CSCS

Annual Report
2019

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

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The cover page depicts the visualization of air bubbles in moving water.
Anyone who has ever taken a walk on the beach knows the phenomenon: foam crowns on the waves. This is, because breaking sea waves capture air and produce bubbles that cluster up as foam. PhD student Petr Karnakov, Postdoc Sergey Litvinov and ETH professor Petros Koumoutsakos from the Computational Science & Engineering Laboratory of ETH Zurich have used the supercomputer “Piz Daint” to investigate how foam is formed and what its formation depends on. The visualization software engineer Jean M. Favre from CSCS has then visualized the simulation results in collaboration with the ETH researchers. The resulting video received the prestigious 2019 APS/DFD Gallery of Fluid Motion Award.

The photographer Alessandro Della Bella has portrayed eight staff members of CSCS: Claudia Alongi-Bühler, Prashanth Kanduri, Jérôme Tissières, Heidi Oggian-Wittwer, Mark Klein, Hussein Harake, Shoshana Jakobovits, Victor Holanda Rusu.

Welcome from the Director

Thomas Schulthess, Director of CSCS.

Since the end of 2019 marks the conclusion of both the year and decade, please allow me to take a brief look back at this period of innovation in which we at CSCS successfully established our computer "Piz Daint" in the petaflop performance class. While we were doing so, the next era of computing was already dominating discussions among high-performance computing (HPC) experts and users. These discussions have centred around the necessity, purpose and viability of exascale computing. As we enter the new decade, extreme-scale computing is already becoming a reality across many areas of science and business. Computers 100 times more powerful than "Piz Daint" will soon be in use worldwide – including in Europe.

The support of ETH Zurich and the Swiss government, coupled with our positive reputation among and integration into European HPC communities, enables us to actively participate in forward-thinking European initiatives. The EuroHPC Joint Undertaking, for example, is actively making extreme-scale systems a reality, and we are honoured and excited to contribute to the project. These new supercomputing systems will make it possible to investigate highly complex and urgent scientific problems in even greater detail and, in turn, hopefully find solutions for the benefit of society – whether in climate research, economics, medicine, or the classical scientific disciplines. This annual report aims to give an overview of the wide range of uses HPC currently offers.

Continuous upgrades of our flagship supercomputer "Piz Daint" have made it the most powerful computer in Europe for six years now. In 2019, two ETH Zurich research teams succeeded in winning the prestigious Gordon Bell Prize, an award presented annually by the Association for Computing Machinery in conjunction with the SC Conference series, using "Piz Daint" for the development of their codes. This is another important achievement in the history of CSCS and a recognition of our efforts as a service institution to provide our users with highly efficient computing power in addition to our expertise.

In order to be just as successful in the coming decade, we at CSCS are focused on embracing the coming era of HPC and therefore working diligently on plans for the successor to "Piz Daint". With the recent software investment of the PASC (Platform of Advanced Scientific Computing) program, we are better equipped than ever to provide our users with new and innovative technologies that can accelerate their research while maintaining high energy efficiency. We recognize that, in the age of cloud computing and artificial intelligence, it is no longer only about the computer architecture, but also about establishing a comprehensive, service-oriented infrastructure that satisfies our users' diverse needs. We will strive to stay tuned-in and attentive, and we look forward to continued cooperation and collaboration with all of our participants and supporters. We thank you all for the trust you have placed in us.

Last but not least, it is important to note that the new year and new decade bring new challenges as well as opportunities — and not only in HPC. As of January 1, 2020, CSCS is no longer organizationally attached to the Vice President for Human Resources and Infrastructure (VPPR). After a new infrastructure was established in tandem with the new building in Lugano, computer-aided research made possible at CSCS is once again brought to the fore. After about 11 years, CSCS will therefore once again report to the Vice President for Research. I would like to take this opportunity to thank Prof. Ulrich Weidmann (VPPR) and his team for their cooperation and support through the years, and I would also like to welcome Prof. Detlef Günther as we embark on an exciting new collaboration.

In closing, I would like to extend my gratitude to my CSCS team, not only for their hard work but also for the trust they placed in me. Thank you!

Content

KEY INFORMATION

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

Production Machines

Piz Daint, Cray XC50, 27.2 PFlops
Piz Daint, Cray XC40, 2.2 PFlops

Granted Resources for User Lab

2019: 50 045 000 node h
2018: 46 709 533 node h

User Community

2019: 124 projects, 1 883 users
2018: 132 Projects, 1 584 Users

Employees

2019: 115
2018: 99

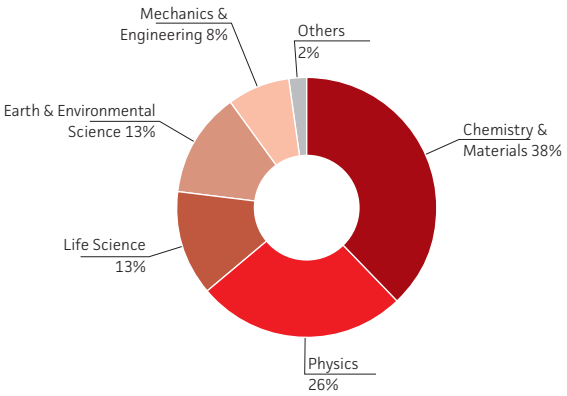
Investments

2019: 2.9 Mio CHF
2018: 2.5 Mio CHF

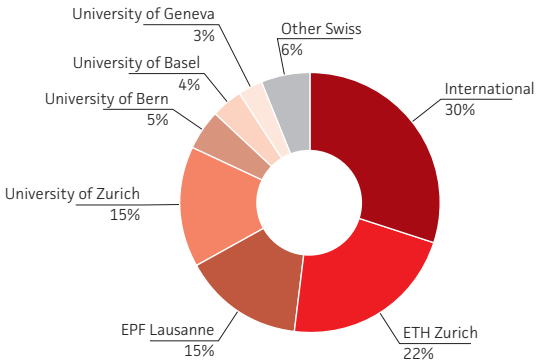
Operational Costs

2019: 21.2 Mio CHF
2018: 19.9 Mio CHF

User Lab Usage by Research Field



User Lab Usage by Institution



Computing Systems Overview

Name	Model	Installation/Upgrades	Owner	TFlops
Piz Daint	Cray XC50/Cray XC40	2012 / 13 / 16 / 17 / 18	User Lab, UZH, NCCR Marvel, CHIPP	27 154 + 2 193
Piz Kesch + Piz Escha	Cray CS-Storm	2015	MeteoSwiss	392
Grand Tavé	Cray X40	2017	Research & Development	437

Claudia Alongi-Bühler – Corporate Controller, Staff Unit

Nationality	Swiss
Working at CSCS since	September 2001
Background	1996-1999 Degree in Economics and Management, Höhere Wirtschaftsmittelschule, Bern 2006-2009 Dipl. Controllerin NDS HF, Swiss Federal Diploma, Schweizerisches Institut für Betriebsökonomie, Zürich
Specialised in	I am specialized in financial data business analysis, data monitoring for management reports and financial data planning. As Corporate Controller, I am acting as the interface between CSCS and the financial department in Zurich. One of my main tasks is to provide financial data reports to the leadership of the centre on a regular basis. Leading the planning process for the annual budget and medium-term strategy is one of the most intense and challenging tasks of my work at CSCS. This process is followed closely by our financial headquarters office at ETH Zurich. The yearly average budget I am managing amounts to CHF 53 Mio, including third party projects and external contractual collaborations.
Working at CSCS means to me	I am very proud to be able to contribute to a future-oriented institution in technology and research like CSCS. I appreciate the opportunity to work in the academic environment, which gives me the chance to perform on a very high educational level and the possibility to follow the latest trends in my activity field.
What I like most about my work	Even though my educational background is mainly based in the financial field, my work at CSCS requires a lot of communication and management skills as well. My language skills are needed to communicate with our head office in Zurich and also with the CSCS staff, making my daily activities diverse and unique. The international environment allows me to be surrounded by interesting people who exchange experiences from all over the world.
What challenges me at my work	My career at CSCS has been very challenging, as it has changed a lot in its dimension and in its activity field. The complexity of processes and rules in the financial sector has grown enormously in the last few years. Because CSCS operates in a very specified field, our needs and requirements are not always comparable to other activities in the public sector. This requires initiative and a good ability to collaborate closely with the Financial and Controlling Department in Zurich in order to find and integrate special business processes and to guarantee a correct and transparent performance in executing CSCS's daily operational business. With the introduction of the new financial system at ETH Zurich within the framework of the project "Refine", I developed and elaborated the new financial and organizational structure for CSCS in collaboration with the financial experts at the headquarters in Zurich.

Prashanth Kanduri – Scientific Software Developer, Scientific Software & Libraries

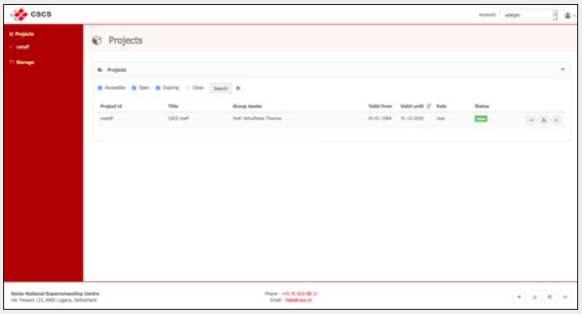
Nationality	Indian
Working at CSCS since	April 2017
Background	2009-2013 Bachelor in Mechanical Engineering, VIT University, India 2013-2017 Master in Computational Science & Engineering (Masters Scholarship), ETH Zurich 2012-2016 Various positions as student researcher/teaching assistant in India and Zürich 2014-2015 Student Developer at AutoForm Engineering GmbH, Zurich 2016-2017 Collaborative thesis project with ETH Zurich and ABB Corporate Research, Zurich
Specialised in	My main project aims to create a library for particle simulations that will empower research in the fields of chemistry, molecular biology, and material science, among others. To achieve this, we co-design with developers of a simulation package called GROMACS. The project cuts through aspects of API design, numerical methods, high performance on current and emerging hardware architectures, understanding workflows/goals of domain experts, etc. In addition, I get to play with new development platforms and assist in porting specific mathematical kernels for emerging hardware, sometimes via secondary projects or through hackathons.
Working at CSCS means to me	It is helping scientific research and enhancing our collective capabilities by building free and open toolkits; making my contributions in the public interest, as opposed to further enriching private companies; and directly impacting the trajectory of research by enabling new kinds of simulations on supercomputers.
What I like most about my work	I like getting to do the above-mentioned tasks while playing with some of the most cutting-edge machines in the world, thus being a part of the newest developments in the world of computing. More importantly, I like having a great learning platform by being among incredibly smart, diverse and very empathic people.
What challenges me at my work	Challenges include learning about fields I wasn't formally trained in, understanding requirements of researchers, constantly being updated with recent developments, forming collaborations with eminent research groups, and living up to the ambitious vision of the ongoing projects.

January

14 Visit the portal

Portal for managing users and projects opens

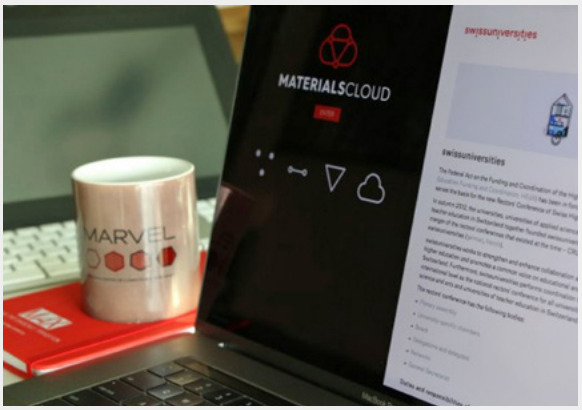
A user-friendly web-based portal was opened that lets users manage their own accounts and lets project leaders access online information and interactively manage their projects and users' membership. This was an important initial step that gives project leaders and users an overview of their accounts and projects at CSCS.



29 Read the article

EPFL researchers, together with CSCS, win grant to scale-up Materials Cloud

A multidisciplinary team made up of people from EPFL and CSCS won a swissuniversities P-5 grant to fund further development of the Materials Cloud web platform for Computational Open Science in the context of NCCR Marvel. The platform enables seamless sharing and dissemination of computational materials science resources, with users all over the world contributing hundreds of different data entries to the project.



30

First Elastic Meetup in Ticino

CSCS welcomed about 40 IT specialists to the first Elastic Meetup in Ticino for an evening of information sharing. The Elastic Stack is an open source solution for managing, searching, and visualizing large volumes of log data. The product has a large community behind it that periodically gathers together to share experiences and define best practices. CSCS relies heavily on the use of many components of the Elastic Stack to centrally collect and visualize log data.

February

04 Read the article

CSCS joined the second phase of the ESiWACE-2 project

The climate and weather prediction community is preparing for exascale through the EU-funded ESiWACE-2 project. This second phase will focus on containers, a technical solution that allows operating-system-level virtualization without the heavy overhead of virtual machines while still offering the full emulation of a computer system. CSCS will help teams from the project partners to "containerize" their models so they can run seamlessly on a variety of platforms. Activities related to this effort include a container unit for the ESiWACE-2 summer school, as well as a one-week container hackathon.

27 Watch the video

Webinar on getting started at CSCS

The CSCS user base acquires a number of new users every year, so the webinar "Getting started at CSCS" is organized as a beginner's guide to the User Lab. Attendees received instruction on how to access CSCS systems, manage the computing and filesystem resources, and run batch jobs.

March

05 Read the article

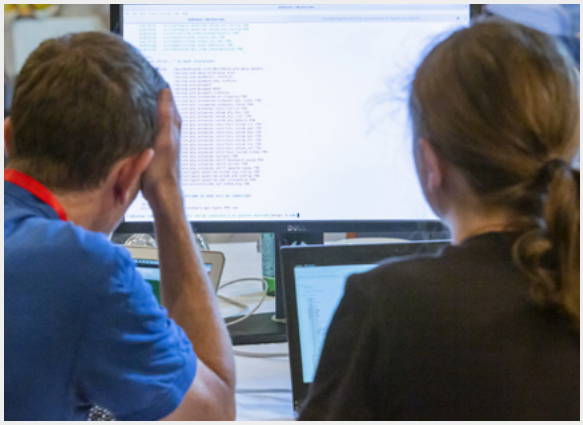
SELVEDAS: A CSCS and PSI joint project funded by swissuniversities

An ambitious project proposed jointly by CSCS and PSI was selected to receive another swissuniversities P-5 grant. The project, called SELVEDAS (Services for Large Volume Experiment-Data Analysis utilising Supercomputing and Cloud technologies at CSCS), aims to enable real-time extreme data workflows and use cases by deploying a cloud interface to access Petascale computational and data resources.

14/15 Watch the videos

Workshop on efficient and distributed training with TensorFlow on "Piz Daint"

A two-day course on efficient and distributed training with TensorFlow was organized to address the use of this tool on the "Piz Daint" system. Attendees had the chance to observe how to run distributed deep learning workloads and learn best practices for building efficient input pipelines that maximize the throughput of deep learning models with TensorFlow.



26 Read the article

Interactive supercomputing with JupyterLab

Users can now interactively access the computational power of CSCS through a JupyterLab interface. JupyterLab allows configures and arranges the user interface to support a wide range of workflows in data science, scientific computing, and machine learning.

April

01 Read the article

"Piz Daint" takes on Tier 2 function in worldwide LHC computing grid

In the future, the "Piz Daint" supercomputer will handle part of the analysis of the data generated by the experiments conducted on the Large Hadron Collider (LHC). This development was enabled by the close collaboration between CSCS and the Swiss Institute of Particle Physics (CHIPP). In the past, CSCS relied on the "Phoenix" cluster being exclusively dedicated to the LHC experiments to provide the same service.

01/04 Read the article

HPC Advisory Council 2019 & HPCXXL user group conferences

The HPC-AI Advisory Council (HPCAIAC), along with CSCS and the HPCXXL Board, held its tenth annual high-performance computing conference on April 1–4 in Lugano. The conference annually draws about 130 professionals to southern Switzerland to discuss the latest technology developments.

03 Read the article

2019 Doron Prize for Thomas Schulthess

At an event in Zug, the Swiss Foundation for the Doron Prize honoured Thomas Schulthess, Director of CSCS and Professor of Computational Physics at the Department of Physics, for his outstanding achievements in the field of supercomputing. The Foundation praised Schulthess as one of the most renowned Swiss and American scientists in the field of supercomputing.

16 Read the article

21.7 Mio. node hours distributed in the User Lab and PRACE Tier-0 calls

A total of 21.7 Mio. node hours were distributed in the first two calls of 2019 — the User Lab Call and PRACE Tier-0 Call 18 — for the allocation period starting on April 1, 2019 and continuing until March 31, 2020.

May

13/14 Watch the videos

Workshop on software management

A two-day workshop on "software management" was organized to help developers who are not familiar with working on large projects as part of a team. The workshop aimed to improve their build, test, version management and collaborative skills using software tools like CMake, Git, EasyBuild, Jenkins and Spack.

June

06 Read the article

Switzerland contributes to EuroHPC

CSCS will represent Switzerland in EuroHPC, a joint endeavour which aims to develop a pan-European supercomputing infrastructure. Specifically, the goal is to acquire, build and deploy a world-class computing and data infrastructure at the CSC - IT Centre for Science in Kajaani, Finland. Nine countries and the EU will participate in this unique project that, by the end of 2020, should deploy one of the fastest and most advanced supercomputers in the world, providing highly competitive HPC resources for Europe's scientific, industrial and public users.

11

European Trilinos User Group Meeting

The Trilinos Project Team and CSCS co-organized a one-day European Trilinos User Group Meeting at ETH Zurich to cover several topics, including an overview of Trilinos capabilities for next-generation parallel computers. Trilinos is an effort to develop algorithms and enabling technologies within an object-oriented software framework for the solution of large-scale, complex multi-physics engineering and scientific problems.

12/14 Read the article

PASC19 Conference

The Platform for Advanced Scientific Computing held its sixth annual interdisciplinary conference in scientific computing and computational science, PASC19, June 12–14 in Zurich. Taking place at the campus of ETH Zurich, the conference set a new PASC attendance record with 428 scientists, industry representatives and experts. The trend toward wider diversity in attendees, something that the PASC conference has strived for since its beginning in 2014, continued to grow with PASC19, as nearly 60 percent of attendees travelled from outside of Switzerland to take part in this expansive scientific computing event.

17/19

CSCS booth at ISC19

Like every year, CSCS and the Swiss HPC community were present at the High Performance Computing Conference and Exhibition, ISC19, in Frankfurt, Germany. Attendees discovered the latest news about CSCS and HPC in Switzerland while enjoying a cup of coffee and some world-famous Swiss chocolate.

19 Read the article

Team RACKlette Earns Success at ISC-HPCAC Student Cluster Competition

ETH Zurich's Team RACKlette participated for the first time in the 2019 ISC-HPCAC Student Cluster Competition. The competition is designed to introduce the next generation of students to the high-performance computing community, and it draws teams of undergraduate students from around the world. RACKlette was very successful, winning the Linpack award for the most performant run and third place overall out of the 14 selected teams from all over the world participating in the competition that took place during ISC19.

14

Information event on Swiss participation in EuroHPC

The goal of this event, jointly organized by the State Secretariat for Education, Research and Innovation (SERI), Euresearch and CSCS, was to inform about Swiss participation in the EuroHPC Joint Undertaking (JU) — a legal and funding entity that aims to enable pooling of EU and national resources in high performance computing (HPC) to develop a pan-European supercomputing infrastructure and to support research and innovation activities.

July

02 / 04 Watch the videos

Workshop on high-performance computing with Python

A three-day course with lectures and hands-on sessions was offered to show how the programming language Python can be used on parallel computer architectures and how to optimize critical parts of the kernel using various tools.

15 / 25

CSCS-USI Summer School 2019

The CSCS-USI Summer School took place at the Steger Center for International Scholarship in Riva San Vitale. The selected 20 participants, from Switzerland and abroad, were comprised of undergraduate students, Ph.D. students, and postdocs interested in learning more about high-performance, data analytics and parallel GPU computing.

August

08 Read the article

Extension of CSCS home page with "social wall"

A "social wall" was added to the home page of www.cscs.ch, to aggregate the feeds of the social channels. At the same time, several small improvements in the layout were implemented to make reading more pleasant.

September

09 Read the article

User Lab Day 2019

The User Engagement & Support team welcomed more than a hundred of their current and possible future users to Lucerne. The day consisted of a Mars-themed scientific keynote from ETH Professor Domenico Giardini, parallel workshop sessions and staff presentations, open discussions with the participants, plus an up-close look at current computing nodes used on the flagship supercomputer "Piz Daint".

25/26 Watch the videos

Workshop on advanced scientific visualization with ParaView

A two-day course was organized for scientists with a strong interest in efficient visualization of 3D data. The focus for the attendees was to learn how to utilise ParaView, an open-source multiple-platform application for interactive, scientific visualization.

30/04

EuroHack19: GPU programming hackathon

The fifth GPU-programming hackathon took place at the Hotel De La Paix in Lugano. EuroHack19 engaged a total of nine teams from Switzerland and around the world for a total of 28 participants. With the support of expert mentors, the hackathon was designed to help researchers port their codes to a hybrid supercomputing environment with GPU.

October

01

24.7 Mio. node hours distributed in the User Lab and PRACE Tier-0 calls

24.7 Mio. node hours were distributed in the final two calls of 2019, the User Lab Call and PRACE Tier-0 Call 19, for the allocation period starting on October 1, 2019 and continuing until September 30, 2020.

07/08 Read the article

Hosting of the 74th HPC User Forum

A group of about 50 high-performance computing specialists and industry experts gathered for the 74th HPC User Forum, sponsored by AMD, Cray, Intel, and Panasas, at the Hotel De la Paix in Lugano. CSCS served as host of the event in the home city of “Piz Daint”.

29 Read the article

Monte Leone shutdown

After five years of successful computing, “Monte Leone” was retired as a production cluster. Monte Leone was the first general purpose diskless cluster to be put into production operations at CSCS. The system also provided the capability of computing on large memory nodes, as a portion of the cluster was configured with 768GB of RAM. The cluster was designed to handle large memory computing needs for the User Lab as well as meet the production computing requirements for a commercial customer. The nodes have found a new life as computing resources in the CSCS Infrastructure as a Service (IaaS) at the Pollux facility.

November

11/13

Workshop on high-performance computing with Python

Due to the very high demand and long waiting list, the three-day workshop on HPC with the programming language Python was offered a second time to 25 new participants, indicating that Python is increasingly used in high-performance computing projects. The goal was to show how the language can be used as a high-level interface to existing HPC applications and libraries, as an embedded interpreter or directly.

18 / 21 Read the article

CSCS at Supercomputing Conference 2019

CSCS and the Swiss HPC community had a brand-new booth at the world's largest supercomputing conference, SC19 in Denver, Colorado, where in a friendly and inviting environment visitors had the opportunity to ask about the latest HPC developments in Switzerland and to have open discussions with the Swiss technical staff attending the conference.

21 Read the article

Gordon Bell Prize awarded to two research groups at ETH Zurich

At SC19 in Denver, the prestigious Gordon Bell Prize by the Association for Computing Machinery was awarded to two research groups at ETH Zurich: The groups of professors Torsten Hoefler, head of the Scalable Parallel Computing Laboratory, and Mathieu Luisier, head of the Integrated Systems Laboratory. Their optimized application will allow a more efficient use of "Piz Daint" for scientific output.

28 Read the article

Extension of the account and resource management tool

The web-based portal to let users manage their accounts and projects was enhanced with new features. Improvements help users to visualize the daily resource utilization of each project in a user-friendly interface and to download such data.

December

03 / 05

Container hackathon for modellers

CSCS organized the first Container Hackathon for Modellers as part of the EsiWACE-2 project effort. Seven teams from all over Europe with a total of 15 participants were working hard for three intense days to containerize their applications with the help of CSCS expert mentors. After the three days, some of the teams applied with a small development project to continue and complete their work of containerization on the CSCS system, "Piz Daint".

05 Read the article Watch the video

Winner of the 2019 APS/DFD Gallery of Fluid Motion Award

A team of ETH-professor Petros Koumoutsakos, chair of computational science at ETH Zurich, and CSCS visualization expert Jean Favre received the 2019 APS/DFD Gallery of Fluid Motion Award. This recognition was announced at the 72nd Annual Meeting of the American Physical Society, the Division of Fluid Dynamics, held in Seattle, Washington from November 23–26, 2019.

Jérôme Tissières – Network & Security Engineer, HPC Operations

Nationality	Swiss
Working at CSCS since	February 2019
Background	1989-1993 Federal diploma of vocational education and training in Electronics, École des métiers, Lausanne 1995-1995 IT infrastructure manager and Novell Supervisor specialization, Écoles des Arches, Lausanne 1995-2008 Network engineer and peering manager at different service providers, Vaud 2008-2010 Senior network and security engineer at IMD Business School, Lausanne 2011-2014 Head of network engineering & operations at Ticinocom SA, Locarno 2014-2019 Senior network systems engineer at Swisscom, Bellinzona
Specialised in	As a network and security engineer, I am sharing my time between network operations and engineering projects. Network operations are the daily activities performed to monitor and manage the CSCS high-speed datacentre network and to analyse and respond to alerts on security, availability or performance issues on the network. Network engineering includes medium- to long-term projects related to the network expansion and evolution, hardware, software or technology assessment and testing, implementation of new clusters, and much more.
Working at CSCS means to me	To be part of an organization that aims to support research and science at a national and international level is very important to me.
What I like most about my work	Working at the cutting edge of information technology and having to learn constantly is a daily challenge, but above all a pleasure. The conviviality and dynamism of working in a human-sized structure like CSCS, where everyone takes responsibility and where trust is essential, is also very pleasant.
What challenges me at my work	Constantly learning to keep up with the rapid development of technology is an important but exciting challenge. Constant learning is the key in the IT field, and network engineers are life-long learners.

Heidi Oggian-Wittwer – Finance and Travel Officer, Business Services

Nationality	Swiss
Working at CSCS since	March 2005
Background	1974-1978 Swiss Federal Commercial Diploma, Basel 1978-1983 Hotel receptionist, Ticino 1983-1990 HR, Finances and Administration officer, Ticino 1990-2005 Maternity leave
Specialised in	After earning my degree, I have been working in different departments of secondary and tertiary sectors of the economy and so became an administrative allrounder. For the past 15 years at CSCS, I have been responsible for the arrangement and cost control of business trips for invited speakers, VIP guests and CSCS staff. When I started this job, the staff consisted of approx. 50 people, whereas today we are more than double the number, spread over three different locations.
Working at CSCS means to me	My aim is to make travelling for CSCS guests and staff something they do not have to think about so they can focus completely on the mission of their trips. It means I must put myself in the travellers' situation and secure the right arrangement for every single case and person.
What I like most about my work	The autonomy is appreciated, and the direct contact with our visitors from around the world and with my collegues is fascinating and makes my work interesting and varied. I enjoy the multicultural surroundings and the exchange in different languages as I find travel solutions that respect the needs of the traveller as well as the ETH regulations. Processing expenses and cost monitoring make the job comprehensive and exciting.
What challenges me at my work	There are tricky situations where good solutions are not easy to find. I must always be aware that even a small mistake can have really annoying consequences for the person who is travelling somewhere in the world. It is inherently demanding, but the real challenge has become finding environmentally friendly travel solutions to keep the carbon footprint as low as possible.

CSCS training program – Keeping pace with the fast-changing world of supercomputing

CSCS has been offering a diverse training program for several years now that helps our community to learn about evolving technologies, new tools, and new architectures. Courses cover many topics of relevance to High-Performance Computing and Data Science and prepare the user to make best use of all CSCS resources.

The CSCS training program is targeting the users of CSCS, helping them with all aspects of high-performance computing, but it is open to other researchers as well. It includes short webinars, one- and multi-day courses at CSCS in Lugano and even an annual summer school.

In 2019 we have had six 2- and 3-day courses covering topics from *HPC with Python or Advanced Programming (C++)* to data science tools *(distributed tensor flow)*. The 10-day summer school, held in collaboration with the Università della Svizzera italiana (USI), has focused on GPU and parallel programming (CUDA, OpenACC, MPI) as well as machine learning. Two "Hackathons" have been held, one about porting applications to GPUs and another one about the use of containers in climate research applications.

Visualization is another cornerstone in the training program. It has traditionally played an important role at CSCS, in no small part due to having Jean Favre in our team, a well-known expert in the field. Visualization is important to analyze and present results of complex simulations; in many cases it conveys an understanding otherwise unachievable. As computational science enters the era of "big data", visualization will inevitably become even more indispensable. Our collaboration with Professor Koumoutsakos (ETH Zurich) and his team is just one example that demonstrates the high level of expertise available at CSCS: Jean Favre's video of the simulation has won the prestigious APS/DFD 2019 Gallery Fluid Motion Award.

Resources allocated in 2019

Usage statistics shows that Chemistry & Materials remains the best-represented field at CSCS, using 38% of the available resources. Physics follows with 26% of the total allocation, Earth & Environmental Science and Life Science with 13% each.

ETH Zurich is the largest user (22%) among institutions, followed by EPF Lausanne (15%), and the Universities of Zurich, Bern, Basel, and Geneva (15, 5, 4, 3%). International utilization remains high at about 30%. User Lab Calls are still the primary path to resource allocation for domestic research institutions, but the major part of international allocation has been granted in PRACE Tier-0 calls.

List of PRACE Tier-0 Projects

Principal Investigator	Organisation	Research Field	Project Title	Node h
Christoph Schär	ETH Zurich	Earth & Environ. Science	Convection-resolving climate on GPUs (gpuCLIMATE)	1 400 000
Massimiliano Bonoli	Institut Pasteur Paris	Chemistry & Materials	DynPil - Functional dynamics of the bacterial type-IV pilus and type-2 secretion system pseudopilus	1 370 000
Gabriele Tocci	University of Zurich	Chemistry & Materials	Ab-initio molecular dynamics for nanoscale osmotic energy conversion	1 200 000
Modesto Orozco	Institute for Research in Biomedicine Barcelona	Life Science	Dynamics of the spliceosome bound to anti-cancer agents	1 176 500
Gabriel Wlazlowski	University of Warsaw	Physics	Investigation of quantum turbulence in strongly interacting Fermi systems	1 162 000
Carlos Martins	University of Porto	Physics	Abelian-Higgs cosmic strings: Network evolution	1 000 000
Szabolcs Borsanyi	University of Wuppertal	Physics	Fluctuations of conserved charges on the cross-over line	1 000 000
Constantia Alexandrou	University of Cyprus & Cyprus Institute	Physics	NPiTwist – The Nπ system using twisted mass fermions at the physical point	1 000 000
Andrew Hung	Royal Melbourne Institute of Technology University	Life Science	Developing new treatments for chronic and inflammatory pain	912 000
Jorge Viera	Technical University of Lisbon	Physics	OptiMom - Optical angular momentum in laser-matter interactions at ultra-high intensities	882 400
Olaf Kaczmarek	University of Bielefeld	Physics	Chiral flavor symmetry and axial U(1) symmetry restoration in (2+1)-flavor QCD	800 000
Andrei Ruban	Royal Institute of Technology in Stockholm	Chemistry & Materials	AMCVD - Ab-initio modelling of chemical vapor deposition for efficient computational design of new advanced coatings	794 120
Fabrizio Petrucci	University Pierre and Marie Curie Paris	Chemistry & Materials	IcePATH - Ice nucleation pathways, thermodynamics and kinetics	647 000
Marco D'Abramo	University of Rome "La Sapienza"	Life Science	TCR_MD - Towards a molecular understanding of the T-Cell receptor dynamical behavior	500 000
Andrei Mesinger	Scuola Normale Superiore di Pisa	Physics	AIfor21CM - Artificial intelligence for 21-cm cosmology	294 120

Largest Projects (> 700 000 Node h)

Principal Investigator	Organisation	Research Field	Project Title	Node h
Petros Koumoutsakos	ETH Zurich	Mechanics & Engineering	Modeling, sensing and control of turbulent flows	2 090 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	Ab-initio exploration of novel 2D materials for logic switch applications and beyond	913 000
Nicola Spaldin	ETH Zurich	Chemistry & Materials	Coupled and competing instabilities in complex oxides	900 000
Andrew Jackson	ETH Zurich	Earth & Environ. Science	Self-excited dynamo action in planets	864 000
Stefan Goedecker	University of Basel	Chemistry & Materials	Structure and dynamics of solids, interfaces and clusters	863 000
Nicola Marzari	EPF Lausanne	Chemistry & Materials	Mapping the structures and properties of all bulk forming binary systems: A high-throughput study	804 000
David Leutwyler	Max Planck Institute for Meteorlogy Hamburg	Earth & Environ. Science	Self-aggregation of deep convection at kilometer-scale resolution	800 000
Sandra Luber	University of Zurich	Chemistry & Materials	Advancing biomimetic water oxidation catalysis via novel Co(II)-based cubanes	800 000
Daniele Passerone	Empa	Chemistry & Materials	Proving regio- and enantioselectivity on PdGa surfaces: The Huisgen reaction	724 000
Urse Wenger	University of Bern	Physics	Flavour singlet physics from lattice QCD at the physical point	714 000
Andreas Fichtner	ETH Zurich	Earth & Environ. Science	Auto-updating full-waveform inversion	700 000
Jose Abdenago Livas-Flores	University of Basel	Chemistry & Materials	Computational evaluation of prospective high-performance p-type transparent conductors	700 000
Jürg Hutter	University of Zurich	Chemistry & Materials	Molecules at interfaces from density functional theory	700 000


D6
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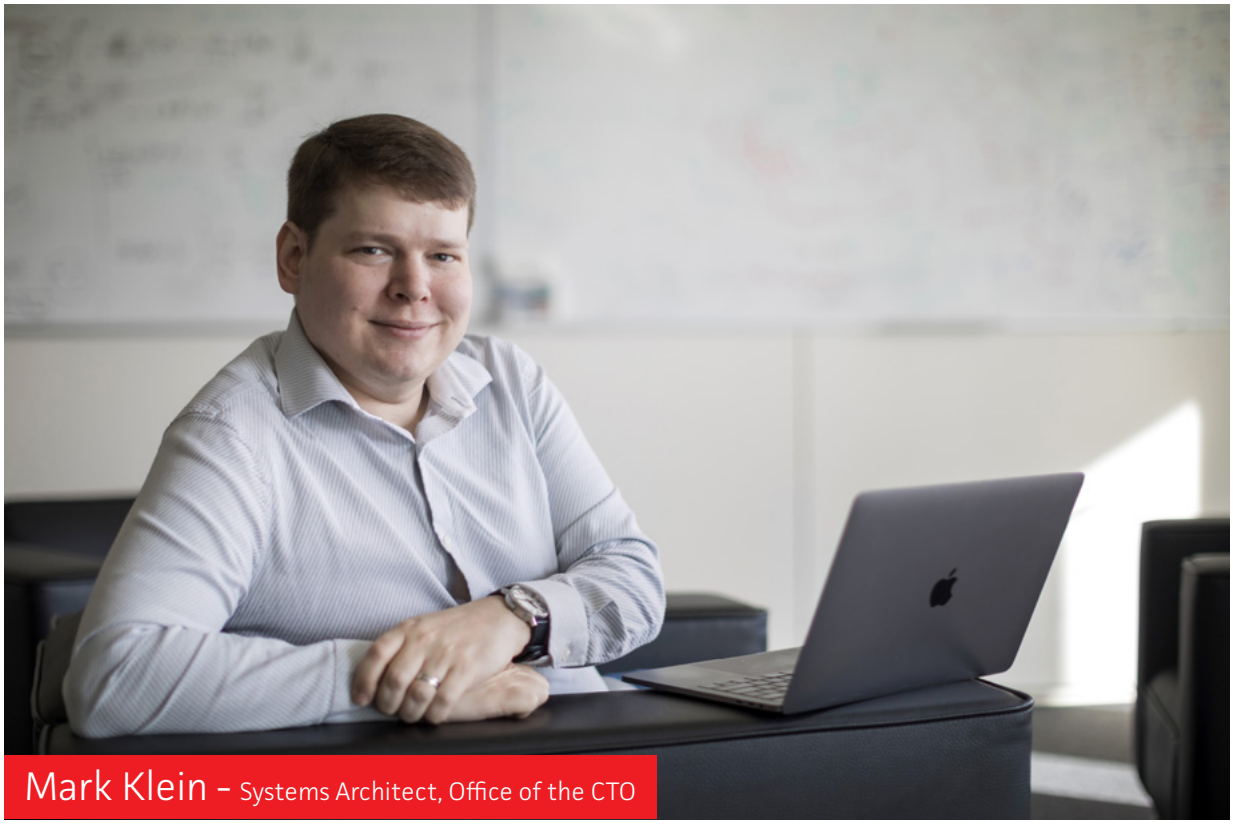
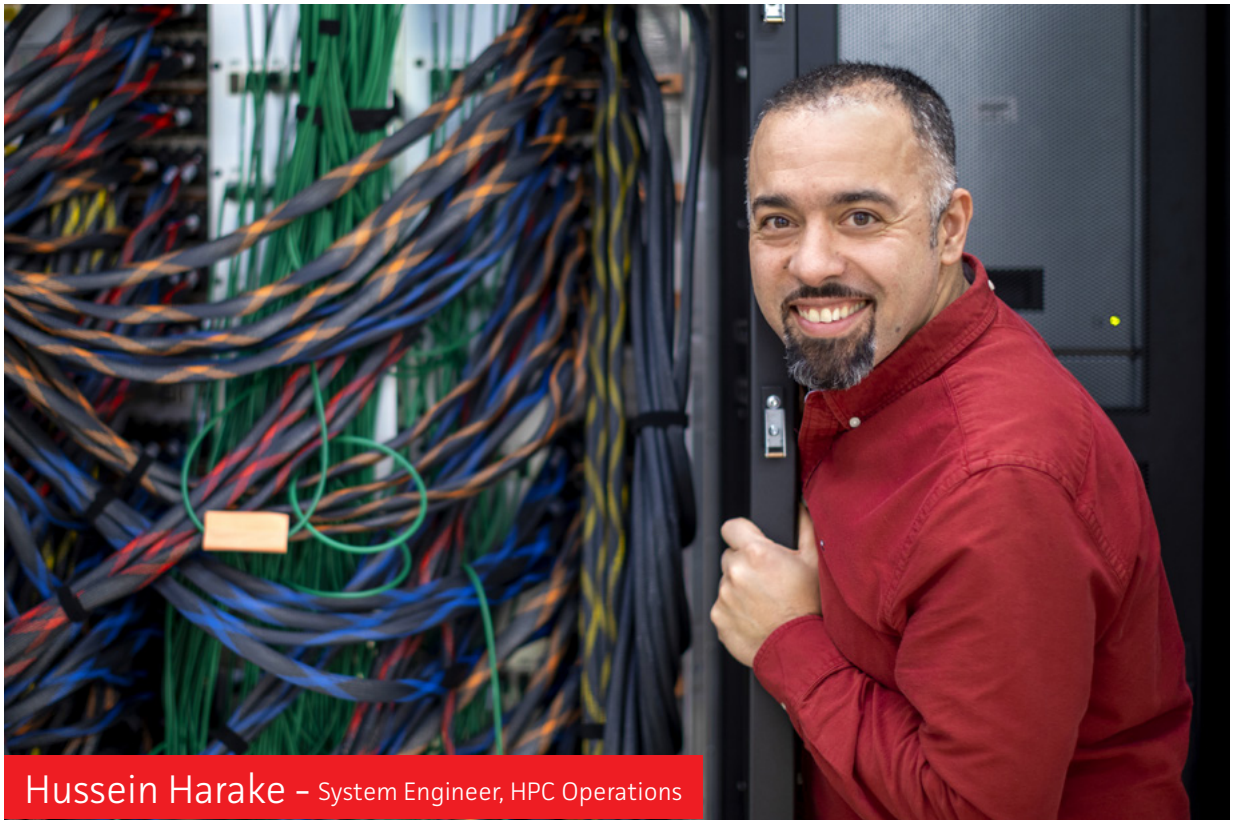
C3



Mark Klein – Systems Architect, Office of the CTO

Nationality	USA
Working at CSCS since	January 2015
Background	2001-2005 Bachelor of Science in Computer Engineering, Iowa State University, USA 2005-2012 Systems Support Specialist, Ames Laboratory, USA 2012-2015 Systems Engineer, National Center for Supercomputing Applications, USA
Specialised in	In the office of the CTO, I oversee many projects relating to the infrastructure of CSCS. This involves interacting with the many groups at CSCS to coordinate efforts towards the overall strategic goals defined by our Director. As a Systems Architect, I design new HPC systems to meet the needs of our customers and partners. This includes running a hardware testbed platform to try out new ideas, as well as constantly staying up to date with the latest technologies and software service offerings in order for CSCS to remain competitive.
Working at CSCS means to me	It means being on the cutting edge of HPC: coming up with new solutions using technologies and ideas that haven't been fully perfected yet, and then figuring out how to integrate these to best support our scientific users' needs.
What I like most about my work	I like that there isn't really a typical day for me, and there are always new things to learn and new technologies to explore. I also really enjoy taking part in world-wide collaborations between other leading HPC centers and vendors to develop new ideas and see how others are tackling similar problems.
What challenges me at my work	Trying to plan years ahead into the future in a rapidly changing landscape can be difficult and sometimes frustrating when roadmaps change unexpectedly, and I have to be able to adapt rapidly as releases get closer. Also, keeping current production needs met while exploring future solutions is a delicate balance, which means that I can't always investigate everything that looks interesting.



Hussein Harake – System Engineer, HPC Operations

Nationality	Swiss and Lebanese
Working at CSCS since	April 2001
Background	1993-1996 Interior design degree, Amlieh Technical School, Lebanon 1996-1998 Technical IT support specialist, EHGT, Lebanon 1998-2000 Owner of TopNetwork, Lebanon Since 2016 Bachelor in Computer Science, Open University, UK
Specialised in	As system engineering, I am specialized in managing and implementing HPC system. Recently I joined the Infrastructure & Development Services group, and my main focus is to bring new technologies to the centre, evaluate it, and bring to production.
Working at CSCS means to me	CSCS is the place where I consolidated and grew my carrier. After 19 years of working at CSCS, I still find it to be a very interesting place. It gives me the opportunity to work on cutting-edge technology and outstanding projects.
What I like most about my work	I like getting my hands on the newest technology and trying to bring new solutions that have never been implemented at CSCS.
What challenges me at my work	Every project is a challenge, and we never repeat ourselves. We must stay up-to-date on every change in the industry and try to bring it to CSCS if it fits with our strategy. It is challenging to constantly keep learning; however, we celebrate the completion and delivery of every successful project.

List of Projects by Institution

EAWAG

SPUX - Scalable high-performance uncertainty quantification for stochastic models in environmental data sciences, Jonas Sukys (Computer Science, 36 000 node h)

Empa

Characterization of on-surface reactions in the fabrication of atomically precise nanographenes with non-hexagonal rings, Carlo Antonio Pignedoli (Chemistry & Materials, 631 000 node h)

EPF Lausanne

Energy-efficient molecular sieving by two-dimensional nanoporous materials, Kumar Varoon Agrawal (Chemistry & Materials, 200 000 node h)

The accuracy and validity of flux-tube gyrokinetic simulations with GENE, Justin Ball (Physics, 300 000 node h)

Exploring the phase diagram of ice from first principles, Bingqing Cheng (Chemistry & Materials, 80 000 node h)

Template-free design of epitope-scaffolds for influenza, Bruno Correia (Life Science 500 000 node h)

Effect of post-translational modifications and polyglutamine expansions on the conformational landscape of Huntingtin's disordered N-terminus, Matteo Dal Peraro (Life Science, 340 000 node h)

NMR crystallography beyond static structures, Edgar Engel (Chemistry & Materials, 600 000 node h)

Performance testing of the EPFL OpenFOAM-based solvers for nuclear reactor analysis, Carlo Fiorina (Mechanics & Engineering, 17 500 node h)

Fusion plasma heating via suprathermal ions in tokamaks and stellarators: Unconventional schemes and plasma regimes, Jonathan Graves (Physics, 129 500 node h)

Deep learning for understanding clouds and precipitation, Jussi Leinonen (Earth & Environmental Science, 10 000 node h)

Surface and subsurface evolution of metals in three-body wear conditions, Jean-François Molinari (Chemistry & Materials, 520 000 node h)

Towards lead-free and stable solar cells, Ursula Röthlisberger (Chemistry & Materials, 600 000 node h)

Molecular dynamics simulations of biological systems: From molecular mechanisms to medicinal chemistry, Ursula Röthlisberger (Life Science, 500 000 node h)

Non-local turbulent transport with ORB5, Laurent Villard (Physics, 600 000 node h)

ETH Zurich

Full-waveform inversion for breast cancer detection with ultrasound computed tomography, Christian Böhm (Life Science, 67 000 node h)

Hunting for gravitational waves – Implementation of seismological machine learning tools for gravitational waves detection, Filippo Broggini (Earth & Environmental Science, 50 000 node h)

Advanced magnetotelluric imaging of volcanic high-enthalpy geothermal systems, Friedemann Samrock (Earth & Environmental Science, 60 000 node h)

Structure of bismuth ferrite surfaces and environmental interactions: A density functional theory study, Chiara Gattinoni (Chemistry & Materials, 160 000 node h)

General large batch methods for scalable and accurate neural network training, Torsten Hoefler (Computer Science, 36 000 node h)

Hypersonic flows with the Lattice Boltzmann method, Ilya Karlin (Mechanics & Engineering, 100 000 node h)

High throughput micro-fluidics, Petros Koumoutsakos (Mechanics & Engineering, 150 000 node h)

Membraneless electrochemical reactors, Petros Koumoutsakos (Mechanics & Engineering, 380 000 node h)

The impact of aerosols, feedbacks and variability on climate, Ulrike Lohmann (Earth & Environmental Science, 500 000 node h)

2-D memristors: Identifying their switching mechanism and designing efficient devices with ab-initio simulations, Mathieu Luisier (Chemistry & Materials, 396 000 node h)

Computing statistical solutions of three-dimensional compressible fluid flows, Siddhartha Mishra (Computer Science, 200 000 node h)

Numerical simulations for understanding the role of dynamical weather systems in shaping the atmospheric water cycle across latitudes, Lukas Papritz (Earth & Environmental Science, 35 000 node h)

Can neural networks derive quantum theory?, Renato Renner (Physics, 4 000 node h)

3D, GPU-accelerated modelling of mantle convection and lithospheric dynamics, Paul Tackley (Earth & Environmental Science, 300 000 node h)

3D Seismic wave simulations for the Mars InSight mission, Martin van Driel (Earth & Environmental Science, 100 000 node h)

JUNO-IZUMO interaction during gamete fusion: Towards understanding the role of forces in the initial phase of fertilization, Viola Vogel (Life Science, 100 000 node h)

Molecular dynamics simulations of glycoproteins, Gregor Weiss (Life Science, 36 000 node h)

Li ion dynamics in LiFePO4 nanocrystals and nanocrystal interfaces, Vanessa Wood (Chemistry & Materials, 136 000 node h)

Friedrich-Alexander University of Erlangen-Nuremberg

Benchmarking a generated phase-field code for simulation of ternary eutectic solidification, Harald Köstler (Chemistry & Materials, 12 000 node h)

IDSIA

Learning learning algorithms, Jürgen Schmidhuber (Computer Science, 150 000 node h)

Imperial College London

On the unsteady 3D physics of industrially relevant turbulent flows, Giorgio Giangaspero (Mechanics & Engineering, 400 000 node h)

Paul Scherrer Institute

Study of deterministic neutron transport solver nTRACER and Monte-Carlo code SERPENT on the basis of the VVER core, Mathieu Hursin (Mechanics & Engineering, 12 000 node h)

Property-driven sampling of the configurational space of supported catalytically active Pt particles, Dennis Palagin (Chemistry & Materials, 100 000 node h)

Physical Meteorological Observatory Davos / World Radiation Centre

Past and future of the Ozone Layer Evolution (POLE), Eugene Rozanov (Earth & Environmental Science, 100 000 node h)

Stanford University

Scaling the Legion programming system, Alex Aiken (Computer Science, 65 000 node h)

SUPSI

MEMbrane destabilizatiOn mechanism dRIven by the prEsence of AB fibrilS (MEMORIES), Mario Agostino Deriu (Life Science, 35 000 node h)

Molecular modeling of fuel-driven supra-molecular self assembly, Giovanni Maria Pavan (Chemistry & Materials, 282 000 node h)

Università della Svizzera italiana

Funnel-metadynamics calculations to unravel the binding of agonists and antagonists of the adenosine*A*2AG protein-coupled receptor, Vittorio Limongelli (Life Science, 36 000 node h)

Understanding iron surface morphology in presence of adsorbed nitrogen, Giovanni Maria Piccini (Chemistry & Materials, 100 000 node h)

Cell biomechanics in flow: Parallel simulations, Igor Pivkin (Life Science, 150 000 node h)

An ab-initio-metadynamics study of methyl acrylic acid free-radical polymerization in water: Investigation of chain-length and protonation effects on propagation, Daniela Polino (Chemistry & materials, 150 000 node h)

University of Bern

Machine-learning the self-consistent and site-dependent DFT+U for large-scale atomistic simulations of transition metal oxides, Ulrich Aschauer (Chemistry & Materials, 300 000 node h)

Mechanistic understanding of dissolution-precipitation processes by pore-scale Lattice Boltzmann modelling and in-situ synchrotron based X-Ray tomography, Sergey Churakov (Earth & Environmental Science, 150 000 node h)

A Palaeoreanalysis to understand decadal climate variability (PALAEO-RA), Ralf Hand (Earth & Environmental Science, 210 000 node h)

ISOCARBON-II (Modelling ISOtopes of CARBON in the Earth System), Fortunat Joos (Earth & Environmental Science, 147 000 node h)

Calibration and performance tuning for the simulation of transitional blood flow past a bioprosthetic aortic valve, Dominik Obrist (Life Science, 12 000 node h)

High-resolution glacial climate conditions over the Alps (HicAp), Christoph Raible (Earth & Environmental Science, 212 000 node h)

Highest-resolution simulations of climate change and land use to project the impact on water resources and human well-being in Kenya, Thomas Stocker (Earth & Environmental Science, 123 000 node h)

University of Cyprus & Cyprus Institute

Precision nucleon structure using lattice QCD, Constantia Alexandrou (Physics, 500 000 node h)

University of Fribourg

Molecular insights on the mechanochemical activation of polymer brushes, Pablo Campomanes (Life Science, 150 000 node h)

Large-scale molecular modeling of lipid droplet biogenesis, Stefano Vanni (Life Science, 335 000 node h)

University of Geneva

Higher-order statistics in large-scale structure: Matter bispectrum covariance matrix and cosmological parameter constraints, Joyce Byun (Physics, 77 200 node h)

Digital blood on CPU/GPU parallel system, Bastien Chopard (Life Science, 100 000 node h)

Photoinduced spin crossover in iron(II) complexes in solution: Insights from ab-initio molecular dynamics studies, Latévi Max Lawson Daku (Chemistry & Materials, 200 000 node h)

Reliable ground state in novel magnetic 2D materials for spintronics and ICT applications, Marco Gibertini (Chemistry & Materials, 67 000 node h)

Effective field theory of dark energy simulations and computation of precision observables with gevolution, Martin Kunz (Physics, 400 000 node h)

Cosmological unequal-time correlators, Francesca Lepori (Physics, 40 000 node h)

Instrument Monte Carlo simulations for the DArk matter particle explorer (DAMPE), Andrii Tykhonov (Physics, 250 000 node h)

University of Lausanne

Identification of protonation events that drive activation of acid-sensing ion channels, Stephan Kellenberger (Life Science, 169 000 node h)

University of Melbourne

High-fidelity simulation of high-pressure turbine stages for model development using machine learning, Richard Sandberg (Mechanics & Engineering, 400 000 node h)

University of Rome 2

Electroosmotic flow in wild-type and mutated CgsG nanopore, Mauro Chinappi (Mechanics & Engineering, 252 000 node h)

University of Southern Denmark

Deciphering host recognition mechanisms of Zika and other Flaviviruses, Himanshu Khandelia (Life Science, 408 000 node h)

University of Zurich

The galactic fountain of youth: Gas accretion in Milky-Way halos with non-equilibrium metal cooling and chemistry, Robert Feldmann (Physics, 50 000 node h)

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

First principles simulations of aqueous metal interfaces, Marcella Iannuzzi (Chemistry & Materials, 300 000 node h)

GPU-based simulations of intermediate mass black holes (IMBHs) in merging dwarf galaxies: From the occurrence e of LISS gravitational wave sources to the nature of dark matter, Lucio Mayer (Physics, 600 000 node h)

Investigating the effects of phosphorylation and prolyl-isomerization on the dynamics and stability of intrinsically disordered protein complexes, Davide Mercadante (Chemistry & Materials, 100 000 node h)

Reduction of aqueous carbon dioxide by the hydrated electron from hybrid DFT and many-body electronic structure theory, Vladimir Rybkin (Chemistry & Materials, 200 000 node h)

Linear-scaling DFT for protein/ligand binding energy evaluation, Alisa Solovyeva (Life Science, 80 000 node h)

ZHAW

Study of laminar separation bubbles, Marcello Righi (Mechanics & Engineering, 30 000 node h)

Weizmann Institute of Science

Tubulin post-translational modifications: The effect on tubulin tail dynamics and interactions, Yaakov Levy (Life Science, 500 000 node h)

Renewals

Empa

Forward and inverse modelling of greenhouse gases, Dominik Brunner (Earth & Environmental Science, 94 000 node h)

EPF Lausanne

Exploring very-large-scale motions in turbulent boundary-layer flows by direct and large-Eddy simulation, Jiannong Fang (Mechanics & Engineering, 100 000 node h)

Materials for energy, Nicola Marzari (Chemistry & Materials, 600 000 node h)

Novel topological phases of materials, Oleg Yazyev (Chemistry & Materials, 100 000 node h)

Atomic scale processes at solid-water interfaces, Alfredo Pasquarello (Chemistry & Materials, 430 000 node h)

Simulation of plasma turbulence in the periphery of tokamak devices, Paolo Ricci (Physics, 510 000 node h)

ETH Zurich

Multiphase fluid flow, evaporation and crystallization in deforming porous materials, Jan Carmeliet (Mechanics & Engineering, 105 000 node h)

Land-climate feedbacks in a changing climate, Edouard L. Davin (Earth & Environmental Science, 228 000 node h)

General large batch methods for scalable and accurate neural network training, Torsten Hoefler (Computer Science, 120 000 node h)

Cloud cavitation collapse in turbulent flows, Petros Koumoutsakos (Mechanics & Engineering, 320 000 node h)

Multiscale in-silico modelling of bone mechanoregulation: From molecule to cell, tissue and organ, Harry van Lenthe (Life Science, 40 000 node h)

Università della Svizzera italiana

Atrial fibrillation in-silico study, Simone Pezzuto (Life Science, 150 000 node h)

University of Basel

Atomization energies from ab-initio calculations without empirical corrections, Dirk Bakowies (Chemistry & Materials, 240 000 node h)

Effects of complex liquid environments on material properties, Giuseppe Fisicaro (Chemistry & Materials, 400 000 node h)

University of Bern

Modelling extreme events in multiple ocean ecosystem stressors (M-OceanX), Thomas Frölicher (Earth & Environmental Science, 100 000 node h)

Pleistocene climate variability – Complex modeling of the Earth system, Christoph Raible (Earth & Environmental Science, 300 000 node h)

University of Geneva

Electronic, magnetic, and structural properties of complex oxides: Vanadates, iridates, and cuprates, Antoine Georges (Chemistry & Materials, 450 000 node h)

University of Zurich

Advancing electronic structure calculations for complex nature-inspired systems, Sandra Luber (Chemistry & Materials, 610 000 node h)

Advancing understanding and design of photosensitizers for artificial water-splitting, Sandra Luber (Chemistry & Materials, 117 800 node h)

SLF

Simulations of drifting and blowing snow over East Antarctica using the Weather Research and Forecasting (WRF) model, Michael Lehning (Earth & Environmental Science, 120 000 node h)


DELL

Computationally designed materials show potential for carbon capture

The German Boxberg lignite-fired power plant. (Image: Torsten Kellermann on Unsplash)

"Flue gas" refers to any gas coming out of type of a pipe, exhaust, or chimney as a product of combustion. However, the term is more commonly used to describe the exhaust vapours exiting the flues of factories and powerplants. These flue gases contain significant amounts of carbon dioxide (CO_2), which is a major greenhouse gas contributing to global warming. Carbon capture and storage is one of the technologies that can mitigate current CO_2 emission: The greenhouse gas carbon dioxide is captured directly from the atmosphere or at its point of origin — for example, at coal-fired power plants. Technical processes and special CO_2-adsorbing materials are methods used to do this, with the aim of slowing down the increase of CO_2 in the atmosphere and thus counteracting global warming.

Materials that seem particularly suitable for this purpose are so-called metal-organic-frameworks (MOFs). However, MOFs that have been optimized for this purpose so far have shown a problem: The water in the flue gases competes with CO_2 for the same adsorption sites and thus reduces the efficiency of CO_2 capture. An international research team led by Berend Smit, professor at the Laboratory of Molecular Simulation of EPFL, has now scanned more than 300 000 MOFs to find suitable candidates that do not interact with water.

CSCS' "Piz Daint" was one of the supercomputers used in this screening study. In collaboration with experimental researchers, the team succeeded in synthesizing two of the promising MOFs. In their publication published in the scientific journal "Nature", the researchers emphasised that it will be necessary to test the performance of these MOFs in an industrial setting and consider the full capture process — including the targeted CO_2 sink, such as geological storage or serving as a carbon source for the chemical industry — in order to identify the optimal separation material.

Reference

Boyd, P at al.: Data-driven design of metal-organic frameworks for wet flue gas CO_2 capture, Nature (2019).

New software may help to unveil origin of our galaxy

Orbiting around Earth, the DAMPE satellite measures high-energy cosmic rays (illustration). The data is anticipated to reveal evidence of dark matter as well as knowledge of the origin of our galaxy. (Image: Video still, Purple Mountain Observatory, CAS, China)

Up to this day, cosmic particles tell the story of how the universe came into existence. Especially high-energy cosmic ray particles can reveal useful information; they originate from the most energetic processes in the universe, like the supernova explosions that generate all matter. But, it is difficult to measure the fractions of these highest-energy particles that carry information about our galaxy and partially from beyond it — meaning particles with an energy in the tera electron Volt (TeV=10^{12} eV) magnitude and higher. Those particles are rare, and their detection in space has been limited due to constraints in weight and size of the detectors. In addition, scientists have to rely on detector simulations to understand the data. Such simulations calculate the decomposition pattern and spectra of particle samples colliding with the detector, thereby allowing differentiation between electrons, protons or gamma rays and making sense of the spectra itself.

Upon colliding with the detector, protons decompose into an avalanche of interactions, creating subatomic particles of variable energy. Unfortunately, the simulation software packages available to date could not handle particles above 10 TeV with reliable accuracy.

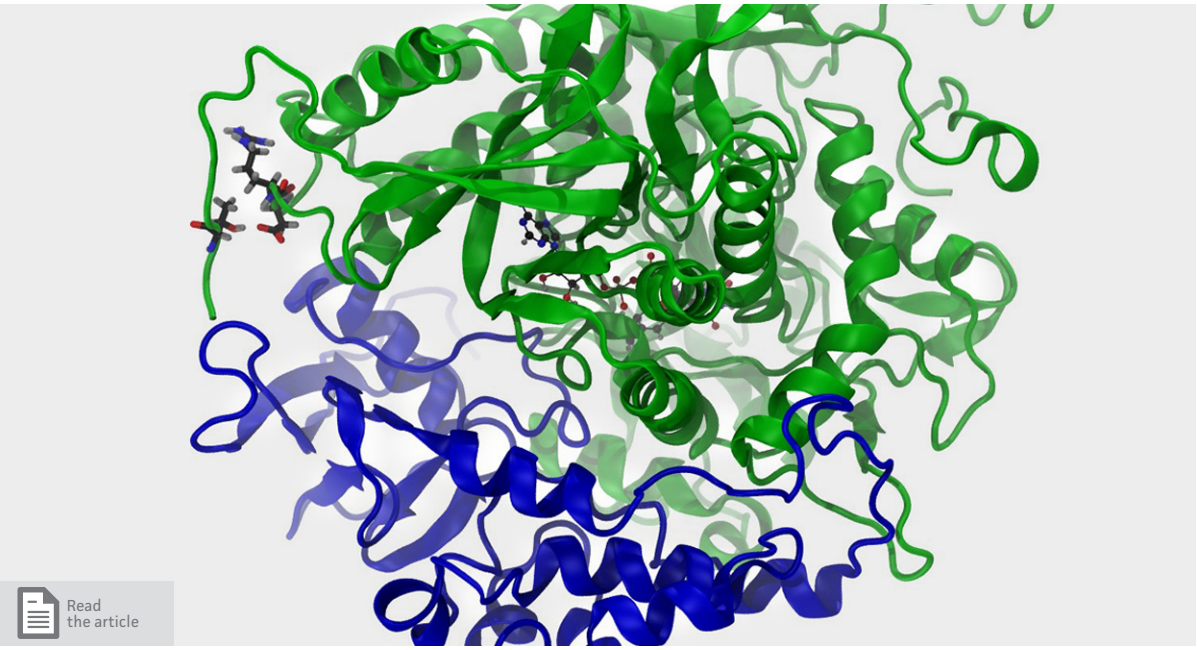
That's why Andrii Tykhonov, an astrophysicist at the University of Geneva, developed new software that allows precise measurement of high-energy cosmic ray protons above 100 TeV. To create a software capable of handling such high-energy proton interactions, Thykonov combined the algorithms of two existing software packages. Specifically, he implemented so-called event generators from the CRMC package into the widely-used Geant4 detector simulation tool kit via a dedicated interface. The scientist made extensive use of the "Piz Daint" supercomputer for feasibility tests, validation and preliminary simulations of high-energy proton data.

In the future, the new software will be used to interpret data collected by the Dark Matter Particle Explorer (DAMPE) satellite. Since December 2015, DAMPE has been orbiting around Earth measuring cosmic radiation with a much better energy resolution and energy reach than any other space experiment.

Reference

Tykhonov, A et al.: TeV-PeV hadronic simulations with DAMPE. Proceedings of Science (2019).

Researchers pinpoint how the immune system gets on the wrong track



How the mutation stabilizes the SDHA-SDHB interactions: Molecular representation of the mutated SDHA (green) and the SDHB (blue) complex, are shown in ribbons. A typical interaction between the mutated residue and adjacent residues in SDHA is highlighted (sticks). (Image: Olivier Bignucolo)

The intact human immune system is a perfect guard: it repels infections and cancer cells without harming the otherwise healthy organism. But, people with a defective immune system usually depend on medical help, like many patients with genetically-caused primary immunodeficiency disorders (PIDs). They suffer from a lack of antibodies, which are normally produced in so-called B cells. As a result, they are susceptible not just to infections, but also to autoimmune and autoinflammatory diseases.

Recently, a team of researchers led by Christoph Hess and Mike Recher, both professors at the University of Basel and the University Hospital of Basel, has succeeded in deciphering an essential molecular process in the B cells of a subgroup of affected patients, thus enabling tailored and more efficient treatment. The researchers found that in the cells of PID-patients, the mitochondria — which are the power plants of the cell — exhibit increased cellular respiration. They also found a mutation in the germ line of a key protein in the respiratory chain called SDHA.

In order to clarify the cause of this increased cellular respiration and the role of SDHA, the team used the supercomputer "Piz Daint" to visualize the molecular dynamics of SDHA in those cells. The simulations enable them to analyse the behaviour of ions, water and ligands together with the protein over time at the atomic level. In this way, the researchers were able to describe the atomic interactions caused by the SDHA mutations.

In practice, the simulations showed that the mutation of the protein SDHA enhances its interaction with the protein SDHB, thus augmenting the activity of the respiratory chain and driving accumulation of a certain salt. This in turn activates a signalling cascade leading to the production of so-called cytokines, which ultimately cause inflammatory reactions. On the basis of these results, the researchers proceeded to treat one patient with an antibody to specifically block cytokine as an inflammation mediator. As expected, this treatment reduced the inflammation — and the patient's condition improved. Decoding of such processes enables more targeted treatments and the production of drugs with fewer side effects.

Reference

Burgener, A et al.: SDHA gain-of-function engages inflammatory mitochondrial retrograde signaling via KEAP1–Nrf2. Nature Immunology (2019).

Transparent electronics research gains momentum

Transparent conductive materials have many futuristic applications, such as touchscreens. (Image: Dolphfyn, Shutterstock.com)

Transparent electronics are the future: they represent the merging of electronical and optical technologies, creating the possibility for devices with completely novel, even previously unimaginable properties. However, the technological development is still hampered by the comparatively low level of conductivity of certain transparent semiconductors. Luckily, conductivity can be optimised by making use of appropriate impurities in the material. The impurities can change the charge carrier density, thus increasing this property.

However, identifying suitable impurities, meaning elements from the periodic table to insert in a material's structure, often involves years of laboratory experimentation. Therefore, researchers of the institute of computational Physics at the University of Basel have been working on speeding up this process with computer simulations using the "Piz Daint" supercomputer at CSCS. The goal is to find the most promising impurity candidates as efficiently as possible.

When it comes to transparent conductors, there is a shortage of high-performance conductors known as P-Type, which stands for positively charged carriers — negatively charged carriers are conversely known as N-Type semiconductors.

Recently, the environmentally friendly and earth-abundant tin monoxide emerged as a promising material for transparent and high-performance P-Type conductors, but only a handful of elements have been examined that could be suitable as impurities for equipping the tin monoxide-based semiconductor with the desired properties.

Thanks to their calculations, the researchers have now been able to identify additional candidates that could be introduced into tin monoxide in order to enable high-performance and transparent P-Type semiconductors: five alkali metals — lithium, sodium, potassium, rubidium and caesium. In addition, the computations established 13 elements suitable for doping with N-Type semiconductors. If it is possible to incorporate these elements into tin monoxide and produce the desired semiconductor, the researchers are convinced that this will open up new paths for a whole range of transparent technologies.

Reference

Graužinytė, M et al.: Towards bipolar tin monoxide: Revealing unexplored dopants, Phys. Rev. Materials 2, (2018).

Papers with Highest Journal Impact Factor[1)]

Nature
Impact Factor: 43.07

P. G. Boyd, A. Chidambaram, E. García-Díez, C. P. Ireland, T. D. Daff, R. Bounds, A. Gładysiak, P. Schouwink, S. M. Moosavi, M. M. Maroto-Valer, J. A. Reimer, J. A. R. Navarro, T. K. Woo, S. Garcia, K. C. Stylianou, B. Smit, Data-driven design of metal–organic frameworks for wet flue gas CO_2 capture, Nature, DOI 10.1038/s41586-019-1798-7.

Nature Materials
Impact Factor: 38.87

A. Narayan, A. Cano, A.V. Balatsky, N. A. Spaldin, Multiferroic quantum criticality, Nature Materials, DOI 10.1038/s41563-018-0255-6.

Nature Nanotechnology
Impact Factor: 33.41

A. Avsar, A. Ciarrocchi, M. Pizzochero, D. Unuchek, O. V. Yazyev, A. Kis, Defect induced, layer-modulated magnetism in ultrathin metallic $PtSe_2$, Nature Nanotechnology, DOI 10.1038/s41565-019-0467-1.

Energy & Environmental Science
Impact Factor: 33.25

R. Wick-Joliat, T. Musso, R. R. Prabhakar, J. Löckinger, S. Siol, W. Cui, L. Sévery, T. Moehl, J. Suh, J. Hutter, M. Iannuzzi, S. D. Tilley, Stable and tunable phosphonic acid dipole layer for band edge engineering of photoelectrochemical and photovoltaic heterojunction devices, Energy & Environmental Science, DOI 10.1039/c9ee00748b.

S. M. H. Hashemi, P. Karnakov, P. Hadikhani, E. Chinello, S. Litvinov, C. Moser, P. Koumoutsakos, D. Psaltis, A versatile and membrane-less electrochemical reactor for the electrolysis of water and brine, Energy & Environmental Science, DOI 10.1039/C9EE00219G.

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Working at CSCS means to me	When I optimize the GPU backend of a linear algebra library, I know that this will allow scientists to run their simulations faster on "Piz Daint" and at other supercomputing facilities around the world. Knowing that my work has this type of impact is very rewarding. I take pride in writing software that is performant, portable and usable, because in doing so, I play a part in advancing scientific research.
What I like most about my work	I feel very fortunate that there are a lot of things I enjoy about my job at CSCS. I am lucky to be surrounded by incredibly friendly and knowledgeable colleagues on my team. I love that I learn new things almost every day, and that our working atmosphere is so cooperative and caring. Last but not least, developing and running code on a nearly daily basis on "Piz Daint", one of the largest supercomputers in the world, is thrilling.
What challenges me at my work	High-performance computing is an exciting and demanding field. I have to keep up with new architectures, new technologies, new libraries and new developments in software engineering in order to take full advantage of them in my work.

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Working at CSCS since	October 2016
Background	2009-2010 Lecturer, Universidade Federal de Pernambuco, Brazil 2010-2014 Doctor in Chemistry, Universidade Federal de Pernambuco, Brazil 2012-2013 PhD Exchange Program, The University of Utah, USA 2014-2016 Postdoctoral training, Laboratory of Physical Chemistry, ETH Zurich
Specialised in	As part of the User Enagagement and Support Unit, I work towards enabling our scientific community to make the best use of the HPC environment. On the support role I help the users with their needs and contribute to the scientific software stack management tools, to a monitoring tool, and to a framework for regression testing and continuous integration of HPC applications. I also work on a particle simulation library which will empower research on different scientific fields. Furthermore, I have been involved in outreach activities as hackathons, teaching, and leading seminars.
Working at CSCS means to me	To contribute to the scientific and HPC community on a global scale and engage in solving dynamic and interesting challenges, all while helping our users to best utilize the resources in order to run applications efficiently on one of the biggest supercomputer systems in the world.
What I like most about my work	I like its dynamic environment. I work in a multi-discipline, multi-cultural software engineering team that provides direct support and proposes solutions to our users' problems. The team is comprised of skilled individuals whose knowledge spans the whole software stack, from systems and computer architecture to scientific applications. There is no regular routine or programming language. One day I can help a user to setup a complex simulation workflow, then code an application in C++, then contribute to a Python-based project, and interact with scientists about their challenges. I like the possibility of digging deep into very complex scientific software while still being able to communicate and interact with people at different levels and help our users, so they can focus on the science while running optimally on our system.
What challenges me at my work	As a member of a production engineering team that monitors the end-user software performance in our systems, it is part of my responsibility to know when/how/what impacts the application's performance, work towards the understanding of the root causes, propose solutions and deploy automatic monitoring systems to alert potential incidents. Due to the number and variety of scientific software in our center and the complexity and scale of our machines, this is a big challenge. Furthermore, we also interact directly with the users. We see first-hand the challenges they face. So, we are always in pursuit of solutions that can empower them and allow efficient use of our resources, as well as make their interactions with the system and us easier.

Knowledge is Computing Power: A Conversation with the HPC Advisory Council Swiss Conference Organizers

The HPC-AI Advisory Council (HPCAIAC), along with the Swiss National Supercomputing Centre (CSCS) and the HPCXXL Board, just held its tenth annual high-performance computing conference April 1–4 in Lugano, Switzerland. The conference annually draws about 130 professionals to southern Switzerland to discuss the latest technology developments.

From left to right: Hussein Harake (CSCS), Gilad Shainer (HPC-AI Advisory Council) and Michele De Lorenzi (CSCS).

About ten years ago, two men who had never met before had an unexpected conversation in a hotel lobby during a Supercomputing conference. Hussein Harake was debating with a colleague the possibility of creating a 3D torus supercomputer topology with InfiniBand, when Gilad Shainer approached the colleagues. That chance meeting inspired Hussein and Gilad to not only become friends, but also to work toward organizing the first conference of the HPC-AI Advisory Council, a global organization dedicated to connecting high-performance computing (HPC) to both current and potential users, software designers, hardware manufacturers and numerous other experts on the leading edge of the HPC frontier, in Lugano.

Harake is currently a system engineer at CSCS, and Shainer currently serves as Senior Vice President of Marketing at Mellanox Technologies, a high-end multi-national supplier of computer networking products and sponsor of the HPC-AI Advisory Council. During the HPCAIAC Swiss conference held this April, Deputy Director of the Swiss National Supercomputing Centre Michele De Lorenzi interviewed the two men, asking them about their decade-old chance meeting; the motivation behind the HPC Advisory Council's conception; how the annual Swiss conference has evolved to address changes in the industry; and what the future of Exascale computing may have in store for both the organization as well as the wider community of HPC professionals and researchers around the world.

Can you tell me the story of why you started this conference?
Harake: Back in 2008, Gilad and I met by luck in a hotel at a supercomputing conference. It happened when a colleague and I were discussing whether we could build a high performance network based on 3D torus topology using InfiniBand, which was just becoming one of the main HPC networks on the market. My colleague said "no." Gilad was passing behind us and heard the question. He said, "I'm Gilad from Mellanox, might I be allowed to answer this question?" And then he described how we really can build a 3D torus topology using InfiniBand. Based on that, we got the idea: 'It is difficult for people to understand these things; we *can* really try to bring these ideas together and teach people, or exchange knowledge with people, about how we can build it and how we can make that possible.'

Shainer: So that was the idea behind establishing the HPC Advisory Council organization in 2008, to bridge the gap between technology and knowledge and to bring more knowledge to more people, by helping with HPC outreach and providing education to more people around the globe.

Harake: We liked the idea of contributing to such events as the workshop, since even we ourselves find that we are missing out on some HPC knowledge and information. We also wanted to bring our people at CSCS to a higher level of knowledge where they could build better supercomputers. We are happy to share our knowledge and learning with others, and to learn from what others bring to this event. It just creates an excellent opportunity for collaboration and sharing between all the academic institutes. That is in fact a key component of the event.

What was the goal for you in doing such an event in Switzerland, and what view of Switzerland did you have at that time?
Shainer: In Europe, the HPCAIAC organization was looking for a strong HPC entity who cared about bringing more education to more people, and actually extending the community of companies or academics that can utilize HPC, in order to do things that can't be done without HPC. Hussein and I had a good collaboration from the start, and we have enjoyed working together ever since. There is willingness on both sides. And Switzerland, I think, is a great European central location, close to multiple countries. And then if you add in the Swiss coffee and chocolate and Lugano… it's kind of a no-brainer.

Harake: There's no border that should block the sharing of knowledge, science and technology. As much as we can collaborate and share, we do. I think that's the way to go in an environment like CSCS or ETH Zurich, where academic sharing is a key component of what we are doing.

How are you celebrating the ten-year milestone for the HPC-AI Advisory Council Swiss Conference?
Shainer: We planned an evening event in one of the best places in Lugano: Monte Brè. That's one of the ways we are going to celebrate the 10 years. We picked this place, which sits at the top of the mountain and has an amazing view of the Gulf of Lugano. But really, we never find the time to celebrate, because there's always the next step to think about. We'll do the 11th and the 12th conference, it just doesn't stop here. So you can have a nice dinner and enjoy the 10-year mark, but from my perspective, that's not a major milestone. We want much more.

In what ways have the needs of the users and the user community you are serving changed over time? How has the technology addressing these needs changed, and how have you changed the contents of the conference over the years to adapt to the new needs?

Harake: When we started 10 years ago, the event in Lugano focused more on high-speed networks, and on the way to manage supercomputers' deployments and build and design HPC platforms. Over time, we expanded the topics covered to include computing architectures, storage technologies, applications and co-design, the use of deep learning, and more. Every year we add more things to the agenda, covering a lot of topics and different technologies, different applications, going from research to sys-admin to application support, to design and system architecture—all of this has been included. Of course, we keep looking out for the next big thing we can offer our community.

Shainer: Over time, technology changes. There are changes in compute elements or networking elements or storage elements or software frameworks; and then you start looking at how to bring deep learning into HPC, and so forth. The technologies are being enhanced or changed over the years, but the one goal of getting the maximum performance and the never-ending demand for high-performance is always there. And what we're doing here is looking at three different areas in the high-performance computing world: One area is the technology itself, what's new and how it's being evolved, and that's why we bring in vendors to discuss that, or other entities who develop the technology; we also have the framework people that actually create the bridge between applications and a technology, and how their software is being evolved over time; and then we have the users who build those infrastructures and run applications, and whose needs change over time. So if you have those three elements, and they come year after year and talk about evolving the technology, evolving the software interface, evolving applications, you keep yourself up-to-date—and you can even conduct discussions on technology before it hits the market, so people can start thinking about what's coming next.

Last year you started a corporation for a joint conference with the HPCXXL User group. Why did you start this, and why did you decide to extend this year's conference an extra day for HPCXXL guests?

Shainer: HPCXXL is a community of supercomputing centers that meet twice a year, once in in the US and once in Europe, and we thought that it would be beneficial for both sides to combine the effort, and have the supercomputing centers that are part of XXL come together to present as part of the HPC Advisory Council Swiss conference. I think both of us give and get from that combination. We have added one more day to this year's conference, dedicated to the specific private meetings of the HPCXXL group. We have gained a lot, as now there are more supercomputing centers that can participate and present different views. And then, those centers also gain not only by hearing more people talk about their needs, but also by learning about new technology and other things being developed in other places.

What will be the biggest challenges in HPC in the next years? How will the conference develop over the next 10 years?

Shainer: It's very hard to say where we are going to be in 10 years, because things change and change very fast. In the next few years, I think we are going to see the first Exascale system being built. So there is going to be a lot of focus around high-performance computing and AI, around building those large infrastructures that enable us to do things that we cannot do today. I believe there is going to be much more importance given to HPC over the next several years, and our mission is to make sure that everyone is working together, driving the leading edge of technology in its usage and building the next generation. That's what is going to keep us busy during the next 10 years and hopefully beyond that.

Harake: I think it will be important to remove the gap between HPC and the Cloud and try to accommodate all the users coming from these two communities, in an HPC machine like ours. So from a user point-of-view, that could be at least a short mission for us, trying to build a system that allows us to accommodate these two communities.

How do you view the relationship between the HPC-AI Advisory Council and CSCS?

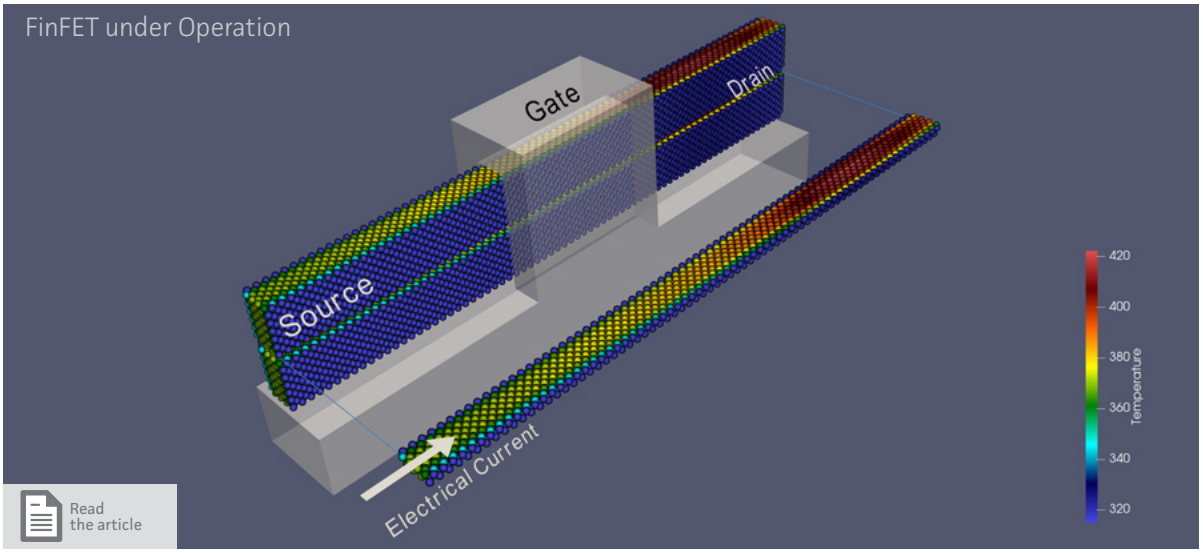
Shainer: CSCS is a leading supercomputing centre, not just in Europe, but worldwide. We're very fortunate to be able to collaborate with CSCS to facilitate the Swiss conferences year after year, and together, to be building the next generation of HPC professionals and researchers. I think there are more things we can be doing together in the future, and I'm looking forward to continue working with CSCS for years to come.

From left to right: Gilad Shainer (HPC-AI Advisory Council) and Hussein Harake (CSCS).

Harake: I would like to thank the HPC Advisory for everything they've done so far. It's really a great organization, a not-for-profit organization that has no business side. They are not biased for any technology, and they are happy to hear from everybody. So please join us at a future HPCAIAC and CSCS Swiss conference, and tell us how good you are in your technology and how good you are at optimizing and running applications!

A “simulation booster” for nanoelectronics wins Gordon Bell Prize

With help of CSCS-supercomputer “Piz Daint” two research groups from ETH Zurich have developed a method that can realistically, quickly and efficiently simulate nanoelectronics devices and their properties. This project earned the researchers the prestigious Gordon Bell Prize, awarded by the Association for Computing Machinery at Supercomputing ‘19 (SC19).



Self-heating in a so-called Fin field-effect transistor (FinFET) at high current densities. Each constituting Silicon atom is coloured according to its temperature. (Credit: Jean Favre, CSCS)

Chip manufacturers are already assembling transistors that measure just a few nanometres across. They are much smaller than a human hair, whose diameter is approximately 20,000 nanometres in the case of finer strands. Now, demand for increasingly powerful supercomputers is driving the industry to develop components that are even smaller and yet more powerful at the same time.

Awarded the Gordon Bell Prize

However, in addition to physical laws that make it harder to build ultra-scaled transistors, the problem of the ever increasing heat dissipation is putting manufacturers in a tricky situation – partly due to steep rises in cooling requirements and the resulting demand for energy. Cooling the computers already accounts for up to 40 percent of power consumption in some data centres, as the research groups led by ETH professors Torsten Hoefler and Mathieu Luisier report in their latest study, which they hope will allow a better approach to be developed. In recognition of this valuable study, the researchers received the most prestigious prize in the field of supercomputing, the ACM Gordon Bell Prize, which is awarded annually at the SC supercomputing conference in the United States.

To make today’s nanotransistors more efficient, the research group led by Luisier from the Integrated Systems Laboratory (IIS) at ETH Zurich simulates transistors using software named OMEN, which is a so-called quantum transport simulator. OMEN runs its calculations based on what is known as density functional theory (DFT), allowing a realistic simulation of transistors in atomic resolution and at the quantum mechanical level. This simulation visualises how electrical current flows through the nanotransistor and how the electrons interact with crystal vibrations, thus enabling researchers to precisely identify locations where heat is produced. In turn, OMEN also provides useful clues as to where there is room for improvement.

Improving transistors using optimised simulations

Until now, conventional programming methods and supercomputers only permitted researchers to simulate heat dissipation in transistors consisting of around 1,000 atoms, as data communication between the processors and memory requirements made it impossible to produce a realistic simulation of larger objects. Most computer programs do not spend most of their time performing computing operations, but rather moving data between processors, main memory and external interfaces.

According to the scientists, OMEN also suffered from a pronounced bottleneck in communication, which curtailed performance. "The software is already used in the semiconductor industry, but there is considerable room for improvement in terms of its numerical algorithms and parallelisation," says Luisier.

Until now, the parallelization of OMEN was designed according to the physics of the electro-thermal problem, as Luisierexplains. Now, Ph.D. student Alexandros Ziogas and the postdoc Tal Ben-Nun – working under Hoefler, head of the Scalable Parallel Computing Laboratory at ETH Zurich – have not looked at the physics but rather at the dependencies between the data. They reorganised the computing operations according to these dependencies, effectively without considering the underlying physics. In optimising the code, they had the help of two of the most powerful supercomputers in the world – "Piz Daint" at the Swiss National Supercomputing Centre (CSCS) and "Summit" at Oak Ridge National Laboratory in the US, the latter being the fastest supercomputer in the world. According to the researchers, the resulting code – dubbed DaCe OMEN – produced simulation results that were just as precise as those from the original OMEN software.

For the first time, DaCe OMEN has reportedly made it possible for researchers to produce a realistic simulation of transistors ten times the size, made up of 10,000 atoms, on the same number of processors – and up to 14 times faster than the original method took for 1,000 atoms. Overall, DaCe OMEN is more efficient than OMEN by two orders of magnitude: on Summit, it was possible to simulate, among other things, a realistic transistor up to 140 times faster with a sustained performance of 85.45 petaflops per second – and indeed to do so in double precision on 4,560 computer nodes. This extreme boost in computing speed has earned the researchers the Gordon Bell Prize.

Data-centric programming

The scientists achieved this optimisation by applying the principles of data-centric parallel programming (DAPP), which was developed by Hoefler's research group. Here, the aim is to minimise data transport and therefore communication between the processors. "This type of programming allows us to very accurately determine not only where this communication can be improved on various levels of the program, but also how we can tune specific computing-intensive sections, known as computational kernels, within the calculation for a single state," says Ben-Nun. This multilevel approach makes it possible to optimise an application without having to rewrite it every time.
Data movements are also optimised without modifying the original calculation – and for any desired computer architecture. "When we optimise the code for the target architecture, we're now only changing it from the perspective of the performance engineer, and not that of the programmer – that is, the researcher who translates the scientific problem into code," says Hoefler. This, he says, leads to the establishment of a very simple interface between computer scientists and interdisciplinary programmers.

The application of DaCe OMEN has shown that the most heat is generated near the end of the nanotransistor channel and revealed how it spreads from there and affects the whole system. The scientists are convinced that the new process for simulating electronic components of this kind has a variety of potential applications. One example is in the production of lithium batteries, which can lead to some unpleasant surprises when they overheat.

Data-centric programming is an approach that ETH Professor Torsten Hoefler has been pursuing for a number of years with a goal of putting the power of supercomputers to more efficient use. In 2015, Hoefler received an ERC Starting Grant for his project, Data Centric Parallel Programming (DAPP).

Reference

Ziogas AN, Ben-Nun T, Fern.ndezGI, Schneider T, Luisier M & Hoefler T: A data-centric approach to extreme-scale ab-initio dissipative quantum transport simulations, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC19), November 2019.

Finances

Expenditures in CHF

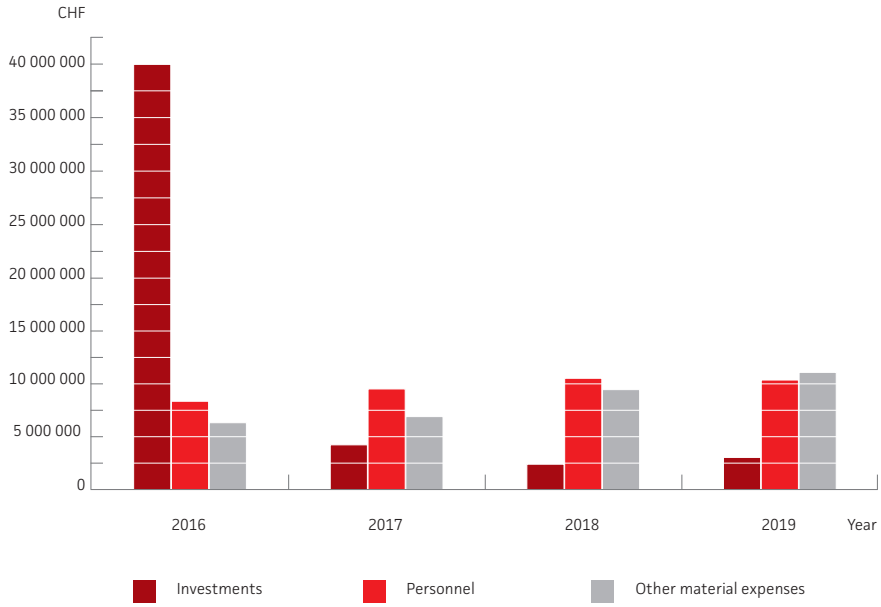
	User Lab	Third Party	Total
IT Investments	**2 998 291.54**	**2 509 025.93**	**5 507 317.47**
Personnel	**10 286 087.88**	**4 872 335.97**	**15 158 423.85**
Payroll	9 973 301.35	4 871 137.65	14 844 439.00
Further education, Recruitment	312 786.53	1 198.32	313 984.85
Material expenses	**11 006 943.26**	**1 653 387.03**	**12 660 330.29**
Maintenance building & technical infrastructure	838 565.66	213 300.94	1 051 866.60
Energy	2 605 070.98	424 031.43	3 029 102.41
Maintenance hardware & licenses	4 250 192.43	423 317.45	4 673 509.88
Remunerations, Marketing, Workshops, Services, Travel, Membership fees	1 648 457.62	592 737.21	2 241 194.83
PASC projects contribution	1 664 656.57		1 664 656.57
Total expenditures	**24 291 322.68**	**9 034 748.93**	**33 326 071.61**

Income in CHF

	User Lab	Third Party	Total
Contribution ETH Zurich	17 453 270.06		17 453 270.06
Contribution ETH-Rat - HPCN Investments	3 396 601.14		3 396 601.14
Contribution ETH-Rat - PASC Initiative	3 246 750.27		3 246 750.27
European projects		3 483 833.48	3 483 833.48
Paying customers		5 196 244.70	5 196 244.70
Other income	194 701.21	354 670.75	549 371.96
Total income	**24 291 322.68**	**9 034 748.93**	**33 326 071.61**

User Lab Expenses Development (CHF)

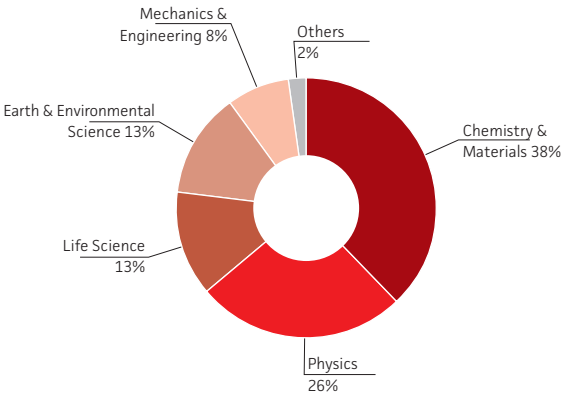
	2016	2017	2018	2019
Investments	40 023 533	4 218 973	2 472 847	2 998 292
Personnel	8 313 178	9 478 260	10 479 422	10 286 088
Other material expenses	6 293 094	6 877 461	9 414 401	11 006 943



Usage Statistics

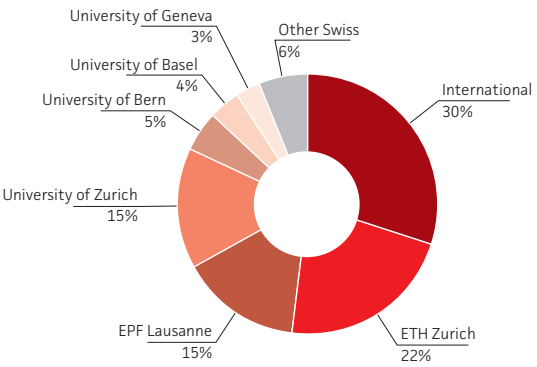
User Lab Usage by Research Field

Research Field	Node h	%
Chemistry & Materials	14986864	38
Physics	10315970	26
Life Science	5320871	13
Earth & Environmental Science	5058587	13
Mechanics & Engineering	3196088	8
Others	979962	2
Total Usage	**39 858 342**	**100**



User Lab Usage by Institution

Institution	Node h	%
International	11993044	30
ETH Zurich	8761567	22
EPF Lausanne	6175551	15
University of Zurich	5860898	15
University of Bern	1893207	5
University of Basel	1505777	4
University of Geneva	1072476	3
Other Swiss	2595822	6
Total Usage	**39 858 342**	**100**



Compute Infrastructure

Computing Systems Overview

Name	Model	Installation/Upgrades	Owner	TFlops
Piz Daint	Cray XC50/Cray XC40	2012 / 13 / 16 / 17 / 18	User Lab, UZH, NCCR Marvel, CHIPP	27 154 + 2 193
Piz Kesch + Piz Escha	Cray CS-Storm	2015	MeteoSwiss	392
Grand Tavé	Cray X40	2017	Research & Development	437

Computing Systems Specifications

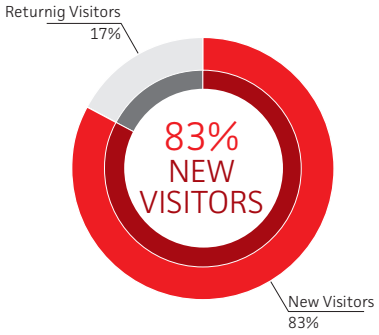
Name	Interconnect Type	CPU Type	No. Cores	No. Sockets per Node	No. Nodes
Piz Daint	Cray Aries	Intel Xeon E5-2690 v3 + Nvidia P100	12	1 + 1	5 704
		Intel Xeon E5-2695 v4	18	2	1 813
Piz Kesch + Piz Escha	Infiniband FDR	Intel Xeon E5-2690 v3 + Nvidia K80	24	2 + 8	12
Grand Tavé	Cray Aries	Intel Xeon Phi CPU 7230	64	1	164

Communications Statistics

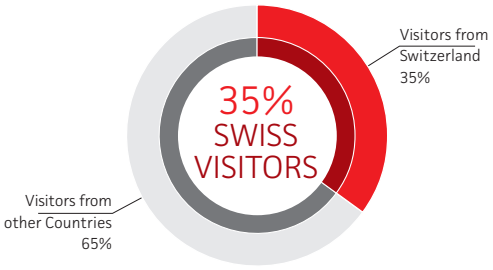
Website cscs.ch

	2018	2019
Total Website Visitors	76 265	76 986
Average Website Visits (Minutes)	2:22	2:17

New Visitors



Visitors Origin



Top 5 Most Visited Website Pages

1. CSCS Homepage www.cscs.ch
2. Piz Daint www.cscs.ch/computers/piz-daint/
3. Staff www.cscs.ch/about/staff/
4. Working at CSCS www.cscs.ch/about/working-at-cscs/
5. Events www.cscs.ch/events/

Twitter

	2018	2019
Followers	1 097	1 480

LinkedIn

	2018	2019
Followers	6 810	7 880

YouTube

	2018	2019
Watch Time (Minutes)	613 000	456 815
Average View Duration (Minutes)	5:21	4:33
Number of Views	114 600	105 500

Facebook

	2018	2019
Followers	181	220

CSCS in the News

	2018	2019
News Websites	341	304
Print	196	254
Radio & TV	7	10

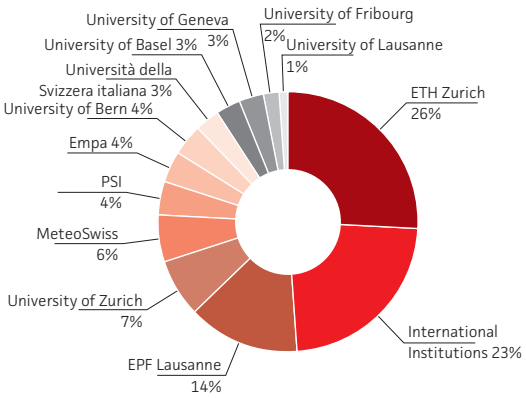
Word Cloud of News Related to CSCS

User Satisfaction

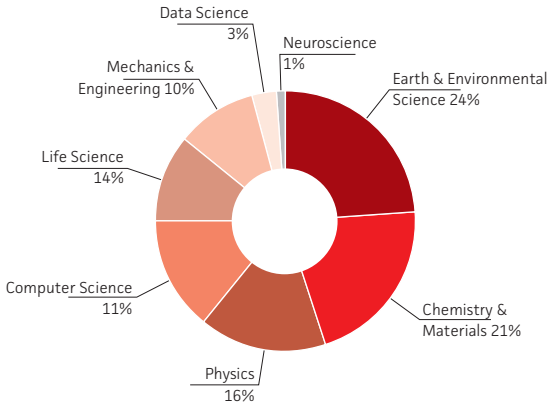
A user satisfaction survey was submitted to 1 883 users in January 2020. The response rate was of 12.9% (243 answers).

User Profile

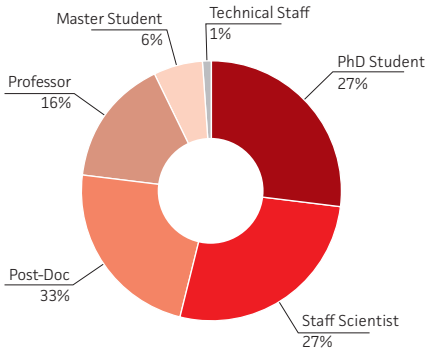
Your institution



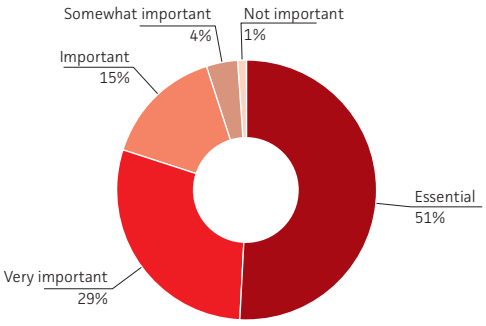
Your scientific field



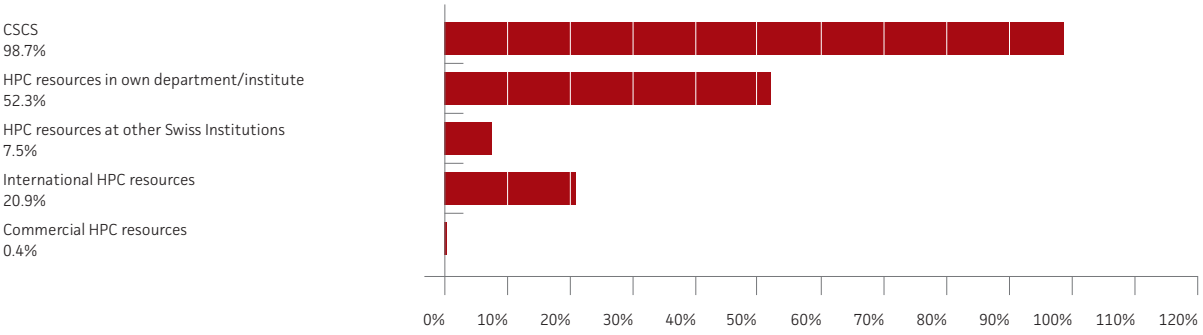
Your position



For my research, CSCS resources are

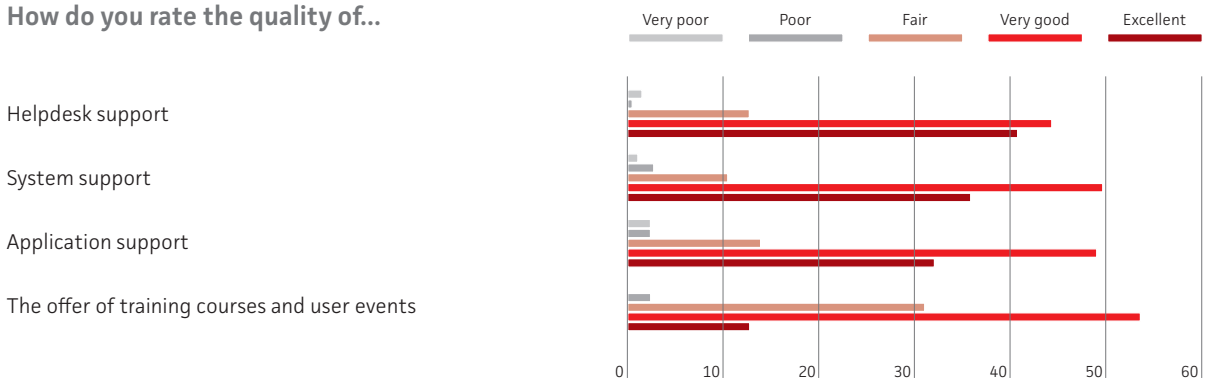


Which HPC resources are you using?

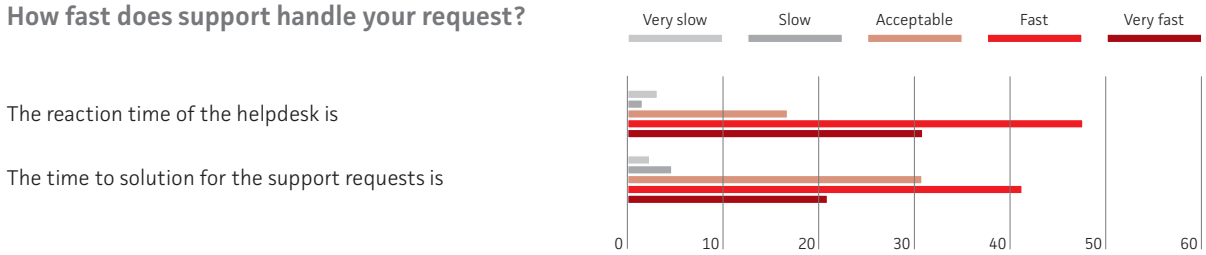


User Support

How do you rate the quality of...

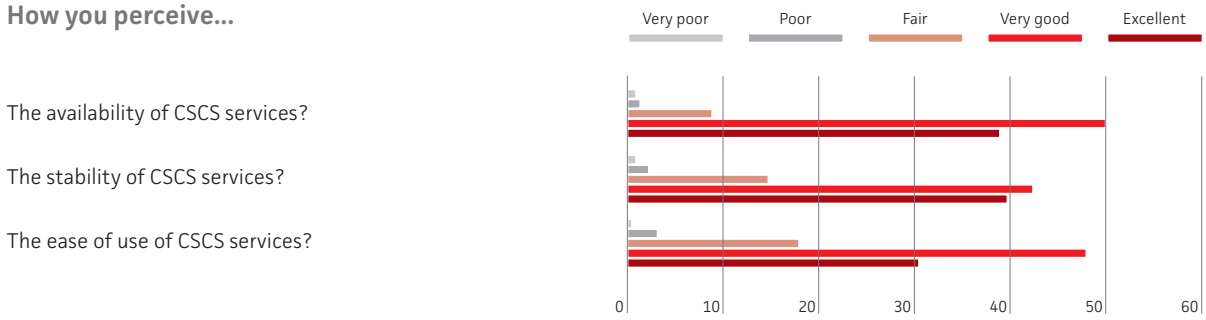


How fast does support handle your request?

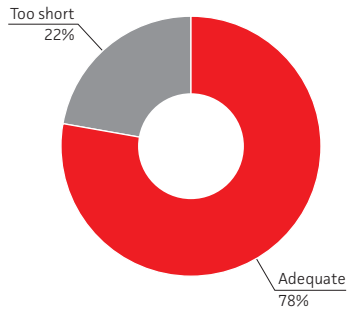


Service Availability, Stability and Usability

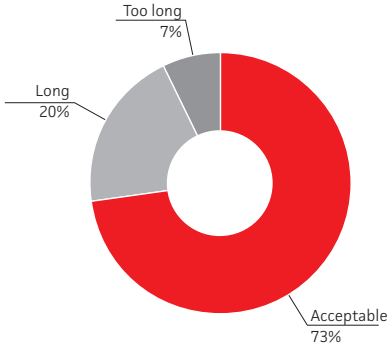
How you perceive...



The run time limits for batch jobs are

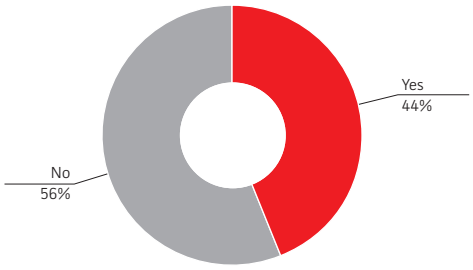


The job waiting time in the queue is

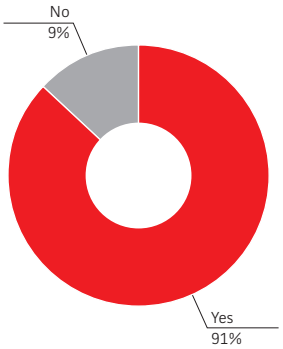


Project Proposal Process

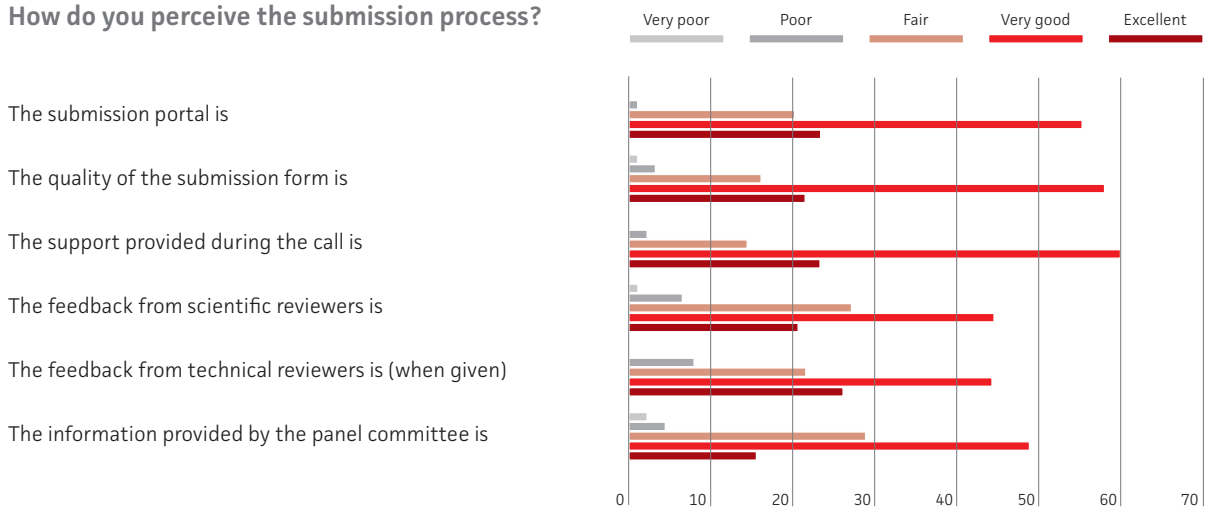
Have you been submitting project proposals to CSCS (as PI or supporting the PI?)



Is the reviewing process transparent?

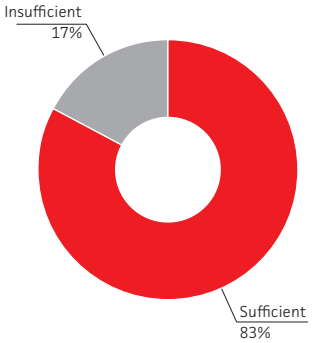


How do you perceive the submission process?

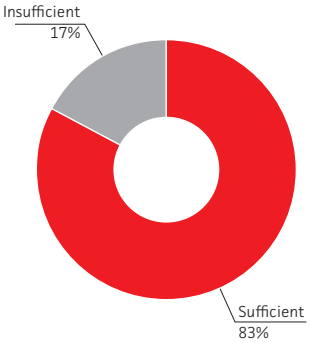


Adequacy of Allocated Resources

The resources assigned to my project are

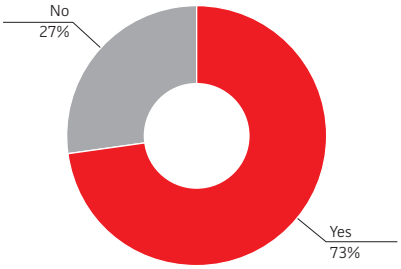


My storage allocation on "project" is

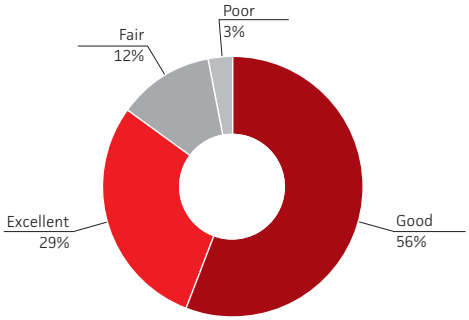


Application Development

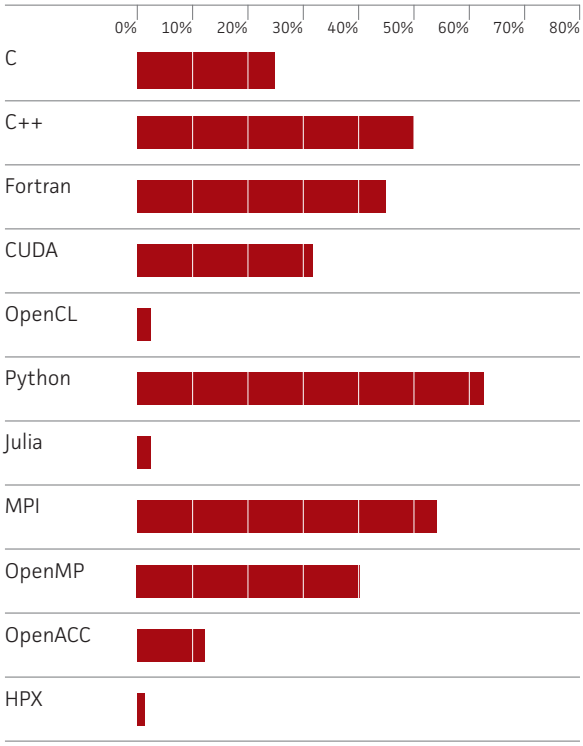
Do you develop and maintain application codes?



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

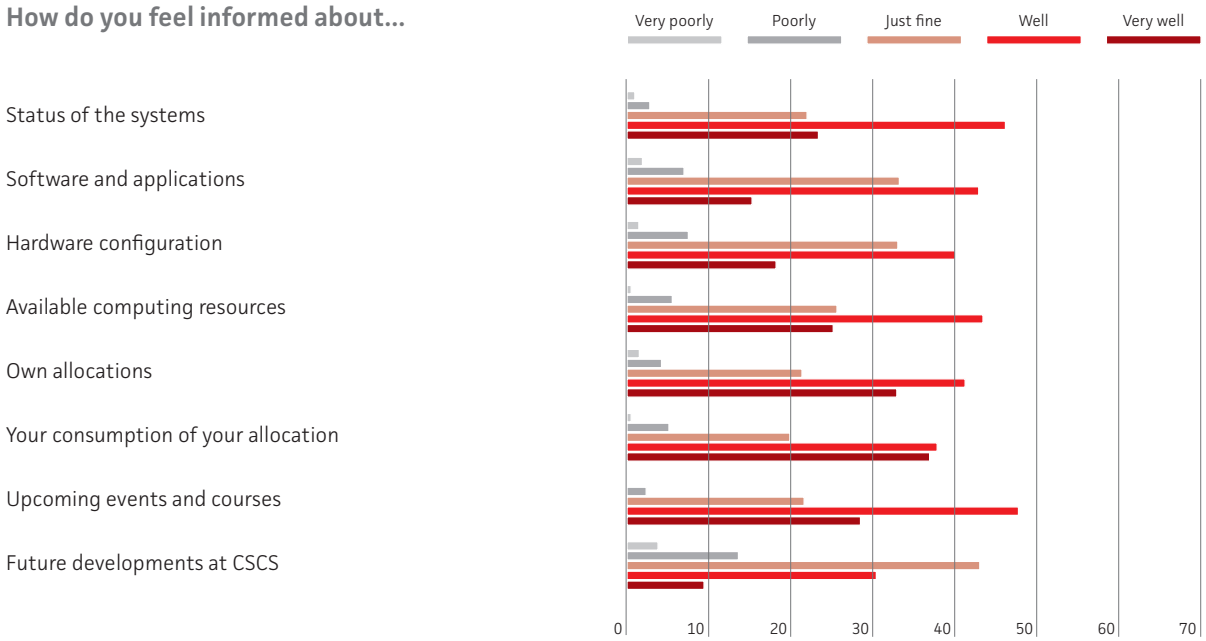


Which programming languages and parallelization paradigms are you using primarily?



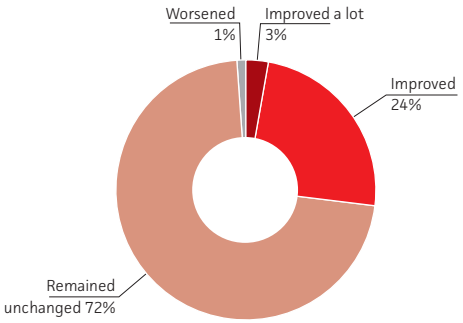
Information & Communication

How do you feel informed about...

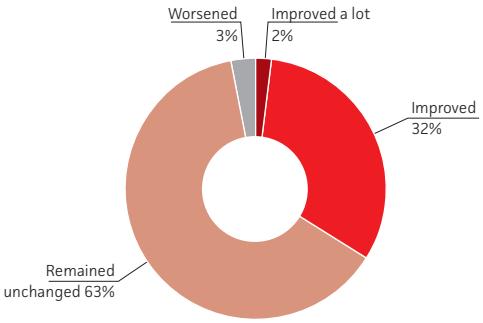


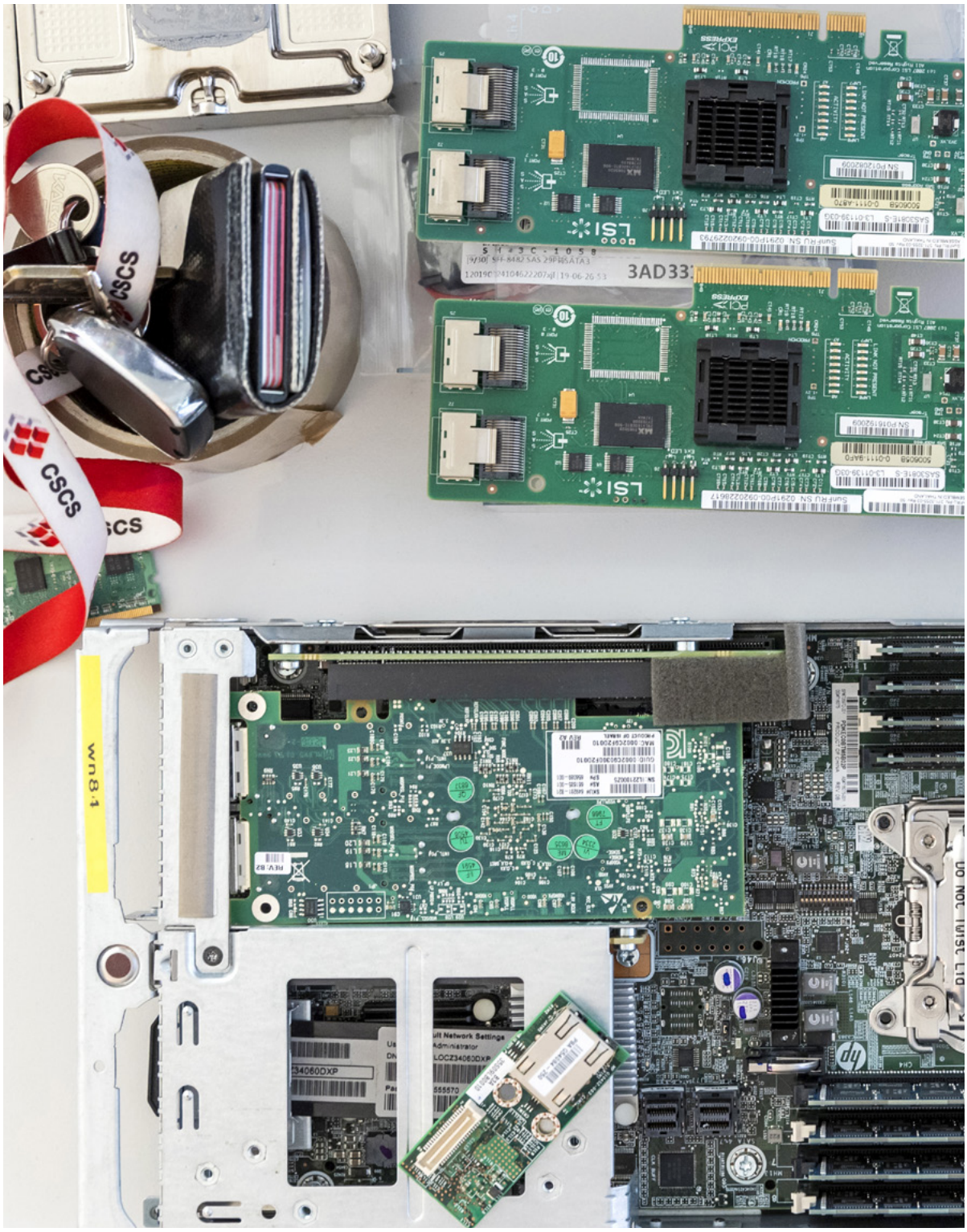
Perception of CSCS

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




CSCS
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