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Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre Annual Report **2016** 







# Annual Report 2016

# CSCS

Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre

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

# Welcome from the Director



Thomas Schulthess, Director of CSCS.

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

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

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

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

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

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

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

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

Prof. Thomas Schulthess Director of CSCS

Schuttte

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

#### Name Andreas Fichtner

Anureas Fichther

Position Assistant professor

Institution ETH Zurich

#### Background

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

#### Area of research

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

#### Specialised in

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

#### HPC means for me

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



### Where the Earth is humming and whistling

Researchers at ETH developed a novel technique to image the sources of incessant, micrometer-scale vibrations of the whole Earth known as the ambient seismic field. With the help of "Piz Daint" they were able to process massive amounts of seismic data recorded world-wide every second over a period of 10 years.

Their method can be used to reduce errors in tomographic imaging of the crust and is in the process of being expanded to a framework for the daily monitoring of hydro-carbon and geothermal reservoirs.

(Image: Andreas Fichtner, ETH Zurich)

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

### **Production Machines**

Piz Daint, Cray XC50, 23.5 PFlops Piz Daint, Cray XC40, 1.7 PFlops

### User Community

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

Investments 2016: 40 Mio CHF 2015: 5.1 Mio CHF Computing Time for User Lab 2016: 43 446 610 node h 2015: 1 201 734 615 CPU h

Employees 2016: 79 2015: 70

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



### Usage by Institution



### Computing Systems Overview

Usage by Research Field

Name	Model	Installation/Upgrades	Owner	TFlops
Piz Daint	Cray XC50/Cray XC40	2012/13/16	User Lab, UZH, NCCR Marvel	23 498 + 1 731
Blue Brain BG/Q	IBM BG/Q	2013	EPF Lausanne	839
Blue Brain Viz	IBM Cluster	2013	EPF Lausanne	13
Monch	NEC Cluster	2013/14	ETH Zurich	132
Phoenix	x86 Cluster	2007/12/14/15/16	CHIPP (LHC Grid)	86
Piz Kesch	Cray CS-Storm	2015	MeteoSwiss	196
Piz Escha	Cray CS-Storm	2015	MeteoSwiss	196
Monte Leone	HP Cluster	2015	User Lab	33
Pilatus	x86 Cluster	2012	User Lab	13

### Computing Systems Specifications

Name	Interconnect Type	СРИ Туре	No. Cores	No. Cores	No. Nodes
Piz Daint	Cray Aries	Intel Xeon E5-2690 v3 + Nvidia P100	12	1	4 936
		Intel Xeon E5-2695 v4	18	2	1 431
Blue Brain BG/Q	IBM BGQ 3D Torus	PowerPC A2	16	1	4 096
Blue Brain Viz	Infiniband FDR	Intel Xeon E5-2670	8	2	40
Monch	Infiniband FDR	Intel Xeon E5-2660 v2	10	2	376
Phoenix	Infiniband FDR	Intel Xeon E5-2670	8	2	64
Piz Kesch	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2	12
Piz Escha	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2	12
Monte Leone	10 Gb Ethernet	Intel Xeon E5-2667 v3	8	2	20
		Intel Xeon E5-2667 v3	8	2	7
		Intel Xeon E5-2690 v3 + Nvidia K40C	12	2	4
Pilatus	Infiniband FDR	Intel Xeon E5-2670	8	2	38



"Supercomputers like 'Piz Daint' are essential in modern cosmology to study the non-linear evolution of matter and fields in the Universe.

Without supercomputers, current and future large astronomical surveys would not be able to realize their full potential. Thanks to the rapid increase in computing power we are, on the theory and data analysis side, able to keep up with the increase in data volume and quality, and the resulting progress in understanding our Universe has been breath-taking."

Martin Kunz, University of Geneva

Name Martin Kunz

Position Associate professor

Institution University of Geneva

#### Background

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

#### Area of research

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

#### Specialised in

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

#### HPC means for me

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



### More realistic simulation of the evolution of cosmic structures

Cosmologists at the University of Geneva are the first to simulate the structure of the universe in a way that consistently accounts for the general theory of relativity using "Piz Daint". This was made possible with a new simulation code developed by the researchers.

(Image: Cosmology and Astroparticle Physics Group University of Geneva)

### January



#### Webinar: Allinea DDT

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

### February

# 03

#### 5 000 followers on LinkedIn

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



# 22

# Webinar: Deep-dive GPU debugging with Allinea DDT

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

### March

# 21/23

#### HPC Advisory Council Switzerland Conference 2016

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

# 31

#### MeteoSwiss and COSMO-1

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





### April



#### More computing power for Swiss research

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



## 29

#### User meeting at EPF Lausanne and ETH Zurich

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

May



#### "Piz Dora"'s upgrade

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

### 10

### Allocation of computer time, April 2016 to March 2017

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

#### June



#### PASC16 Conference

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



# 10

## CSCS director meets the scientific community at EPF Lausanne

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

# 12/14

#### ADAC workshop Switzerland

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

# 20/22

#### CSCS at ISC16

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

#### ISC Best Visualization award

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

### July

# 04/08

#### Second EuroHack

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





#### Summer School 2016

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



### September



#### Data science with [a] Spark

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



# Allocation of computer time, October 2016 to September 2017

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

# 26/28

#### Workshop on advanced C++ for HPC

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

# 29/30

#### Workshop on task-based programming with HPX

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

### October



#### "Albis" & "Monte Lema" shutdown

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



# 04

#### "Monte Leone": a new small high memory cluster

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



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

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



### 17

#### "Piz Daint"'s major upgrade

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



# 19

#### 25 Years anniversary celebration

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



### November

# 11

# World-leading HPC Centres partner to form accelerated computing institute

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

# 14/17

#### CSCS at Supercomputing 2016

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



### 15

### CSCS and MeteoSwiss winners of the SwissICT Award 2016

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





# 30

#### Webinar: "Piz Daint" upgrade - What's new?"

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

### December



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

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



#### "Piz Daint" back in service

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





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

Mathieu Luisier, ETH Zurich

#### Name

Mathieu Luisier

Position

Associate professor

Institution ETH Zurich

#### Background

1998-2003 Studies of electrical engineering, ETH Zurich

- 2003-2007 PhD at the Integrated Systems Laboratory, Department of Information Technology
  - and Electrical Engineering, ETH Zurich
- 2007Post-doc at the Integrated Systems Laboratory, ETH Zurich2008-2011Research assistant professor, Network for Computational Electronics, Purdue University, USA
- 2011-2016 SNF assistant professor, Integrated Systems Laboratory, ETH Zurich
- Since 2016 Associate professor, Integrated Systems Laboratory, ETH Zurich

#### Area of research

Computational nanoelectronics, computer-aided design of nanoscale devices.

#### Specialised in

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

#### HPC means for me

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



### Ab-initio simulation of electron flow trough a nanowire

Two research teams from ETH Zurich combined two software programs and also developed a new algorithm to maximise the throughput rate for hybrid computer systems. This enabled them

to reduce the time taken to simulate nanoscale devices by one fifty times and to increase the size of the nanocomponents to 100 000 atoms. (Image: Jean M. Favre, CSCS)

### Yet another exciting year

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

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

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

### Resources allocated in 2016

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

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

### List of CHRONOS Projects

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

# **Usage Statistics**

### Usage by Institution (%)

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



### Usage by Research Field (%)

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



### 17 Largest Projects

Principal Investigator	Organisation	Research Field	Project Title	Node h
Stefan Goedecker	University of Basel	Chemistry & Materials	Structure prediction of solids, surfaces and clusters	1 000 000
Alireza Rahmati	University of Zurich	Physics	Spatially adaptive radiation-hydrodynamical simulations of cosmic reionization in a representative volume	1 000 000
Franco Vazza	Hamburg Observatory	Physics	Galaxies in filaments: a high-resolution view from adaptive mesh refinement MHD simulations	822 530
Michael Francis	EPF Lausanne	Chemistry & Materials	Stress controlled surface chemistry: towards the rational design of core-shell nanoparticles catalysts	800 000
Matthias Liebendörfer	University of Basel	Physics	The isotropic diffusion source approximation for the simulation of faint and failed supernova explosions with additional degrees of freedom in the equation of state	750 000
Ulrike Lohmann	ETH Zurich	Earth & Environ. Science	The impact of aerosols in the past, present, and future climate	737 000
Francesco Miniati	ETH Zurich	Physics	Transonic MHD intracluster turbulence	700 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	First-principles simulation of van der Waals homo- and hetero-junctions for optoelectronic applications	600 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	Ab-initio simulations of conductive bridging memristors for application as plasmonic optical switches	600 000
Jürg Hutter	University of Zurich	Chemistry & Materials	Properties of liquids, solutions, and interfaces from density functional theory	600 000
Jan Burjánek	ETH Zurich	Earth & Environ. Science	Numerical modeling of seismic response unstable rock slopes	550 000
Maximilian Amsler	Northwestern University	Chemistry & Materials	Discovery of energy materials through large-scale lattice dynamics	550 000
Jonathan Graves	EPF Lausanne	Physics	Energetic particle physics in magnetically confined configuration	500 000
Paolo Ricci	EPF Lausanne	Physics	Simulation of plasma turbulence in the periphery of tokamak devices	500 000
Ursula Röthlisberger	EPF Lausanne	Chemistry & Materials	Multiscale simulations of biological systems and bioinspired devices	500 000
Nicolas Noiray	ETH Zurich	Mechanics & Engineering	Identification of thermoacoustic instability driving mechanism in a new generation gas turbine combustor	500 000
Martin Kunz	University of Geneva	Physics	Relativistic cosmological simulations with gevolution	500 000

# List of Projects by Institution

#### CERN

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

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

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

#### **EMPA**

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

#### **EPF** Lausanne

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

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

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

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

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

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

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

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

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

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

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

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

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

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

#### ETH Zurich

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

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

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

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

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

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

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

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

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

#### Northwestern University

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

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

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

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

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

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

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

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

#### **ETH Zurich**

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

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#### University of Geneva

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

#### University of Lausanne

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

#### University of Zurich

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# The spleen and its effect on red blood cells



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

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

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

#### Micro filter for red blood cells

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

There is no experimental technique currently available that allows us to observe this process in vivo. Therefore, Igor Pivkin and colleagues used "Piz Daint" to simulate the mechanical filter function of the interendothelial slit and how red blood cells are squeezed through the tiny openings. The simulations are based on the red blood cell (RBC) model which Pivkin started to develop during his PhD studies at Brown University in the group of George Karniadakis. Based on the size of the slits and taking into account the prevailing pressure difference across them, the researchers determined possible sizes and mechanical characteristics of red blood cells that would allow them to pass through the slits. They combined their simulations with a theoretical analysis, by investigating how the geometry of the slits and the blood cells influenced the process.

#### Survival of the fittest

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

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

#### Support for drug development

The findings improve the understanding of the functioning of the spleen, and how the 'filter' may influence disease like sickle cell anaemia or malaria. They also can provide new insights in drug treatments, for example to explain why specific malaria drugs which stiffen healthy and malaria-infected red blood cells, could lead to severe anaemia. Co-author Subra Suresh, president of Carnegie Mellon University, emphasizes that the results offer better understanding of how the circulatory bottleneck for the red blood cell in the spleen could affect a variety of acute and chronic disease states arising from hereditary disorders, human cancers and infectious diseases, with implications for therapeutic interventions and drug efficacy assays. The work on modelling of the RBC passage through the endothelial slits in the spleen began when Pivkin joined Subra Suresh's group at MIT as a postdoctoral researcher. However, the first significant results were obtained years later, after Pivkin moved to USI in Lugano. For experts the study shows that blood-cell and blood-flow modeling and simulation have reached a stage where they can contribute significantly to the understanding and treatment of blood-related disorders.

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# Supercomputers on the trail of dark matter

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

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

#### Quark condensates couple to the Higgs-boson

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

Quarks interact mutually via gluon particles, and quarks with gluons via their respective colour charges, which may be red, green or blue. The strong force acting and being transmitted by the gluons – called the strong interaction – is one of the four fundamental forces of physics along with the weak interaction, the electromagnetic interaction and gravitation. The research field of Alexandrou and her team is quantum chromodynamics (QCD), which theoretically describes the strong interaction



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



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

between quarks and gluons, and hence explains the origin of the nucleon large mass as well as what binds together neutrons and protons in atomic nuclei. For without the strong interaction, protons, for example, with their similar electrical charges, would repel each other rather than sticking together in the nucleus. And that would negate the existence of matter as we now understand it.

#### Heavy mass from binding energy

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

#### Strong force with extremely short radius of action

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

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



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

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

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

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

#### Name Matthias Krack

Position

Group leader

Institution Paul Scherrer Institute

#### Background

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

#### Area of research

Materials science, chemistry, multiscale modelling.

#### Specialised in

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

#### HPC means for me

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



### Simulating chemical evolution

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

#### **INSIGHTS**

# IV

## Twenty-five years supporting Switzerland as a research hub



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

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

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



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

From left to right: Piero Martinoli and Ralph Eichler.



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



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



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

Fulvio Caccia.



Beatrice Fasana, member of the ETH Board.

Lino Guzzella, president of ETH Zurich.



Paolo Beltraminelli, president of the Ticino State Council.



Cristina Zanini Barzaghi, city of Lugano.



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



Boas Erez, rector of Università della Svizzera italiana.

#### The beginning

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

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

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

In December 2009, the Swiss parliament approved a strategy for high-performance computing and networking (HPCN) drawn up by the ETH Board on behalf of the Swiss State Secretariat for Education, Research and Innovation (SBFI). The Swiss federal government, ETH domain and universities thereby laid the foundation for an internationally competitive Swiss supercomputing network. Three years later, CSCS moved into a state-of-the-art new building in Lugano and took receipt of "Piz Daint", a Cray XC30 supercomputer that was Switzerland's first petaflop machine and can perform millions of billions of calculations a second. One of the goals of the HPCN strategy was to support top-level research in Switzerland and thereby secure the country's competitiveness.

#### Today: Most powerful supercomputer in Europe

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

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

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

# More computing power for Swiss research



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

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

ETH Zurich has invested CHF 40 million in the upgrade of "Piz Daint" – from a Cray XC30 to a Cray XC50 – in order to provide an infrastructure that will accommodate the increasing demands in high performance computing (HPC) up until the end of the decade. The upgrade involved replacing two types of compute nodes as well as the deployment of a novel technology from Cray Inc. known as DataWarp. DataWarp's 'burst buffer mode' quadruples the effective bandwidth to and from storage devices, markedly accelerating data input and output rates and so facilitating the analysis of millions of small, unstructured files. Thus, "Piz Daint" is able to analyse the results of its computations on the fly. The revamped "Piz Daint" remains an extremely energy-efficient and balanced system where simulations and data analyses are scalable from a few to thousands of compute nodes.







"'Piz Daint' has enabled our group to build a 'multiscale-scope' for computational science to study phenomena from the atomistic to the macroscale. 'Piz Daint' has been instrumental to our research efforts ranging from the detection of metastatic cancer cells to revealing the hydrodynamics behind the beauty of fish schools." Petros Koumoutsakos, ETH Zurich

#### Name

Petros Koumoutsakos

Position Professor

Institution ETH Zurich

#### Background

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

#### Area of research

Computing.

#### Specialised in

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

#### HPC means for me

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



### In silico lab-on-a-chip

State-of-the-art simulations of the flow of micron-sized red blood cells and tumour cells through mm-long microfluidic channels. The so-called "in-silico lab-on-a-chip" emulates laboratory

experiments looking at how rare tumour cells could be filtered out of the blood thus allowing for the early diagnosis of metastatic cancer. (Image: Christian Conti, CSElab)

# V

# Finances

## Expenditures

	CHF
Investments	40 023 532.86
Equipment and Furniture	8 035.15
Personnel	8 313 178.80
Payroll	6 469 583.30
Employer s contributions	1 113 631.20
Further education, Travel, Recruitment	729 964.30
Other Material Expenses	6 234 696.37
Maintenance building	655 516.81
& Technical Infrastructure	
Energy	1 499 835.87
Administrativ expenses	11 565.79
Hardware, Software, Services	3 529 306.73
Remunerations, Marketing	522 197.97
Workshops, Services	
Other	16 273.20
Extraordinary Income / Expenditures	50 362.37
Membership fees	50 362.37
Total Expenses	54 629 805.55

## Income

	CHF
Basic Budget	52 819 584.26
Contribution ETH Zurich	52 819 584.26

Other Income	164 687.02
Services / Courses	61 929.55
Reimbursements	8 517.97
Other Income	94 239.50

Total Expenses	54 629 805.55	Total Income	52 984 271.28
Balance current year			-1 645 534.27
Rollover Project Fund Investments 2016	5		2 879 930.61
Total Balance User Lab 2016			1 234 396.34
./. Rollover Project Fund Investments 20	)17		29 561.50
Balance operational Funds CSCS - Rollov	ver to ETH 2016		1 204 834.84

#### Third-Party Contributions

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

## Development of Overall Expenses

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



# **Usage Statistics**

## Usage by Research Field

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



## Usage by Institution

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


# **Compute Infrastructure**

### HPC Systems

-				Node Specifications		
Name	Model	Interconnect Type	СРИ Туре	No. Cores	No. Sockets	No. Nodes
Piz Daint	Cray XC50 Cray XC40	Cray Aries	Intel Xeon E5-2690 v3 + Nvidia P100 Intel Xeon E5-2695 v4	12 18	1 2	4 936 1 431
Blue Brain BG/Q	IBM BG/Q	IBM BGQ 3D Torus	PowerPC A2	16	1	4 096
Blue Brain Viz	IBM Cluster	Infiniband FDR	Intel Xeon E5-2670	8	2	40
Monch	NEC Cluster	Infiniband FDR	Intel Xeon E5-2660 v2	10	2	376
Phoenix	x86 Cluster	Infiniband FDR	Intel Xeon E5-2670	8	2	64
Piz Kesch	Cray CS-Storm	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2	12
Piz Escha	Cray CS-Storm	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	12	2	12
Monte Leone	HP DL 360 HP DL 360 HP DL 380	10 Gb Ethernet	Intel Xeon E5-2667 v3 Intel Xeon E5-2667 v3 Intel Xeon E5-2690 v3 + Nvidia K40C	8 8 12	2 2 2	20 7 4
Pilatus	x86 Cluster	Infiniband FDR	Intel Xeon E5-2670	8	2	38



#### Website cscs.ch

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



### Top 5 most visited website pages







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

## Facebook Find us on f November 2015: creation of the CSCS page

	2015	2016	
Followers	-	89	

#### CSCS in the News

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

#### Word Cloud of News Related to CSCS

istituto computing supercomputing schweizer stunden

petaflops hardware federale franken

forschung national ticino usi simulationen calcolo

bereich ricerca zukunft swiss supercomputer forschungsanstalten rechnenleistung

CSCS psi piz ict schweiz

zürich meteoschweiz hochschulen lugano daint award

centro data rat mitteilung svizzero epfl millionen scientifico

università hochleistungsrechnenzentrum svizzera zurigo scienze facoltà rechnen

## **User Satisfaction**

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

#### User Profile



Your scientific field



Your position



For my research, CSCS resources are:



Which HPC resources are you using besides CSCS?



#### User Support



### 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:



75



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:



### **Application Development**

Do you develop and maintain application codes?



Which programming languages and parallelization paradigms are you using primarily?



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



#### 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:





## Impressum

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