was formed no later than 2.5 billion years ago. While computer models have greatly improved our understanding of the Earth's dynamics, how much and how quickly continental crust formed in the planet's early history is not entirely clear.

#### Coupled, three-dimensional representation

Together with his team, Paul Tackley, a professor of geophysics at ETH Zurich, has spent the last few years developing and refining a model that can be used to illustrate physical processes on Earth in a coupled, three-dimensional manner. Although it is a heavily simplified model that does not reproduce all the conditions on Earth realistically, it is sufficient to simulate the fundamental mechanisms for its issues stresses Tobias Rolf, a doctoral student under Tackley. Rolf used the model to examine the impact of the world's entire existing continental crust on convection in the Earth's interior and on the formation of oceanic crust. The results of the study, which Rolf achieved in collaboration with Nicolas Coltice from the University of Lyon, were published in the journal *Geology*.

#### **Crustal differences influence dynamics**

Today, continental crust makes up around thirty percent of the Earth's surface. The continental crust differs greatly from the oceanic crust in terms of thickness, density and its deformation and flow properties. This contrast influences plate-tectonic processes and the heat flow through the Earth's surface: while the MOR heat is conducted away from the Earth's interior, by comparison continents have a thermally insulating effect.

Consequently, the scientists calculated the heat flow through the oceanic crust for a ten, thirty, fifty and seventy-percent continental crust cover of the Earth's surface on the supercomputer "Monte Rosa" at CSCS. Via the local heat flow, they used a standard method to determine the approximate age of the seafloor and the statistical age distribution in the ocean basin. Based on these calculations, the scientists were able to extrapolate the production rate of the oceanic crust depending on the individual continent size and could determine how this production rate varied. The results reveal that as the size of the continents increases, the production rate of the oceanic crust can as much as double. "As a consequence, the mean age of the seafloor found in the ocean basin decreases", says Rolf. Today's ocean beds are a maximum of 200 million years old, the reason being that the basaltic seafloor cools over millions of years and becomes so heavy that it sinks back into the Earth's mantle: the oceanic plate mostly becomes submerged beneath the less dense continental plate and a so-called subduction zone is formed.



The researchers simulated how the local age distribution of the seafloor looks like under the assumption that the global share of the continental curst is 30 per cent. The grey area represents the continental cover. (Source: Coltice N et al., Geology 2014)

# **Researching how stars explode**

Supernovae are exploding stars. The light from such an explosion and its remnants enable numerous conclusions to be drawn about the former star. To this day, however, it has not been possible to explain how these stellar explosions come about. Astrophysicist Matthias Liebendörfer from the University of Basel and his colleagues are getting to the bottom of it with the aid of supercomputers at CSCS.

At the end of their "lives", stars shine brighter than ever before: during their explosion their luminosity is a million or billion times more intense. This event, referred to as a supernova, can be observed for up to 100 days with telescopes in space and on Earth. If a supernova occurs in our galaxy, such as the famous Kepler's Star of 1604, it can even be seen with the naked eye in good visibility.

#### Neutron stars as remnants

At least two mechanisms can cause a star to become a supernova. These mechanisms leave behind different end-products and are based on the star's initial mass: in the case of a large mass, a black hole can form through the collapse of the star's core. If the initial mass is lower but at least eight times higher than that of our sun, a neutron star is formed. Matthias Liebendörfer, a lecturer in astrophysics at the University of Basel, primarily focuses on the supernova mechanism that is triggered by a core collapse and leaves a neutron star behind. When it comes to evaluating the various theories, the only tool researchers like Liebendörfer have at their disposal is simulating the process on high-performance computers. He uses the supercomputers at CSCS.

Back in 1938, the Swiss physicist and astronomer Fritz Zwicky was the first to suggest that the energy for a supernova explosion might come from the gravitational collapse of a star. As we know today, the chemical elements of a star pass through a chain of nuclear fusions during their lifetime, which spans several tens of millions of years. This fusion chain only stops when elements from the iron family are formed. With the most binding energy per nucleon, iron is the final link in the fusion chain. For another fusion to take place, energy would need to be added. Instead, iron now accumulates in the star's core until the latter becomes unstable and collapses as it is no longer able to counter the gravitational forces at work.



A collage of a three-dimensional supernova simulation (centre left) and the Kamiokande neutrino detector (right). The simulation shows a cross-section from inside the collapsing star. The inner blue sphere corresponds to the neutron star formed. On the left in blue, cold, collapsing outer layers; in red, hot layers between the neutron star and the shockwave. The centre displays the structure of the magnetic fields entangled by turbulences. The black curve represents the expected neutron emission, which was detected for SN1987A in the Kamiokande neutrino detector for the first time. (Source: M. Liebendörfer)



This Hubble telescope image shows the supernova's triple-ring system, including the bright spots along the inner ring of gas surrounding the exploded star. A shock wave of material unleashed by the stellar blast is slamming into regions along the inner ring, heating them up, and causing them to glow. (Source: Wikipedia)

In the event of a collapse, the core is compressed enormously. Before collapse the density is about 10 billion grams per cubic centimetre, but after collapse, a massive 1 quadrillion grams per cubic centimetre. The process releases a tremendous amount of energy: after compression, a one-cubic-centimetre cube weighs 500,000 tons – as much as around 1,500 jam-pa-cked jumbo jets.

#### Neutrino shower proves collapse theory

Contrary to their natural state, the negatively charged electrons are compressed in such a way during the collapse in the star's core that the positively charged protons can capture them. As a result, neutrons form through the release of neutrinos.

As neutrinos only interact weakly, they can diffuse the high density generated by the compression from the core and ultimately stream out of the core. This "neutrino shower" can be detected in our galaxy with special measuring devices and interpreted as an indication of a pending supernova. The first time this was achieved successfully was for the supernova in the Magellanic Cloud in 1987: the neutrino shower observed and the disappearance of the progenitor star provided the researchers with a strong indication that the collapse theory was correct.

It is apparent that under certain conditions following a star's collapse, the neutrons remaining in the core will form a neutron star with a diameter of about twenty kilometres and a mass equivalent to about 1.4 suns. Exactly which physical mechanisms ultimately trigger the stellar explosion after the core collapse, however, remains unclear to this day. The strong interaction between the atomic nucleuses in the star causes the collapse of the innermost shells to stop suddenly as soon as a certain extremely high material density has been reached, explains Liebendörfer. The enormous forces exerted in the process trigger a shockwave that propagates itself towards the exterior through the rest of the star. As it spreads, it interacts with the layers it penetrates and exchanges energy.

#### Shockwave forms new elements

On the way, the shockwave also triggers so-called nucleosynthesis where new elements form, including ones that are heavier than iron, such as germanium, gold or uranium. The newly-formed elements are initially in an excited – energetically higher – state, and return to their ground state gradually through radioactive decay. In the process, the material is heated up and emits light. These light spectra provide an indication of the development of the supernova and its remnants, an emission nebula made of gas, dust and the outer, exploded layers of the star. "Based on these light spectra and the materials ejected from the exploding star, a kind of velocity map of the ejecta can be produced and the elements that form during nucleosynthesis determined", says Liebendörfer. Although the explosion process is undisputed, it remains unclear via which physical mechanisms the shockwave gains sufficient energy to explain the nucleosynthesis observed that takes place in the jettisoned external layers.

Astrophysicists have enlisted the aid of computer simulations to reconstruct supernova explosions since the late 1960s. They initially attempted to reconstruct the explosion mechanism based on spherical, shell-like models. Scientists calculated hundreds of shells and observed the impact of one shell on another, explains Liebendörfer. Nonetheless, they failed to create an intrinsically consistent explosion: "When a simulation seemingly produced the result that had been hoped for, the models used always failed to physically pan out", says the astrophysicist.

Around the turn of the millennium, physicists had models at their disposal that they believed displayed the most important physical and relativistic processes, including neutrino transportation through the star. According to Liebendörfer, however, the simulations only ever ended in a black hole, never in a neutron star formation. They then realised that a key process had not been factored into the models, namely multidimensional upheavals such as convections or turbulences. This work was followed by the introduction of very elaborate two-dimensional models, he says. The fact that the cause of the explosion could still not be explained unequivocally was due to the enormous computer resources that were necessary for a realistic simulation, but also to the extreme physical conditions that prevail in a supernova.

#### **Realistic 3D model**

Together with scientists from the University of Geneva, Liebendörfer and his colleagues have spent the last few years developing a three-dimensional model to simulate a supernova in the project High-Performance and High-Productivity Computing (HP2C). Thanks to their efforts it is now possible to consider processes that require three dimensions, such as the detailed development of convection and the magnetic field. This should now enable the stellar explosions to be modelled more realistically. However, Liebendörfer remains only cautiously optimistic. The model still needs to be put through its paces to see whether what it calculates is actually correct. One of the most difficult processes to model is the transportation of neutrinos through the core and star, which scatter at high densities but flow at lower densities.

The researchers needed to devise new algorithms here, as the earlier ones would be far too computationally demanding for use in multi-dimensional space. Consequently, the scientists identified the most essential processes for every phase of a supernova and incorporated them into the model. In this way they can calculate the key aspects of the respective phases in the simulation of the collapse or spread of the shockwaves, and omit the less important processes.

"The new method already works extremely well for one and two-dimensional models", says a delighted Liebendörfer.

In the follow-up project, the Platform for Advanced Scientific Computing (PASC), the neutrino model will be made accessible to all researchers as a radiation transport library, produced in collaboration with scientists from the University of Zurich.

However, it might be some time before a supernova can be reconstructed successfully in the three-dimensional model. Liebendörfer points out how many decades and how much painstaking theoretical work it took to get to the present state of research. But if the scientific community does not succeed in producing a realistic, physically credible supernova with the three-dimensional model on the supercomputer after extensive testing, we will know for sure that something is fundamentally wrong with the model, he says. Nevertheless, if he can show that standard physics does not correctly describe the extreme conditions of a supernova that are unattainable on Earth, it would be just as exciting for him as a definitive understanding of the supernova explosion with the physics we know.



Pipes distributing water from Lake Lugano are ready to be connected to additional heat exchangers.

# Papers with Highest Journal Impact Factor<sup>1)</sup>

#### Nature

#### Impact Factor: 42.35

R. Mankowsky, A. Subedi, M. Forst, S. O. Mariager, M. Chollet, H. T. Lemke, J. S. Robinson, J. M. Glownia, M. P. Minitti, A. Frano, M. Fechner, N. A. Spaldin, T. Loew, B. Keimer, A. Georges, A. Cavalleri, Nonlinear Lattice Dynamics as a Basis for Enhanced Superconductivity in YBa2Cu3O6.5, Nature, Doi 10.1038/ nature13875.

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#### Impact Factor: 33.27

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P. Moffa Sánchez, A. Born, I. R. Hall, D. J. R. Thornalley, S. Barker, Solar forcing of North Atlantic temperature and salinity over the past millennium, Nature Geoscience, Doi 10.1038/ ngeo2094.

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Backplane optical connectors in a Cray XC40 cabinet.

28

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#### **Dirk Bakowies, ETH Zurich**

D. Bakowies, Simplified Wave Function Models in Thermochemical Protocols Based on Bond Separation Reactions, Journal of Physical Chemistry A, Doi 10.1021/jp510249v.

#### Rubén Cabézon, University of Basel

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# Bits and bytes in pictures



A snapshot of the in-situ visualisation on "Piz Daint". (Source: NVIDIA)

Scientists are using "Piz Daint's" graphics processors for displaying the results of their simulations while they are being calculated by the supercomputer. This "in-situ" visualisation of high-resolution simulation reveals the origins of the Milky Way in near film quality.

Scientific discovery is based on observation, theoretical consideration, experiment, and, in many areas, computer simulation. But inspiration and intuition on the part of the scientist play a crucial role too. And it is precisely these senses that are readily stimulated by visual images. When simulating complex systems, in-situ visualisation – where the results from simulations are continually converted to images "on-the-fly" – can thus provide researchers with important insight, without the need for complicated post-processing of the data. This approach is anything but standard, and besides expert knowledge, it requires a suitable supercomputer. This is where "Piz Daint", the flagship supercomputer of CSCS, comes in. Not only do the Tesla graphics processors of the Cray XC30 make "Piz Daint" highly efficient in its calculations; as the term "graphics processors" suggests, they also have exceptional graphics capabilities.

#### Ingenious combination

The challenge of in-situ visualisation lies in combining two completely different data structures – simulation and visualisation – while a simulation is underway. A team of scientists from the Dutch institutions SURFsara, the Centrum Wiskunde & Informatica and Leiden University, and experts from CSCS and the GPU manufacturer NVIDIA succeeded in doing exactly that on "Piz Daint" in 2014. Headed by Simon Portegies Zwart from Leiden University, the team simulated the long-term development of the Milky Way, from the origin of the bar structure to the full formation of the galaxy's spiral arms, in a novel way and at an unprecedented resolution, before adapting the basic software to enable in-situ visualisation.

The simulation software has the ability to distribute the stars and dark matter particles – which are dispersed irregularly in space – evenly onto the compute nodes in such a way that the simulations run at maximum speed. The particles are then redistributed to allow all nodes to contribute to the rendering of the images. This ingenious coupling of the two processes enables an in-situ visualisation to run on over 2,000 nodes of the supercomputer. In this way, the graphics processors are used for both simulation and visualisation, and the scientist can view the formation of the Milky Way from different angles and perspectives during the calculation. The advantage of visualisation on-the-fly is not limited to fuelling inspiration and intuition, however. Removing the need to save data for later retrieval and processing saves time, energy and space on the file system. The approach could thus prove essential for the effective use of future supercomputer generations – after all, writing-out and storing data already takes a lot of time and disk capacity in today's petaflop-class supercomputers. With the next generation computers the process will pose an enormous challenge for both the users and the operators of computer centres: exaflop supercomputers will perform a thousand times more computer operations – a total of one billion billion (i.e. eighteen zeros) per second – and yet they will not be much faster at reading and writing data to external files. CSCS is therefore working closely with its users to develop in-situ visualisation solutions on "Piz Daint".

#### **Pioneering method**

In-situ visualisation is not only valuable for astrophysics and other physical sciences (such as meteorology, earth science and materials science) but can also benefit medicine and neuroscience. For example, in the Human Brain Project it could provide a real-time rendering of the complex processes taking place inside the human brain. One of the short-term goals of in-situ visualisation is the ability to intervene in a running simulation and monitor what happens if a particular parameter is altered. One day, simulations with in-situ visualisation could thus be used to guide complicated surgical procedures inside the human body.



Milky Way in-situ visualisation on 2000 nodes of "Piz Daint".

# Universal computing platform offers comprehensive services

CSCS is convinced that the computer centres of the future will need to offer heterogeneous platforms of multifunctional supercomputers, delivering comprehensive scientific computing services. The "Piz Daint" supercomputer and its sister "Piz Dora" provide the basis for this at CSCS.

One machine that can do everything. That is the dream of both industry and computer centres. The latter would like to have a supercomputer that can not only carry out computations but also process data, being capable of analysing, structuring, visua-lising and storing it – all in one. Until now, CSCS has operated different systems to meet these different requirements. However, with the introduction of "Piz Dora" – an extension to its "Piz Daint" flagship supercomputer – in the second half of 2014, the centre has now laid the foundations for exactly this kind of platform, with one universal supercomputer. The main purpose of the platform is now to provide services.

#### A heterogeneous all-rounder

In "Piz Daint", a Cray XC30, the new platform has one of today's most energy-efficient petaflop computers in the world at its disposal. Thanks to its hybrid system based on graphic processors (GPUs) and conventional CPUs, and with the help of special software, it is able to visually depict the results of computations

even while simulations are running (see the article on "Bits and bytes in pictures" on page 44). By adding "Piz Dora" – a Cray XC40 with 1,256 compute nodes consisting solely of CPUs – to the computing system, the platform can now not only carry out conventional calculations and visualisations but also analyse and structure data. This enables it, for example, to filter out what is important from a vast volume of data – a vital function in this age of Big Data.

The computing system comprising "Piz Daint" and "Piz Dora" is connected by a shared cache memory that is used while a computation is being carried out (scratch space) and by what is currently one of the most powerful networks in the world.

The "Piz Dora" extension is also assuming of the tasks performed by "Monte Rosa", the former CSCS flagship supercomputer, and the University of Zurich's Schrödinger cluster. The University of Zurich has taken a stake in "Piz Dora", bringing with it other research institutions which, for reasons of either space or efficiency, are unable or unwilling to maintain their own computing centre. "Piz Dora" therefore also accommodates the cluster resources of the Paul Scherrer Institute and the National Centre of Competence in Research (NCCR) MARVEL (Materials' Revolution: Computational Design and Discovery of Novel Materials). In addition, scientists from ETH Zurich use



46 Overview of the 2000 square metres machine room with supercomputers and cooling islands.

"Piz Dora" as a tool for data analysis. Individual computers belonging to other institutions that are operated at CSCS are also to be integrated into the new platform in the medium term.

#### User-optimised infrastructure

According to CSCS Director Thomas Schulthess, the core business of computing centres will change in the future. The focus will no longer be on the computing infrastructure, but on providing a comprehensive service platform which is able to support users in all aspects of scientific computing. This is because computer-assisted research is increasingly attracting attention not only from traditional users in fields such as physics, chemistry, materials research and earth and climate sciences, but also from newer areas of research where users sometimes have little experience of working with supercomputers. These users are to be supported by the extended range of services in the areas of software and applications.

The aim is to offer users the flexibility they need to solve their problems without any difficulty using the most suitable computing system. When continuously expanding the platform, the biggest challenge therefore lies in the software, stresses Schulthess. The CSCS Director believes that this heterogeneous platform offering comprehensive services will pave the way for closer cooperation with the providers of publicly available cloud computing solutions. After all, scientists should ideally be able to move their work as required between their local computer for example their laptop - and publicly available cloud services or the CSCS supercomputers.

#### The future lies in services

CSCS believes that the future of high-performance computing lies in the consolidation of computer infrastructure and services, on which it has already embarked. Interdisciplinary projects to improve software and applications as well as hardware have been underway since the launch of the High-Performance Computing and Networking (HPCN) initiative in 2009. These have, for example, helped to enhance computing algorithms, develop codes and optimise modern computer architectures, and they continue to do so. However, last but by no means least, the further successful expansion of the platform also depends on the industry, which in some cases is still refining the technologies required. That is why researchers from the user side and CSCS are working closely with hardware manufacturers to improve hardware and software. It is thanks to this cooperation that the new platform at CSCS now boasts such an extraordinarily efficient network, which enables the compute nodes to communicate with one another and plays such a vital role in the computing speed and efficiency of the computer.



# Inauguration of "Piz Daint"

On 21 March, the president of the ETH Board Fritz Schiesser, the president of ETH Zurich Ralph Eichler, and guests from research, politics and industry inaugurated "Piz Daint". This supercomputer at CSCS is named after one of the highest mountains in Val Müstair in the canton of Grisons. It is currently the most powerful computer in Europe and the flagship of supercomputing in Switzerland.

"Piz Daint" is the culmination of the first phase of the national High-Performance Computing and Networking Strategy (HPCN Strategy), which ran from 2009 to 2014 and was implemented successfully by the ETH Board on behalf of the Swiss government and CSCS. "Nowadays, research relies on tremendous computer capacity to make progress in an increasing number of fields", says Fritz Schiesser. "'Piz Daint' is Switzerland's response to this challenge".



Welcoming address given by Fritz Schiesser, president of ETH Board.



Before the curtain was lifted: The cloaked powerful and yet energy-efficient Cray XC30 "Piz Daint" at the inauguration ceremony.



Prof. Thomas Lippert, Director of Jülich Supercomputing Center.



Prof. Joost VandeVondele, ETH Zurich.



Prof. Ralph Eichler, Prof. Thomas Schulthess and Fritz Schiesser.



# Finances

# Expenditures

	CHF
Investments	8 118 445.92
Equipment and Furniture	45 293.29
Personnel	7 538 405.74
Payroll	5 841 526.81
Employer's Contributions	1 004 747.35
Further education, Travel, Recruitment	692 131.58
Other Material Expenses	8 153 553.64
Maintenance Building	
& Technical Infrastructure	1 061 973.52
Energy & Media	2 551 644.31
Administrative Expenses	25 761.48
Hardware, Software, Services	4 245 922.69
Remunerations, Marketing, Workshops	
Services	259 580.71
Other	8 670.93
Extraordinary Income / Expenditures	69 158.81
Membership Fees / Overhead	69 158.81
Total Expenses	23 924 857.40

#### Income

CHF
4 772 633.00
.6 791 800.00
5 000 000.00
2 900 000.00
80 833.00

Other Income	183 135.05
Services / Courses	44 001.79
Reimbursements	65 257.86
Other Income	73 875.40

Total Expenses	23 924 857.40	Total Income	24 955 768.05
Balance current Year			1 030 910.65
Rollover Project Fund Investments 2013			2 619 818.92
Total Balance User Lab 2014			3 650 729.57

#### Third-Party Contributions

UZH	2 358 000.00
MARVEL	1 500 000.00
CHIPP	1 386 383.70
Euler Cluster	1 237 950.55
MeteoSwiss	1 223 000.00
Blue Brain	830 258.57
Mönch Cluster	682 250.00
EU Projects	598 194.81
USI	450 000.00
C2SM	160 000.00
PSI	65 000.00
Other	18 000.00

**2014** 8 118 445.92

7 538 405.74

8 268 005.74

#### Personnel 7 530 745.80 6 388 608.00 7 249 675.71 **Other Material Expenses** 4 818 411.67 6 825 156.15 5 900 556.39 Mio CHF 35,0 32,5 30,0 27,5 25,0 22,5 20,0 17,5 15,0 12,5 10,0 7,5 5,0 2,5 0 2011 2012 2013 2014 Year Other Material Expenses Investments Personnel

2011

15 777 324.43

2012

17 320 218.00

2013

32 555 142.22

# Development of Overall Expenses

Investments

# **Usage Statistics**

# Usage by Research Field

Research Field	CPU h	%
Chemistry & Materials	484 940 392	56
Physics	273 271 671	31
Earth & Environmental Science	63 269 199	7
Mechanics & Engineering	35 663 479	4
Life Science	14 808 114	2
Others	2 838 617	0
Total Usage	874 791 472	100.0



### Usage by Institution

Institution	CPU h	%
ETH Zurich	309 454 420	35
EPF Lausanne	177 484 182	20
University of Zurich	170 048 986	20
Other International	104 960 561	12
University of Geneva	38 872 416	5
University of Basel	38 518 203	4
Università della Svizzera italiana	17 768 793	2
Other Swiss	17 683 911	2
Total Usage	874 791 472	100



# **Compute Infrastructure**

# HPC Systems for User Lab

	Supplier	Installation /	
Name	& Model	Upgrade	СРИ Туре
Piz Daint	Cray XC30	2012/2013	Intel Xeon E5-2670 & Nvidia Tesla K20X GPU
Piz Dora	Cray XC40	2014	Intel Xeon E5-2690 v3
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	Intel Sandy Bridge 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

	No. of	Interconnect	Peak Performance
Name	Cores	Туре	(TFlops)
Piz Daint	42 176 + 5 272 GPUs	Cray Aries	7 784
Piz Dora	29 952	Cray Aries	1 246
Monte Rosa	47 872	Cray Gemini	402
Tödi	8 704 + 272 GPUs	Cray Gemini	429
Pilatus	704	Infiniband FDR PCI Gen 3	15
Rothorn	256	SGI Numalink	3
Matterhorn	8 192 simultaneous hardware threads	Cray Gemini	NA

# HPC Systems for Third Parties

		Supplier	Installation /		
	Name	& Model	Upgrade	User	СРИ Туре
	Blue Brain 4	IBM BG/Q	2013	EPF Lausanne	BGQ (PowerPC – 1.6GHz) + Intel Xeon 2.6GHz
	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	2007/12/14	CHIPP (LHC Grid)	Intel Xeon CPU E5-2670 2.6 GHz + Intel Yeon E5-2690 v2
-	Albis	Cray XE6	2012	MeteoSwiss	AMD Opteron 6172 2.1 GHz

	No. of	Interconnect	Peak Performance
Name	Cores	Туре	(TFlops)
Blue Brain 4	65 536 (BGQ) + 640 Intel Xeon	IBM BGQ 3D torus + Infiniband FDR	839 + 13
Mönch	7 520	Infiniband FDR PCI Gen 3	132
Monte Lema	4 032	Cray Gemini	34
Phoenix	1 504	Infiniband QDR PCI Gen 2	32
Albis	1 728	Cray Gemini	15

# **User Satisfaction**

A user satisfaction survey was submitted to 523 users in January 2015. The response rate was of 25% (132 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	Very poo	r Poor	Fa	ir G	ood	Excellent
Helpdesk support					<u> </u>	
System support						
Application support			_			
The offer of training courses and user events			_			
	0 10	20	30	40 5	0 60	70
How fast does support handle your request?	Very slov	/ Slow	Ассер	table F	ast	Very fast
The reaction time of the helpdesk is						
The time to solution for the support requests is			-			
	0	10 2	) 30	40	50	60

## System Availability, Stability and Usability







14%



Have you been submitting project proposals to

**Project Proposal Process** 

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:



56

### **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?

	0%	10%	20%	30%	40%	50%	60%	70%	80%	90%
С										
C++										
Fortran										
CUDA										
OpenCL										
Python										
MPI										
OpenMP										
OpenACC										
PGAS										

# 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



How often do you access the following communication channels:	Never	Infrequently	Monthly	Weekly	Dail	y	Hourly
www.cscs.ch	-	_		-			
user.cscs.ch	_	_					
www.twitter.com/cscsch	-						
www.youtube.com/cscsch		-					
www.hpc-ch.org	0 10	20 30	40	50 60	70	80	90

Improved 49%

# 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:

Worsened 4%

Remained unchanged 45% Improved a lot 2%



Front doors of a cooling island reflecting the adjacent island.

# Impressum

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