CSCS

Annual Report **2020**

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

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The photographers Alessandro Della Bella and Daniel Rihs have portrayed six female scientists of different scientific fields who use CSCS supercomputers for their research work: Nicola Spaldin (ETH Zurich), Cécile Münch-Alligné (HES-SO Valais-Wallis), Florina Ciorba (University of Basel), Marina Krstic Marinkovic (ETH Zurich), Ulrike Lohmann (ETH Zurich), Viola Vogel (ETH Zurich).

Welcome from the Director

Thomas Schulthess, Director of CSCS.

Our Annual Report 2020 covers more science than previous editions. This is, for once, a positive consequence of the pandemic, which caused conferences and trainings to be cancelled, making the activity report a bit shorter than usual. More reports on user research at CSCS were included instead. However, these highlights represent only a small sample of the exciting and often highly ambitious projects enabled by the CSCS research infrastructure. These range from pure, basic research to the targeted search for solutions to highly relevant social questions, such as the search for a vaccine or medication against the SARS-Cov-2 virus. CSCS supported research in this latter area by participating in the Swiss National Science Foundation's (SNSF) special call for proposals for research into the SARS-Cov-2 virus, as well as in the Partnership for Advanced Computing in Europe (PRACE) through the PRACE Fast Track call for proposals. As always, an overview of the results achieved with our flagship supercomputer "Piz Daint" can be found in the list of publications.

We began installing the successor to "Piz Daint" — called "Alps" — in the summer, with four computer cabinets completed so far. In order to continue supporting research at a high level, the new system will be based on an innovative, software-defined infrastructure that will enable highly efficient operation and provide our users with many more services tailored to their needs. Expansion will take place in three phases; but until completion and the commissioning of the new system in spring 2023, "Alps" will be available to researchers together with "Piz Daint". More detailed information about "Alps" and our procurement strategy can be found in my interview on page 68, but the main point is this: With "Alps", we are not simply procuring a new computer that will be integrated into the unchanged computer centre, but we are rather retrofitting our data centre in several phases in the next three years.

Our core task remains, of course, to continuously operate and improve a research infrastructure at CSCS that supports researchers in the best possible way. It is therefore essential for me and my team to keep expanding our own expertise. To this end, we often work closely with researchers from various Swiss universities. I would like to take this opportunity to thank not only our partners in the various academic, research and service institutions, but also the Executive Board of ETH Zurich and especially my team.

Lastly, I am particularly pleased this year to introduce some of the female researchers in high-performance computing who are excelling within our research infrastructure. A brief portrait of each researcher can be found between the different chapters of the report. With all that said, I now invite you to browse through our annual report and discover some of the exciting stories of scientific achievement at CSCS in 2020.

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
2020: 54 955 535 node h
2019: 50 045 000 node h

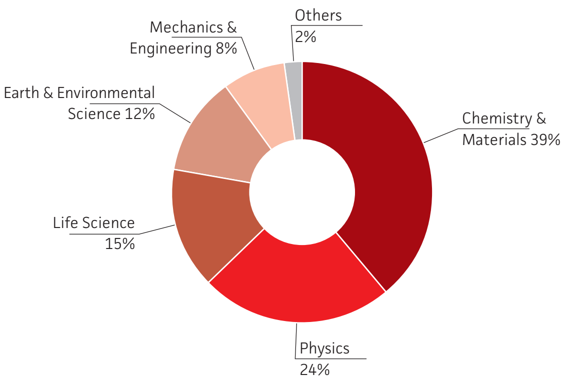
User Community
2020: 134 projects, 2 270 users
2019: 124 projects, 1 883 users

Employees
2020: 116
2019: 115

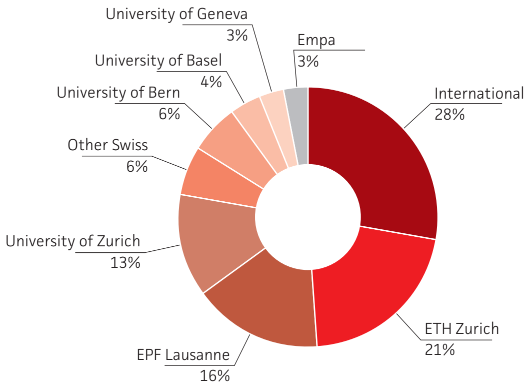
Investments
2020: 9.8 Mio. CHF
2019: 2.9 Mio. CHF

Operational Costs
2020: 23.6 Mio. CHF
2019: 21.2 Mio. CHF

User Lab Usage by Research Field



User Lab Usage by Institution



Computing Systems Overview

Name	Model	Installation/Upgrades	User	TFlops
Piz Daint	Cray XC50/Cray XC40	2012 / 13 / 16 / 17	User Lab, UZH, NCCR Marvel, CHIPP	27 154 + 2 193
Grand Tavé	Cray X40	2017	Research & Development	437
Tsa/Arolla	Cray CS-Storm 500	2020	MeteoSwiss	1 126
Alps	HPE Cray EX	2020	User Lab, Research & Development	4 719

Nicola Spaldin – ETH Zurich

“We’re tremendously fortunate that the team at CSCS has been able to keep the computers and support services running throughout the pandemic, so in turn we have been able to continue our research and education activities almost uninterrupted”.

Name
Nicola Spaldin

Position
Full Professor, Department of Materials

Institution
ETH Zurich

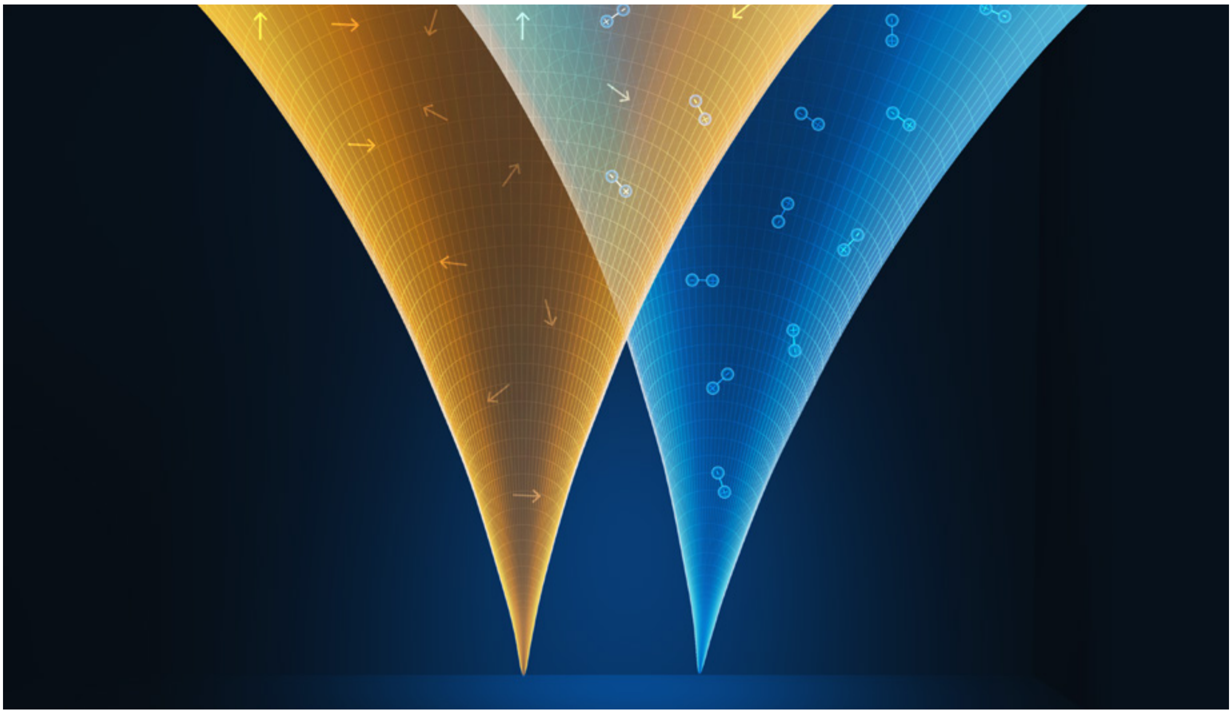
Background

1991-1996	PhD in chemistry, University of California at Berkeley, USA
1996-1997	Postdoc in applied physics, Yale University, USA
1997-2010	Assistant, Associate and Full Professor in materials science, University of California at Santa Barbara, USA
2011-Present	Professor, ETH Zurich

Area of research
Materials theory.

Specialised in
Electronic structure theory.

HPC means for me
The computer is my laboratory. It allows us to characterize our virtual materials in minute detail, seeing exactly where the electrons go and what they do — and why.



Multiferroic Quantum Criticality

A peculiarity of quantum mechanics is that small things like electrons can move around even at zero temperature, when classically they should have no energy. Nicola Spaldin and her team used high-performance computations to show how this property causes the electric charges and the magnetic dipoles of electrons to interact in unexpected ways, and that this can affect their properties even at high temperature. This understanding could one day lead to a room-temperature superconductor. (Image: Nicola Spaldin)

January

15/16 Read the article

Peer review of PASC activities

The peer review of the projects and core program activities supported by the Platform for Advanced Scientific Computing (PASC) took place on January 15-16 at the Università della Svizzera italiana in Lugano. The platform's overarching goal is to position Swiss computational sciences in the emerging exascale-era. It is complementary to the supercomputing-hardware-focused elements of the Swiss High-Performance and Networking (HPCN) initiative.

February

19

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

17

COVID-19 Pandemic: First impact on CSCS operations

On Saturday, March 14, the canton of Ticino declared a state of emergency. As of Tuesday, March 17, access to CSCS buildings was reduced to the absolute minimum; and as a consequence, all staff except on-call service started working from their homes. Despite these considerably more challenging circumstances, the centre was able to provide all services without interruption and to remain effective and efficient.

24 Read the article

CSCS joined the PRACE COVID-19 Fast Track Call for Proposals

On March 24, PRACE announced the COVID-19 Fast Track Call for Proposals to help scientists from all over Europe mitigate the impact of the pandemic by granting easy access to the European Tier-0 HPC facilities with a prompt and fast review process.

April

01

23.6 Mio. node hours distributed in the User Lab and PRACE

A total of 23.6 Mio. node hours were distributed in the first national call for proposals and in the PRACE Tier-0 Call 20 for the allocation period between April 1, 2020 and March 31, 2021.

14

Webinar on "How to prepare the Technical Report for proposal submission"

The webinar provided applicants with guidelines for the preparation of the Technical Report for the National and Tier-0 Calls for Proposals.

May

16 Read the article

Interruption of services after cyber-incident

Many HPC data centers worldwide, including CSCS, were paralyzed by a cyber-incident. CSCS closed external access to the supercomputer infrastructure for one week to restore a safe environment. The services provided to MeteoSwiss for weather forecasts were not affected. An analysis of the cyber-incident did not show any loss of information for our users.

28 Read the article

UK and Switzerland's top supercomputers join COVID-19 HPC Consortium

UK Research and Innovation (UKRI) and CSCS joined as first European organizations the COVID-19 High Performance Computing Consortium, which calls on government, industry, and academia to volunteer free compute time and resources on their world-class machines for COVID-19 research.

June

29/01

PASC20 Conference

The PASC20 Conference — with the theme "New Challenges, New Computing Paradigms" — should have taken place at the University of Geneva, Switzerland. Due to the pandemic, the organizing committee decided to postpone the event by one year. The 2021 edition of the conference is planned to take place from July 5-8, 2021, at the same location.

July

06/08

Webinar 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.

09

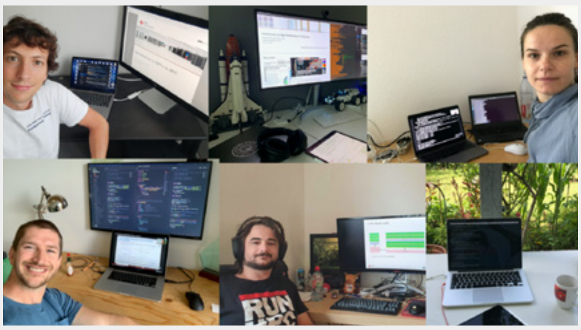
Webinar on best practices for ParaView

A webinar was organized to discuss the new features available in ParaView 5.8, the procedures for connecting to CSCS machines from remote desktops, and some tips and tricks about data I/O and the use of Python to drive both interactive and batch sessions. The webinar included interactive live demonstrations and gave users the chance to ask questions not just about ParaView, but also about 3D scientific visualisation in general.

13/24 Read the article

Online CSCS-USI Summer School 2020

CSCS and Università della Svizzera italiana hosted their annual Summer School online this year due to COVID-19 restrictions, but attendance tripled thanks to the remote accessibility of the program. A total of 100 students and working professionals logged on for the two-week series of lectures and "hands-on" labs to learn about CPU/GPU hybrid high-performance computing systems with a special focus on data analytics.



August

08

Call for PASC project proposals

In this call, PASC is seeking proposals for HPC software development projects that address the broad availability, the quality, and performance of software on GPU-accelerated supercomputing platforms.

31 / 01

Online User Lab Day

CSCS welcomed current and possible future users to two half-day online sessions on August 31 and September 1. Attended by researchers from a diverse range of scientific backgrounds as well as hardware technicians and software developers, the virtual event provided ample time for conversation with CSCS staff about the current best practices and resources, as well as the future services already on the horizon.

September

01

Start of EuroCC collaboration project

The goal of EuroCC is to support and strongly increase the national strengths of high-performance computing (HPC) competences, as well as high-performance data analytics (HPDA) and artificial intelligence (AI) capabilities. The aim is to close existing gaps, increase usability of these technologies in the different states, and provide a European excellence baseline. Within the EuroCC project, CSCS is tasked with establishing a National Competence Centre (NCC) in the area of HPC in Switzerland.

07 / 08

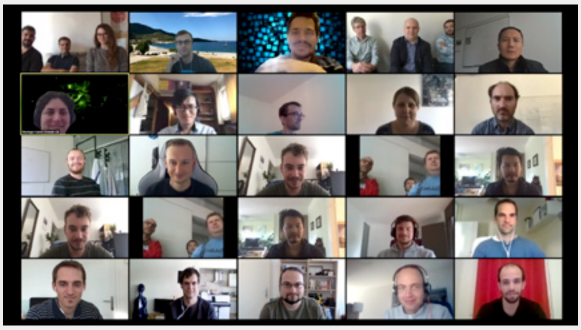
Multi GPU training with TensorFlow on "Piz Daint"

A two-day course on efficient and distributed training with TensorFlow was organized to address the use of this tool on “Piz Daint”. 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.

21 / 30 Read the article

Online EuroHack20: GPU programming hackathon

The 6° GPU-programming hackathon took place online and 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 GPU-hybrid supercomputing environment.



October

01

24.0 Mio. node hours distributed in the User Lab and PRACE

A total of 24.0 Mio. node hours were distributed to scientists in the second national call for proposals and in the PRACE Tier-0 Call 21 for the allocation period between October 1, 2020 and September 30, 2021.

12

Visit from the ETH Zurich Vice President for Research

Vice President for Research Prof. Detlef Günther paid an inaugural visit to the CSCS, so to speak, with a delay because of the pandemic. Since the beginning of 2020, he has been responsible of the computing centre.

12/13

Workshop on scientific visualization

This two-day online course was organized for scientists with a strong interest in efficient visualization of 3D data. The focus for the attendees was to introduce several well-known standalone OpenGL applications.

22

Online workshop on parallel I/O

This webinar introduced parallel I/O on "Piz Daint" and discussed best practices. After a general introduction, the focus was on ADIOS2, a parallel I/O library that addresses shortcomings of commonly used I/O libraries for large-scale computing.

hpc-ch Forum

The 21st Community Forum on Access Abstraction to HPC Resources was hosted by Empa. Representatives of the Swiss HPC Service Provider Community met to discuss computational resources abstraction and efficient management of data.

Acceptance of first four cabinets of "Alps" research infrastructure

The first cabinets of the "Alps" research infrastructure have been installed and accepted at the end of October. This phase comprises of 1'024 compute nodes based on the HPE Cray supercomputing architecture with Slingshot interconnect, and HPE ClusterStor storage system. Each node is equipped with two AMD EPYC(TM) 7742 64-Core processors. The scratch storage capacity is 10 PetaBytes.

26

Read the article

Shutdown of Escha and Kesch supercomputers

After more than five years of successful and reliable computing, Escha and Kesch were retired at the end of October 2020 as MeteoSwiss' operational clusters. The systems have been replaced by a successor, called Arolla and Tsa, that is similar in technology but also provides innovative solutions in respect to fail-safe and on-demand computing capabilities.

November

12/19

Read the article

CSCS virtually meets students from SUPSI and USI

Different staff members represented CSCS in two events related to the topic of careers, organized by Scuola universitaria professionale della Svizzera italiana and Università della Svizzera italiana. The events, targeted to all students and alumni, focused on their professional futures and provided the environment to get insights into internships, career paths and technical skills required to work at CSCS.

December

10

Call for internships for 2021

CSCS opened a call for applications for different types of internships in the field of HPC, particularly for the development and optimization of scientific applications, in order to exploit the coming generations of supercomputing devices. The call is dedicated to master students in computer science, mathematics, physics or related fields. The internship has to be a mandatory part of the curriculum of studies.

Cécile Münch-Alligné - HES-SO Valais-Wallis

Person Detail

“Within our present project, GPU-SPHEROS, we use an in-house, GPU-accelerated, particle-based solver to simulate full, realistic multi-jet Pelton turbine flow — all on ‘Piz Daint’, one of the most powerful GPU-powered supercomputers in the world. We expect to contribute to a better understanding of the complex phenomena developing in the machine under harsh operating conditions”.

Name
Cécile Münch-Alligné

Position
Professor UAS (University of Applied Sciences), Hydroelectricity Research Group

Institution
HES-SO Valais-Wallis

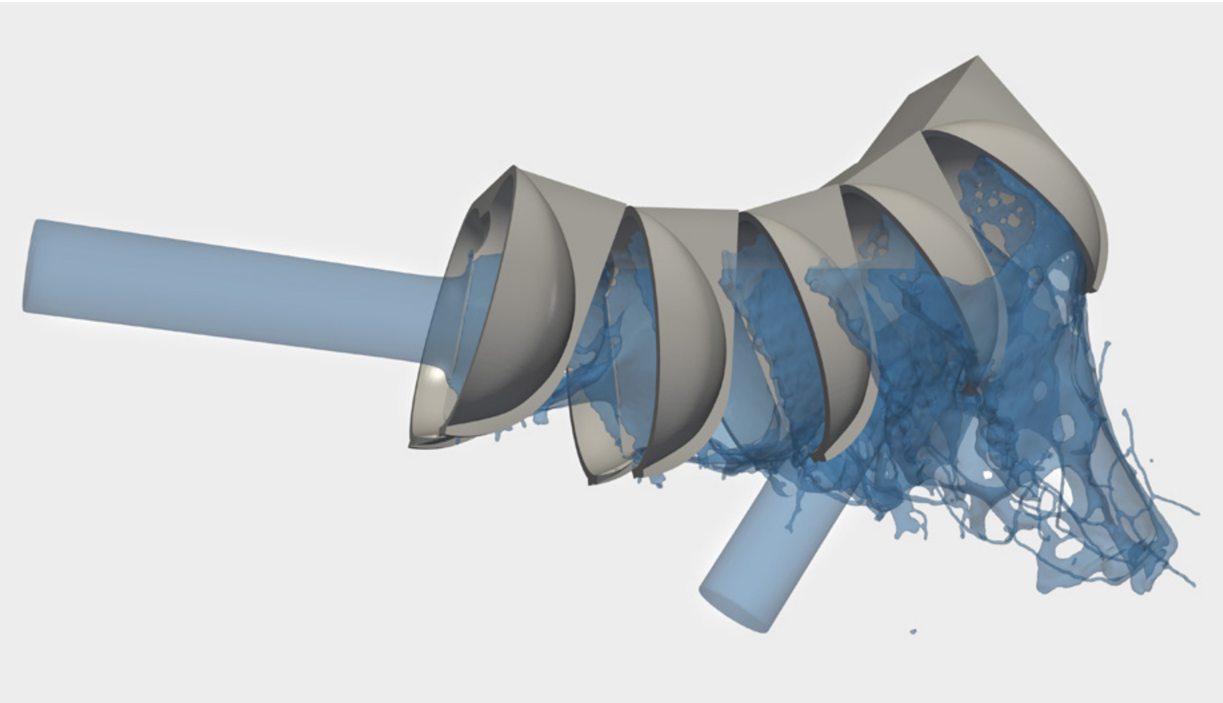
Background

2002–2005	PhD in numerical simulation of turbulence, INPG, France
2006–2010	Postdoc, Laboratory for Hydraulic Machines, EPF Lausanne
2010–2018	Invited Professor, Laboratory for Hydraulic Machines, EPF Lausanne
2010–Present	Professor UAS in hydraulic energy, HES-SO Valais-Wallis

Area of research
Flexibility of large and small hydropower plants.

Specialised in
Numerical simulations, turbulence, and fluid-structure interactions for hydraulic machines.

HPC means for me
HPC means for me an amazing instrument which allows to predict very complex hydrodynamic phenomena such as the one, we want to simulate in Pelton turbines within the GPU-SPHEROS solver using "Piz Daint".



Numerical simulations of hydraulic machines

Numerical simulation of two adjacent jets impacting five buckets of a rotating Pelton runner is carried out with the solver GPU-SPHEROS. Flow simulations in a full, multi-jet Pelton turbine with six injectors and a complete runner are carried out on "Piz Daint" to better predict complex phenomena developing in the machine under specific conditions. (Image: Siamak Alimirzazadeh)

High-Performance Computing at the service of society: Fighting COVID-19

CSCS has been joining a number of initiatives to provide HPC resources to scientists to mitigate the impact of the COVID-19 pandemic and to help them understand the nature of SARS-CoV-2, an aggressive virus that has taken the world by surprise, dramatically impacting modern society.

SARS-CoV-2 has reached Europe and America by early 2020, either one nearly unprepared and the virus has changed life from one day to the other. Public health systems of several countries were strained to the extreme and many lives were lost, especially among the elderly. After a moment of shock, however, essential research infrastructure was put together and scientists started to think how they could contribute helping society to overcome the threat of COVID-19.

Already in March of that year CSCS joined the PRACE (Partnership for Advanced Computing in Europe) initiative to launch an extraordinary Fast-Track Call for Proposals, allocating significant compute resources to promising computational projects that focused on understanding and fighting the disease. Scientists in Switzerland were further encouraged to apply for CSCS resources through the SNF (Swiss National Foundation) COVID-19 Special Call, which addressed both computational and experimental studies. A few weeks later CSCS joined the COVID-19 High Performance Computing Consortium, an international effort led by the US.

CSCS received eight 6-month project proposals focusing on various aspects of COVID-19, including the characterization of relevant proteins, drug design studies, and fluid dynamics studies of virus dissemination in closed rooms filled with people. Collaborative international efforts have demonstrated again that science knows no borders, neither between countries nor between disciplines, and that supercomputers and data services form an important ingredient to modern research infrastructure. Involved parties have synchronized their efforts to accelerate their fight against a very dangerous disease. Results have been made available on a rolling basis and peer-reviewed publications are starting to appear.

Impact of Covid-19 on User Lab

The pandemic has had an impact on the operations of the centre and on the User Lab. However, even with the staff working remotely for most of 2020, CSCS was able to keep up to speed and to provide all services without interruption. We had to adapt, though! We had to quickly learn how to continue our Training Program and provide courses and the User Lab day in an enjoyable online format. The positive result of going virtual has been the ability to reach a much broader audience, a lesson learned that will need to be kept in mind also once the pandemic is over.

Resources allocated in 2020

Usage statistics shows that Chemistry & Materials remains the best-represented field at CSCS, using 39% of the available resources. Physics follows with 24% of the total allocation, followed by Earth & Environmental Science, Life Science and Mechanics & Engineering with 15, 12 and 8% each.

ETH Zurich is again the largest user (21%) among institutions, followed by EPF Lausanne (16%), and the Universities of Zurich, Bern, Basel, and Geneva (13, 6, 4, 3%), other Swiss institutions are sharing the remaining 6% of the resources. International utilization remains high at about 28%. Like in previous years, the User Lab Calls are still the primary path to resource allocation for domestic research institutions, but the majority of the 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
Gabriel Włazlowski	University of Warsaw	Physics	Dissipative dynamics in fermionic superfluids	1 255 000
Vladimir Rybkin	University of Zurich	Chemistry & Materials	Structure of the excess electron in liquid methanol from many-body electronic structure theory	1 176 000
Nikolina Ban	University of Innsbruck	Earth & Environ. Science	Mountain Climate at the Kilometer-Scale Resolution (kmMountains)	1 169 000
Marco Giorgetta	Max Planck Institute for Meteorology Hamburg	Earth & Environ. Science	The Quasi-Biennial Oscillation in a changing climate (QUBICC)	1 060 000
Carmen Domene	University of Bath	Life Science	TRPs - Structure-based characterization of novel TRPV inhibitors	1 044 000
Lucie Delemotte	Royal Institute of Technology in Stockholm	Life Science	Lipid modulation of membrane protein functional cycle	1 030 000
Nicola Marzari	EPF Lausanne	Chemistry & Materials	ELGEN - The electronic-structure genome of materials	1 029 000
Christoph Schär	ETH Zurich	Earth & Environ. Science	kmCLIM - Kilometer-resolution climate modeling on GPUs	1 000 000
Carlo Camilloni	University of Milan	Life Science	PDLCA - Protein dynamics and toxicity in light chain amyloidosis	1 000 000
Carlos Martins	University of Porto	Physics	Coding the cosmos: From cosmic strings to superstrings	1 000 000
Stefano Vanni	University of Fribourg	Life Science	FATstor - The role of Bernardinelli-Seip congenital lipodystrophy type 2 protein (BSCL2 - seipin) and its pathological variants in intracellular fat accumulation	1 000 000
Hansel Gomez	Nuritas Ireland	Life Science	Combining Deep Learning and Language Modelling Techniques to improve prediction of bioactive peptides from natural sources	1 000 000
Constantia Alexandrou	University of Cyprus & Cyprus Institute	Physics	NPiTwist – The Nπ system using twisted mass fermions at the physical point	750 000
Davide Modesti	Delft University of Technology	Mechanics & Engineering	INTAkE--understandINg Turbulence over porous surfaces: towards efficient Acoustic linErs for aircraft engines	735 000
Gabriele Tocci	University of Zurich	Chemistry & Materials	Ab-initio molecular dynamics for nanoscale osmotic energy conversion	588 200

Largest Projects (> 600 000 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	947 000
Michele Ceriotti	EPF Lausanne	Chemistry & Materials	Efficient and reliable crystal structure prediction using quantum Monte Carlo and Machine Learning	900 000
Nicola Spaldin	ETH Zurich	Chemistry & Materials	Coupled and competing instabilities in complex oxides	900 000
Stefan Goedecker	University of Basel	Chemistry & Materials	Structure and dynamics of solids, interfaces and clusters	863 000
Andreas Fichtner	ETH Zurich	Earth & Environ. Science	Full-waveform inversion of the Alpine belt	860 000
Tomasz Kacprzak	ETH Zurich	Physics	Measuring dark energy with deep learning	750 000
Sandra Luber	University of Zurich	Chemistry & Materials	Guiding the design of novel and highly efficient water reduction catalysts by ab initio methods	707 000
Urs Wenger	University of Bern	Physics	Double-virtual neutral pseudoscalar meson transition form factors $FP\gamma*\gamma*$ from Lattice QCD at the physical point	700 000
Jürg Hutter	University of Zurich	Chemistry & Materials	Molecules at interfaces from density functional theory	700 000
Ursula Röthlisberger	EPF Lausanne	Chemistry & Materials	Towards lead-free and stable solar cells	700 000
Carlo A. Pignedoli	Empa	Chemistry & Materials	Characterization of on-surface reactions in the fabrication of atomically precise nanographenes with non-hexagonal rings	631 000
Constantia Alexandrou	University of Cyprus & Cyprus Institute	Physics	Precision nucleon structure using lattice QCD	600 000
Nicola Marzari	EPF Lausanne	Chemistry & Materials	Materials for Energy	600 000

List of Projects by Institution

Aix-Marseille University

Ab-initio calculations of parton distribution functions for the LHC and the EIC, Savvas Zafeiropoulos (Physics, 490 000 node h)

Dalle Molle Institute for Artificial Intelligence Research IDSIA

Learning to replace human-engineered reinforcement learning algorithms, Jürgen Schmidhuber (Computer Science, 400 000 node h)

Model based meta reinforcement learning using recurrent world models, Luca Gambardella (Computer Science, 8 000 node h)

Delft University of Technology

Unveiling turbulence-radiation interactions (TRI) in participating non-gray media, Rene Pecnik (Mechanics & Engineering, 350 000 node h)

EAWAG

Calibration and uncertainty quantification of stochastic models with spux: Applications to hydrology and ecology, Marco Bacci (Earth & Environmental Science, 100 000 node h)

Empa

Harmonic free energy corrections to thermodynamics and kinetics in PdGa-catalysed chemical reactions, Daniele Passerone (Chemistry & Materials, 100 000 node h)

EPF Lausanne

Basic study and experimental modeling of internal transport barriers with gyrokinetics, Justin Ball (Physics, 300 000 node h)

A single-cell atlas of spinal cord injury, Quentin Barraud (Life Science, 168 000 node h)

Surface-centric design of epitope-scaffolds for influenza, Bruno Correia (Life Science, 480 000 node h)

Characterization of SARS-CoV-2 envelope small membrane protein (E), Matteo Dal Peraro (Life Science, 147 000 node h)

Molecular dynamics simulations to assist the engineering of protein-based nanopores for DNA sequencing, Matteo Dal Peraro (Life Science, 365 000 node h)

Computational screening of covalent- and metal-organic frameworks for applications in photocatalysis, Maria Fumanal (Chemistry & Materials, 510 000 node h)

Towards validated, first-principles turbulence simulations of the boundary region of magnetically confined fusion plasmas, Christian Theiler (Physics, 500 000 node h)

Novel topological phases of materials, Oleg V. Yazyev (Chemistry & Materials, 240 000 node h)

ETH Zurich

Elastic metastructures for tailored wave control, Andrea Colombi (Mechanics & Engineering, 36 000 node h)

Estimating glaciers contribution to sea-level rise since the 1970s from historical satellite data, Amaury Dehecq (Earth & Environmental Science, 11 250 node h)

Towards truly data-constrained marine micronutrient biogeochemistry: Deciphering the marine Zn cycle, Gregory de Souza (Earth & Environmental Science, 90 000 node h)

Multi-scale magnetotelluric imaging of mid-enthalpy geothermal systems: Insights from Tsenkher hot springs, Mongolia, Samrock Friedemann (Earth & Environmental Science, 95 000 node h)

Understanding precipitation formation in mixed-phase orographic clouds, Jan Henneberger (Earth & Environmental Science, 220 000 node h)

Validation of a high-resolution 3D velocity model for the Visp area (Wallis) based on standard spectral and horizontal-to-vertical ratios, Walter Imperatori (Earth & Environmental Science, 34 000 node h)

COVID-19 study, Petros Koumoutsakos (Mechanics & Engineering, 500 000 node h)

VISIONNANO – Viscoelastic properties, entanglements, and polymer dynamics in ionic nanocomposites, Martin Kröger (Chemistry & Materials, 320 000 node h)

Molecular mechanisms behind membrane binding and pore creation of gasdermin A3, Kristyna Pluhackova (Life Science, 100 000 node h)

Resolving clouds, Sebastian Schemm (Earth & Environmental Science, 36 000 node h)

Simulating the first steps in fertilization, Viola Vogel (Life Science, 270 000 node h)

Exciton-lattice coupling in lead-halide perovskites, perovskite nanocrystals, and NC thin-films, Nuri Yazdani (Chemistry & Materials, 309 000 node h)

Friedrich-Alexander University of Erlangen-Nuremberg

Slug flow investigations with phase-field modelling, Harald Köstler (Mechanics & Engineering, 440 000 node h)

HES-SO Valais-Wallis

GPU-SPHEROS: A GPU-accelerated particle-based solver for erosion prediction in hydraulic turbines, Cécile Münch-Alligné (Mechanics & Engineering, 200 000 node h)

Institute for Snow and Avalanche Research SLF

Small-scale simulations of drifting snow using Large Eddy simulations and a Lagrangian stochastic model, Michael Lehning (Earth & Environmental Science, 100 000 node h)

Effects of blowing snow on the Antarctic surface mass balance, Michael Lehning (Earth & Environmental Science, 100 000 node h)

Simulating post glacial migration of tree species to better understand their interactions with the mega-faunaparatory project, Heike Lischke (Earth & Environmental Science, 211 000 node h)

Using the Intermediate Complexity Atmospheric Research Model (ICAR) for studying snow atmosphere interactions and climate change assessments, Rebecca Moss (Earth & Environmental Science, 110 000 node h)

Nuritas

Characterisation of a peptide network with a combined anti-viral and anti- inflammatory activity against COVID-19, Hansel Gomez (Life Science, 588 000 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, 16 000 node h)

Thermodynamic insights into strong metal-support interaction of transition metal nanoparticles on titania, Dennis Palagin (Chemistry & Materials, 135 000 node h)

Pore-scale modeling of realistic rock-core dissolution experiments, Nikolaos Prasianakis (Earth & Environmental Science, 120 000 node h)

High-throughput discovery of high temperature multiferroics, Georg Schusteritsch (Chemistry & Materials, 258 000 node h)

Physical Meteorological Observatory Davos / World Radiation Centre

Past and future of the Ozone Layer Evolution (POLE), Eugene Rozanov (Earth & Environmental Science, 94 000 node h)

SUPSI

eluciDating the moleculaR mechanism responsible for the protective role of trodUsquemine aGainst Alzheimer's Disease (DRUGAD), Gianvito Grasso (Life Science, 35 800 node h)

Learning to control exchange dynamics in supramolecular polymers, Giovanni M. Pavan (Chemistry & Materials, 200 000 node h)

Tata Institute of Fundamental Research Mumbai

Characterising the Lyman-alpha forest into the epoch of reionization, Girish Kulkarni (Physics, 200 000 node h)

University Hospital Zurich

Artificial intelligence dermatological imaging (AIDI), Javier Barranco García (Computer Science, 22 000 node h)

Università della Svizzera italiana

Kinetics, pathways and rates of agonists/antagonists unbinding from the adenosine A2A G protein-coupled receptor, Vittorio Limongelli (Life Science, 150 000 node h)

Supersolidity and superionicity of materials under high pressure using ab initio nuclei-exchange path integral enhanced sampling, Myung Chang Woo (Chemistry & Materials, 50 000 node h)

Kinetics of H_2CO_3 formation and decomposition in aqueous solution and in supercritical CO_2 via enhanced ab initio molecular dynamics, Daniela Polino (Chemistry & Materials, 430 000 node h)

REDAC: REpositioned drugs against COVID-19, Vittorio Limongelli (Life Science, 350 000 node h)

GPU based computational geophysics using Utopia, Patrick Zulian (Earth & Environmental Science, 20 000 node h)

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General relativistic MHD simulations of large-scale black hole jets, Oliver Porth (Physics, 200 000 node h)

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SAVECARBON, Fortunat Joos (Earth & Environmental Science, 287 000 node h)

Effect of inflow conditions on leaflet fluttering in bioprosthetic aortic heart valves, Dominik Obrist (Life Science, 60 000 node h)

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The role of water-ethanol mixture and ionic strength on the aggregation of mixed-monolayer-protected gold nanoparticles, Stefano Vanni (Life Science, 183 000 node h)

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Dark energy and modified gravity with gevolution, Martin Kunz (Physics, 224 000 node h)

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Using deep equilibrium nets to solve large-scale dynamic stochastic overlapping generation models, Simon Scheidegger (Economics, 49 600 node h)

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University of Rome 2

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COVIDYN, Himanshu Khandelia, (Life Science, 514 700 node h)

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University of Zurich

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Black hole feedback in massive galaxies at high redshift, Robert Feldmann (Physics, 90 000 node h)

Liquid-liquid phase separation of highly charged disordered proteins, Milos Ivanovic (Life Science, 100 000 node h)

The PHOEBOS simulation: Unveiling the pathway to direct collapse black holes in primeval galaxies, Lucio Mayer (Physics, 200 000 node h)

Advancing real-time propagation methods for spectroscopy in the condensed phase, Sandra Luber (Chemistry & Materials, 98 000 node h)

Predictive models of galaxy formation, Romain Teyssier (Physics, 350 000 node h)

ZHAW

Large Eddy simulation of laminar separation bubbles and hybrid modelling techniques, Marcello Righi (Mechanics & Engineering, 50 000 node h)

Renewals

EPF Lausanne

Exploring very-large-scale motions in turbulent boundary-layer flows by direct and large-eddy simulation, Jiannong Fang (Mechanics & Engineering, 50 000 node h)

Fusion plasma heating via suprathermal ions in tokamaks and stellarators: Unconventional schemes and plasma regimes, Jonathan Graves (Physics, 120 000 node h)

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

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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, 400 000 node h)

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Multiphase fluid flow, evaporation and crystallization in deforming porous materials, Jan Carmeliet (Mechanics & Engineering, 100 000 node h)

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Data driven in-silico nanofluidics, Petros Koumoutsakos (Chemistry & Materials, 200 000 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)

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Computing statistical solutions of three-dimensional compressible fluid flows, Siddhartha Mishra (Mechanics & Engineering, 541 000 node h)

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Imperial College London

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

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Scaling the Legion programming system, Alex Aiken (Computer Science, 60 000 node h)

Università della Svizzera italiana

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University of Basel

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University of Bern

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

University of Geneva

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

Photoinduced spin crossover in iron(II) complexes in solution: Insights from ab initio molecular dynamics studies, Latévi Max Lawson Daku (Chemistry & Materials, 240 000 node h)

University of Zurich

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

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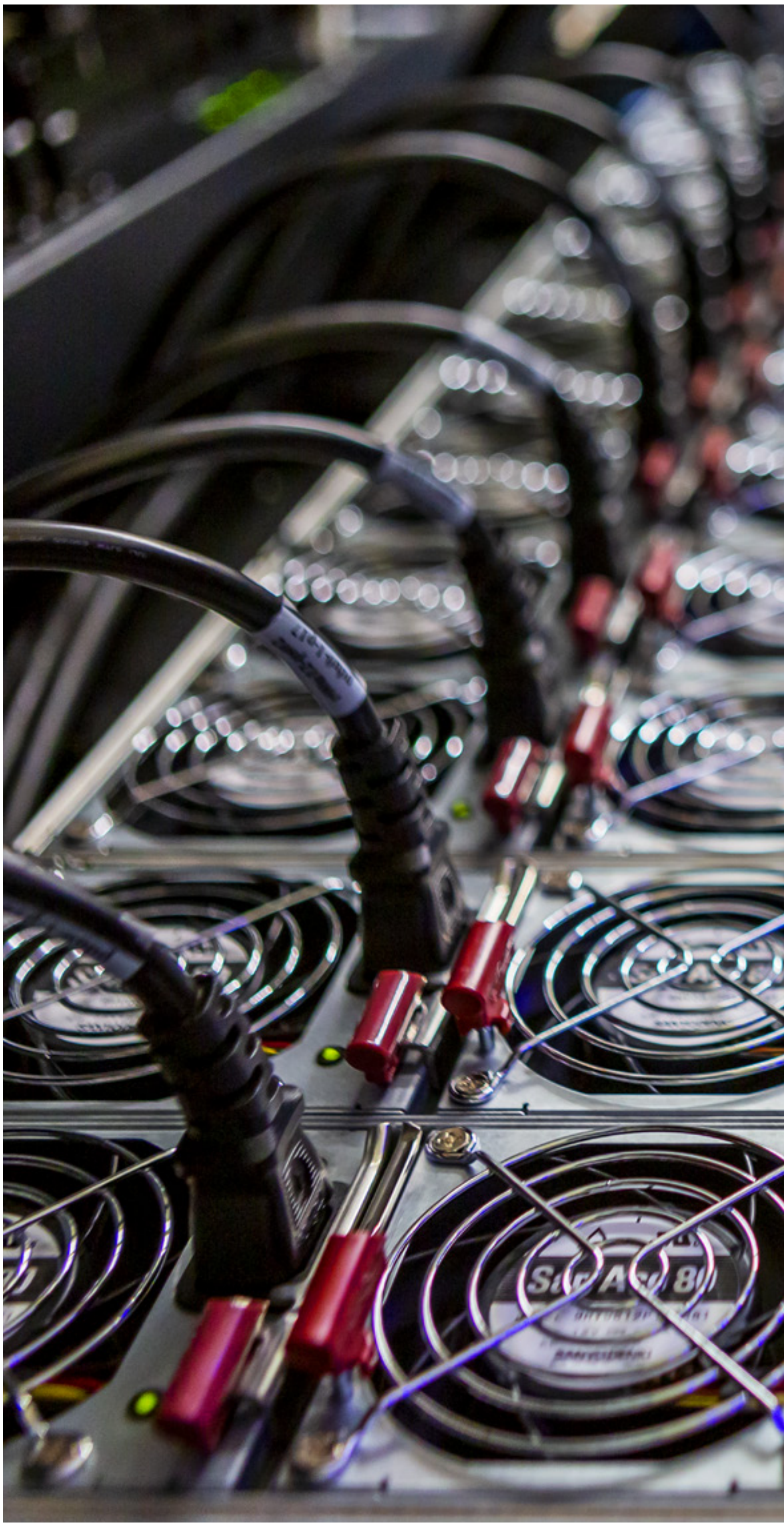
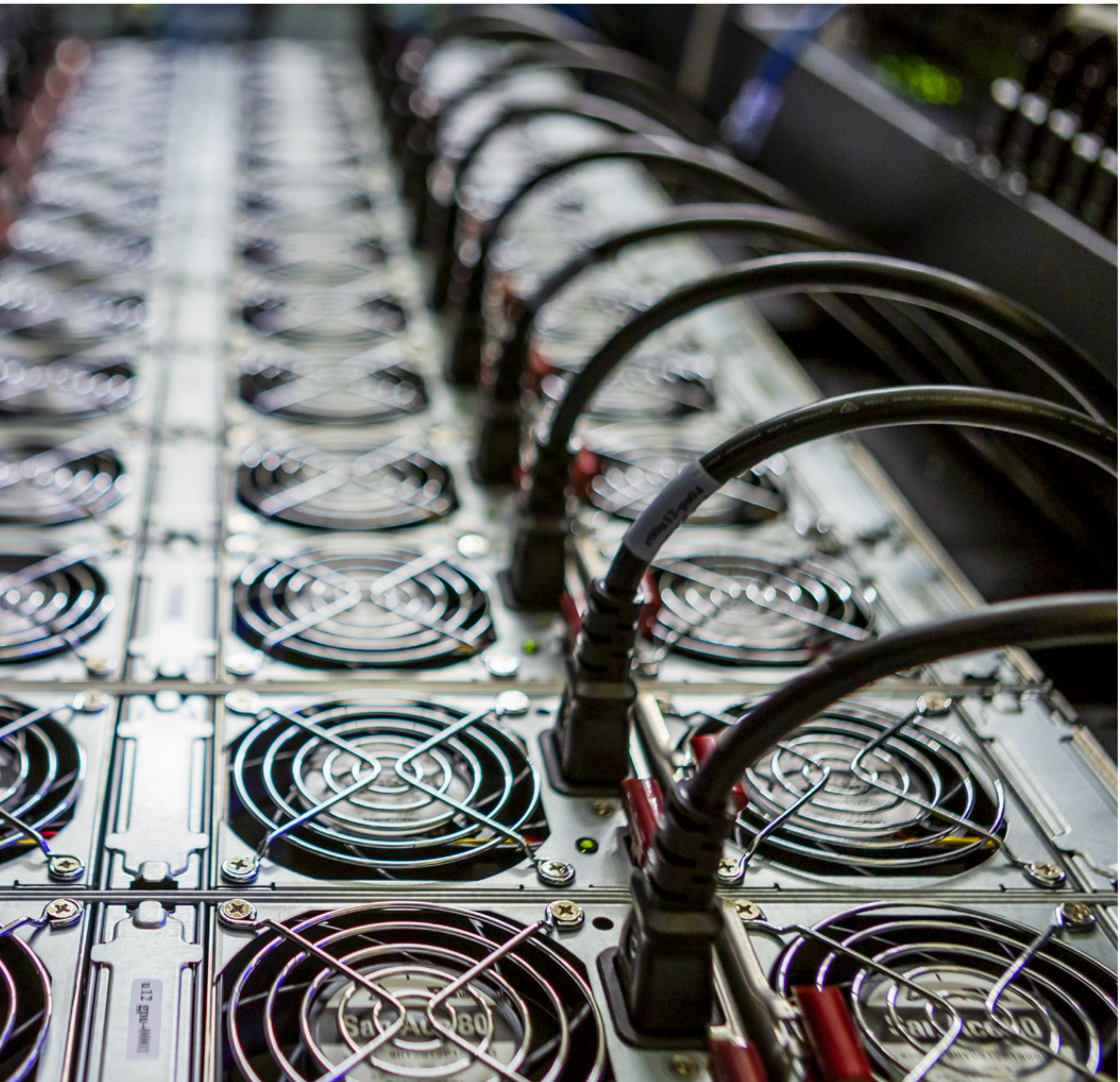
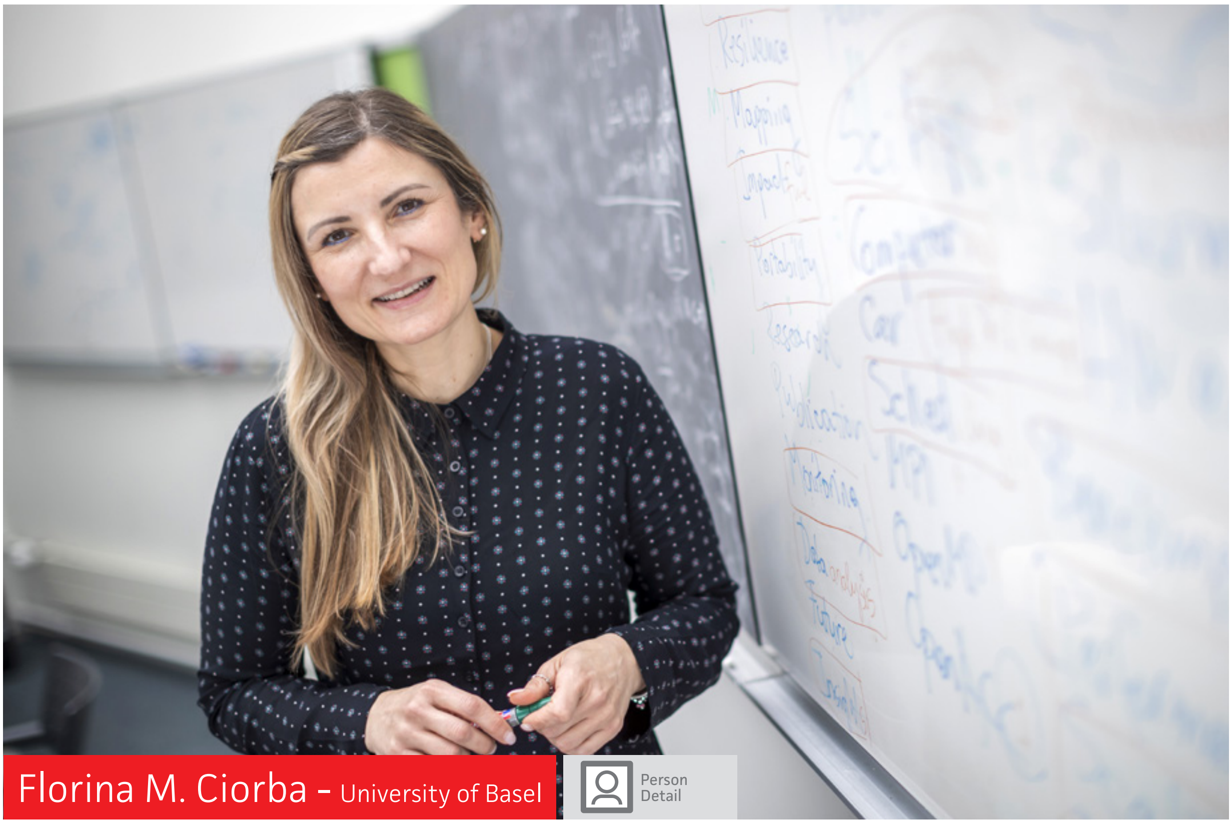






“*Parallelism* and *distribution* are ubiquitous, both in life and in computers. High-performance computers support extreme scales of parallelism and distribution in scientific computation, big data analysis, high-speed communication, and vast storage. Intelligent *resource allocation* and efficient *scheduling* are very important for enabling accelerated scientific discovery in areas ranging from accurate weather prediction, climate modelling, study of the universe’s evolution and of planet formation, to law, drug discovery, epidemiology, and medicine”.

Name
Florina M. Ciorba

Position
Associate Professor of high-performance computing

Institution
University of Basel

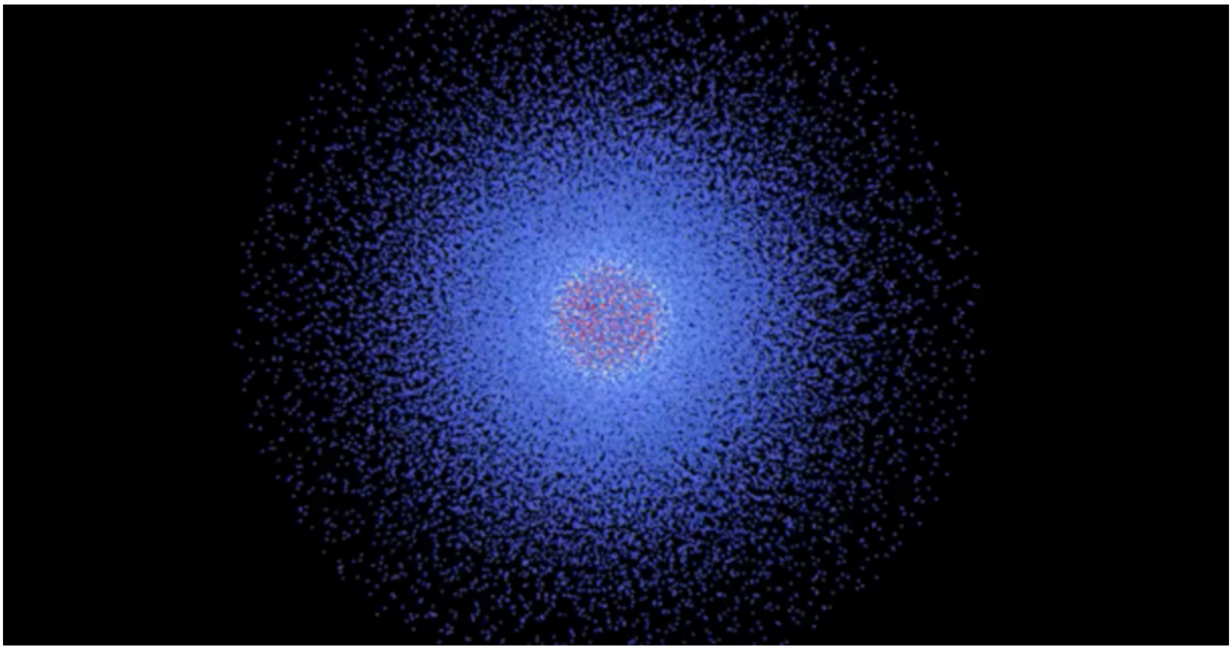
Background

2002–2008	PhD, National Technical University of Athens, Greece
2008–2010	Postdoc, Mississippi State University, USA
2010–2015	Postdoc and Senior Scientist, Dresden University of Technology, Germany
2015–Present	Professor, University of Basel

Area of research
Computer science, parallel and distributed systems, high-performance computing.

Specialised in
Performance optimization of scientific applications via adaptive scheduling and load balancing; performance modelling, simulation, and analysis; monitoring and operational data analytics.

HPC means for me
I am fascinated by the manifestation and intersection of parallelism and distribution in high-performance computing and in real life. Performance optimization through dynamic resource allocation and scheduling is needed at multiple levels in both worlds. Such performance optimization solutions need to be efficient, resilient, adaptive to change, and incur low overhead.

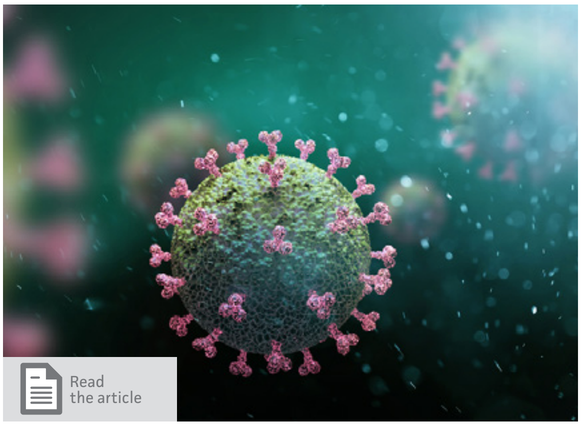


Develop a highly scalable astrophysics simulation code

Florina Ciorba and her team of computer scientists, together with astrophysicists from University of Basel and University of Zurich, developed a highly scalable astrophysics simulation code (SPH-EXA) that implements the smoothed particle hydrodynamics (SPH) method. In 2020, they used “Piz Daint” to perform large-scale hydrodynamical simulations with high efficiency approaching 70%. They will continue to develop the code with the aim to simulate the formation, growth, and mergers of super-massive black holes in the early universe, as well as planet formation, core-collapse and Type Ia supernovas. By employing state-of-the-art SPH and computer science methods (scalable and fault-tolerant algorithms, adaptive scheduling and load balancing), SPH-EXA targets to be the first SPH code to simulate 10^{12} particles on hybrid Tier-0 computing architectures (such as “Piz Daint”). (Image: Florina Ciorba)

PRACE funding accelerates COVID-19 research at CSCS

Throughout the pandemic, CSCS supported special national and international calls to study COVID-19 by participating in the SNF (Swiss National Science Foundation) special call for research on the SARS-Cov-2 virus, as well as in the PRACE (Partnership for Advanced Computing in Europe) Fast Track Call for Proposals. Matteo Dal Peraro, associate professor at EPF Lausanne, is one of the five PIs that successfully applied via PRACE for a computing grant. In an interview with CSCS's Simone Ulmer in May 2020, Dal Peraro explains the research team's scientific goal behind the project: to study the membrane protein which envelopes the SARS-Cov-2 virus.



Matteo Dal Peraro, you are an expert in multiscale modeling of large molecular systems, especially membrane protein systems. Tell us about your research on the envelope protein E of the corona virus SARS-CoV-2, carried out using the "Piz Daint" supercomputer.

Dal Peraro: The primary expertise I am using in our proposal for researching COVID-19 is based on our longstanding interest in membrane proteins. Since my PhD and postdoctoral training, I have been working on membrane proteins. When I established my lab at EPF Lausanne, I continued working on it. Now I have several lines of research on membrane-protein interactions, which we tackle using mainly computational chemistry for molecular simulation and modelling, integrated with experimental data. One key aspect is to study their evolution in a realistic environment, or as realistically as we can reproduce it with a computer. To do this, we must run molecular simulations on HPC (high-performance computing) supercomputers.

Why the E protein?

Compared with what other people in our community are studying, protein E is not in the spotlight. Most groups are studying the spike protein or the nucleocapsid protein; this is a natural choice, as they are the main targets to develop vaccines or drugs, for instance. Rather than to duplicate their efforts, we wanted instead to best use our specific expertise on membrane proteins by looking at the E protein, a pentameric channel that allows the transfer of ions into membrane compartments. These functional properties can be relevant for blocking the occurrence or the progress of COVID-19. This has a potentially therapeutic outcome, although, at the moment, the biology of the virus cycle is not yet well understood, nor is the role of protein E.

Specifically, what are you studying?

When we look at the genome of this virus, some proteins are heavily post-translationally modified, like the spike protein as well as the membrane M and E, for instance, which are palmitoylated. This means that some of their cysteine residues are acylated to provide an anchor point to the membrane. Membrane protein E of the coronavirus has three sites of palmitoylation, and one of the goals of the research is to study their role for stability and assembly of the channel formed by protein E. We know that the two membrane proteins of SARS-CoV-2, M and E, are actually very important for assembly in the virus cycle — for the transport and reassembly of the virus in the host cells. However, they are not yet well structurally characterized. The molecular biology of the virus, and protein E in particular, is still poorly understood. One of the first goals of our proposal is therefore to refine the current structural information that we have for the protein E. Our simulations will test and refine the structural information available so far. We have to characterize states of this channel that can be targeted by small molecules, which can be later developed into effective antivirals. Of course, we also hope to provide some basic additional information about this protein that is mostly unknown at the moment.

How will you go about it?
As I mentioned, protein E is expected to form a pentameric channel. Using molecular modeling and simulation, we plan to probe and see if this conformation is stable in the membrane environment; in the simulations, we model it to be as close as possible to the composition of the membrane compartments where protein E is trafficking, the endoplasmic reticulum and the Golgi apparatus. Protein E is known to conduct cations, but its channel lumen is highly hydrophobic. Molecular simulations will thus be helpful to better understand its functional mechanism.

You wrote in your research proposal that you would like to draw on your experience studying the influenza A M2 channel, as you see functional similarities between the two viruses. What are those similarities?

In influenza A virus, the M2 protein forms a channel that is one of the main targets for antiviral drug development. In SARS-CoV2, the E protein, being also able to form ion channels, could have similar functions. Inhibiting it could provide an additional therapeutic strategy, as we know that viruses not expressing E are much less virulent.

Is there a lot of exchange with other research groups?
My idea for this project is to be completely open, to share the information and not compete with anybody, and to try to collaborate with other people. Even within my group, we are trying to do this together – as a PI, I normally assign a project to one person, but for this project, many people are contributing. We will likely collaborate with other groups from the experimental and computational side as well. This is an unusual type of approach, motivated by the fact that in these days, there is a necessity for us to make results available very quickly, even before publication, to most people in the scientific community. My feeling is that everything is much more open, and this also seems to be the case for other research groups working on COVID-19 programs — now there is more collegiality. People are sharing and are more open to exchange of information so that we can proceed faster than usual. I think this is a great opportunity for the scientific community to explore and get used to different ways to work together.

Apart from the fact that theoretical calculations sent from home to the supercomputer "Piz Daint" are currently easier to perform than laboratory experiments, what is the advantage of simulations over laboratory experiments in this case?

Simulations can give you information that experiments sometimes cannot. Of course, there needs to be an interplay between experimental and computational work. The type of simulations we do need to start from experimental data, but they can then provide new, richer information that is not visible in the experiment. For instance, experiments offer a static snapshot of these proteins in one particular state, which might be, in our case, not the most physiologically relevant one. With the simulations, we are able to expand these static snapshots and add dynamic information. Our simulated protein can be explored in other states based on temperature effects and different environmental conditions, like a specific membrane compartment, for instance. In this case, we take the structure of E protein stabilized in micelles and explore its state in a phospholipid bilayer that is modelled in a way to mimic the endoplasmic reticulum or Golgi apparatus. In the same spirit, palmitoylation is something that is not captured structurally in experiments, at least the ones we have available now, so this can instead be modelled in the simulation. We can probe to find the effect of these post-translational modifications for the stability and conduction of the channel, which is extremely difficult to do experimentally; but computationally, we have theoretical models and techniques that are very robust and reliable to study protein function.

And beyond that?
What the simulations provide on top is a realistic molecular movie of these proteins. You can observe all the atoms of the system, one by one, and gain a detailed understanding of the molecular mechanism that proteins use to interact with each other or with the membrane. This is highly informative, especially when you want to develop interacting entities like a drug. Even for vaccine design, people are using this kind of approach, i.e. structure-based, to engineer proteins that mimic the epitope of some of these viral proteins. Now, we have the next six months to develop some basic understanding of this protein, which is much less characterized than others in the SARS-CoV-2 virus; based on our findings, we can think about the next steps.

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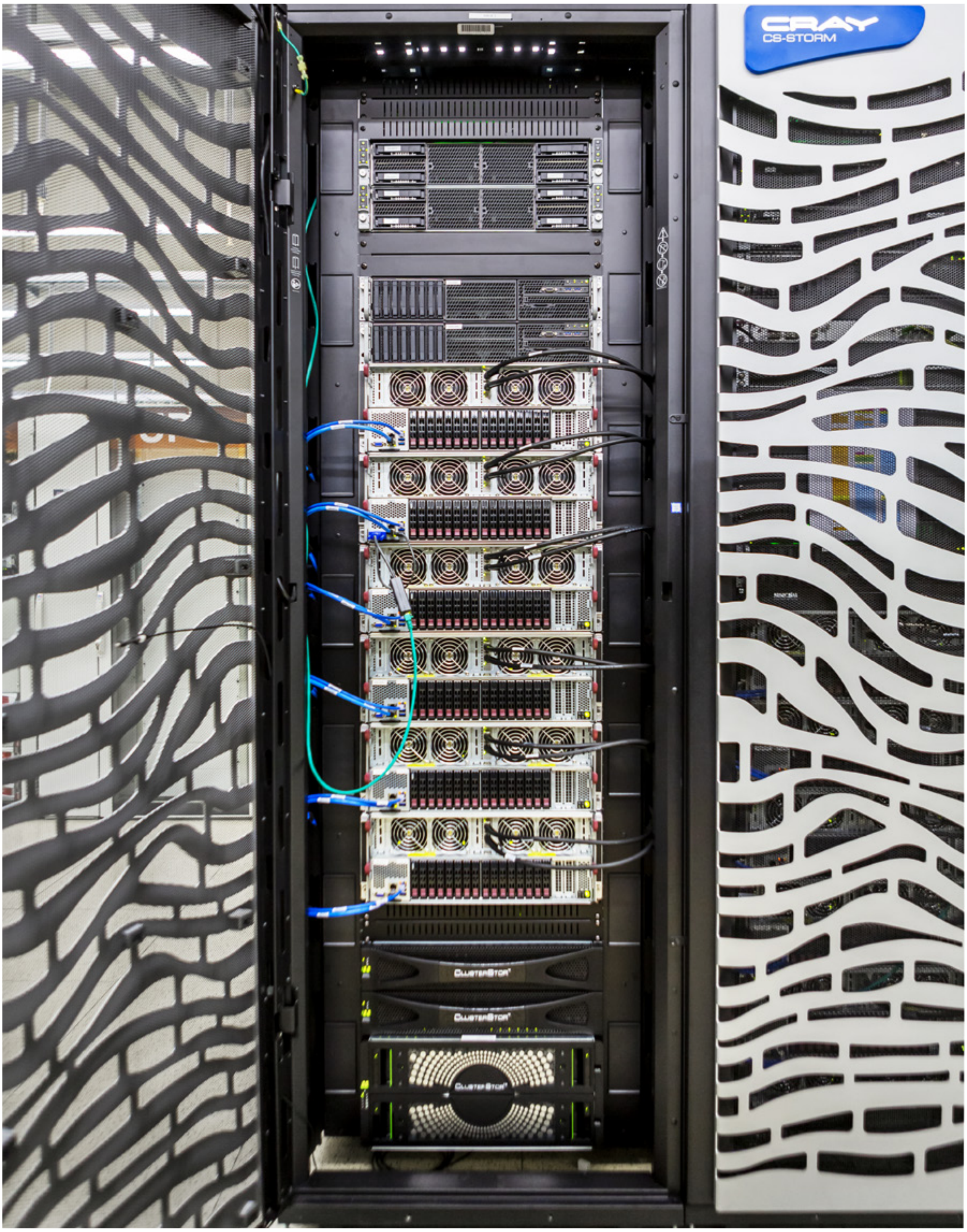
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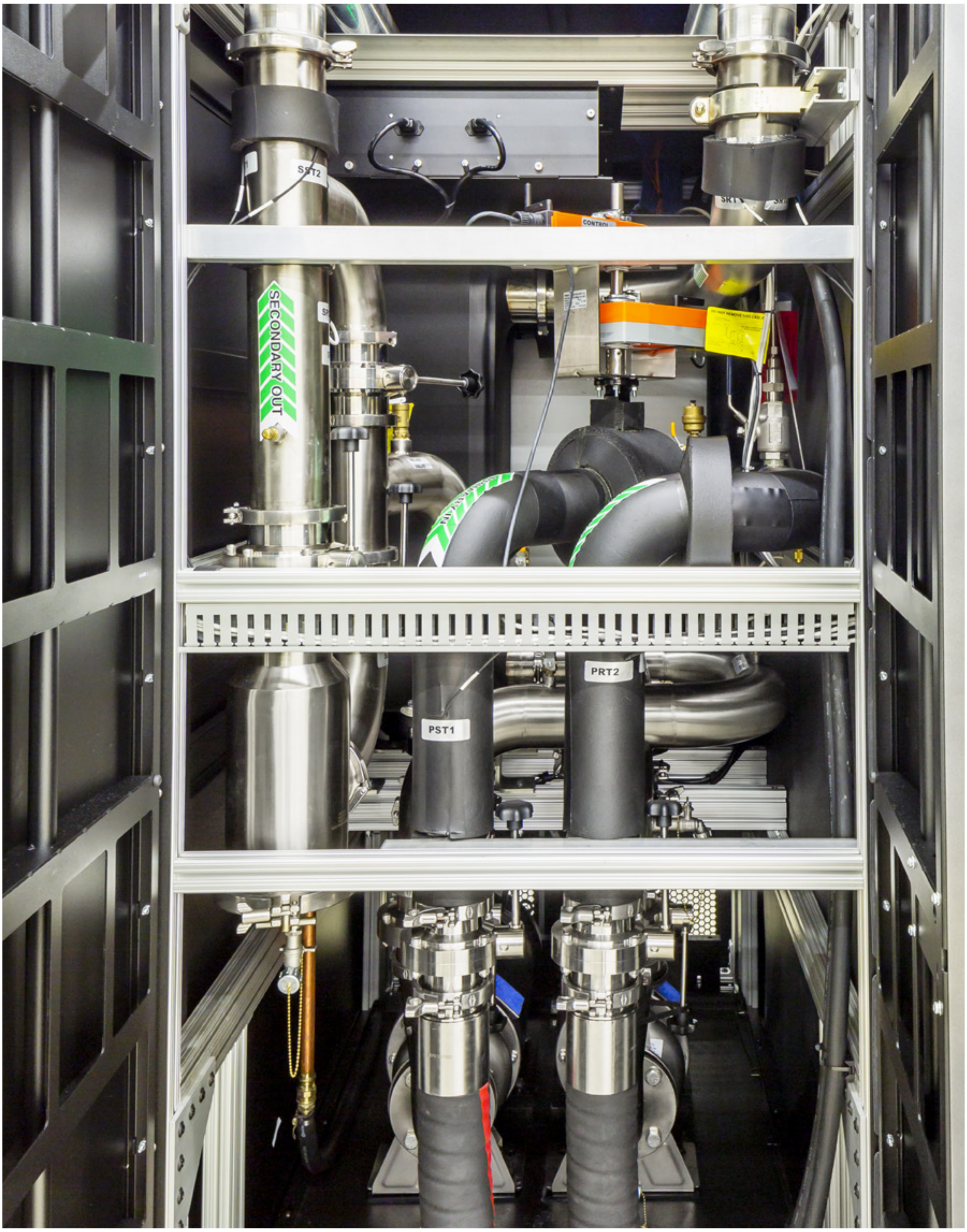
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Marina Krstic Marinkovic - ETH Zurich

Person Detail

“The relationship between my research field of lattice quantum chromodynamics (lattice QCD) and high-performance computing (HPC) is a two-way street: the progress of the field relies on powerful supercomputing facilities, such as CSCS with ‘Piz Daint’; and at the same time, lattice QCD has been driving the development of the field of high-performance computing in the past decades. This synergy allows us to use numerical simulations of strong interaction to learn about new physics beyond our current best theoretical description of particle physics”.

Name
Marina Krstic Marinkovic

Position
Assistant Professor, Institute for Theoretical Physics

Institution
ETH Zurich

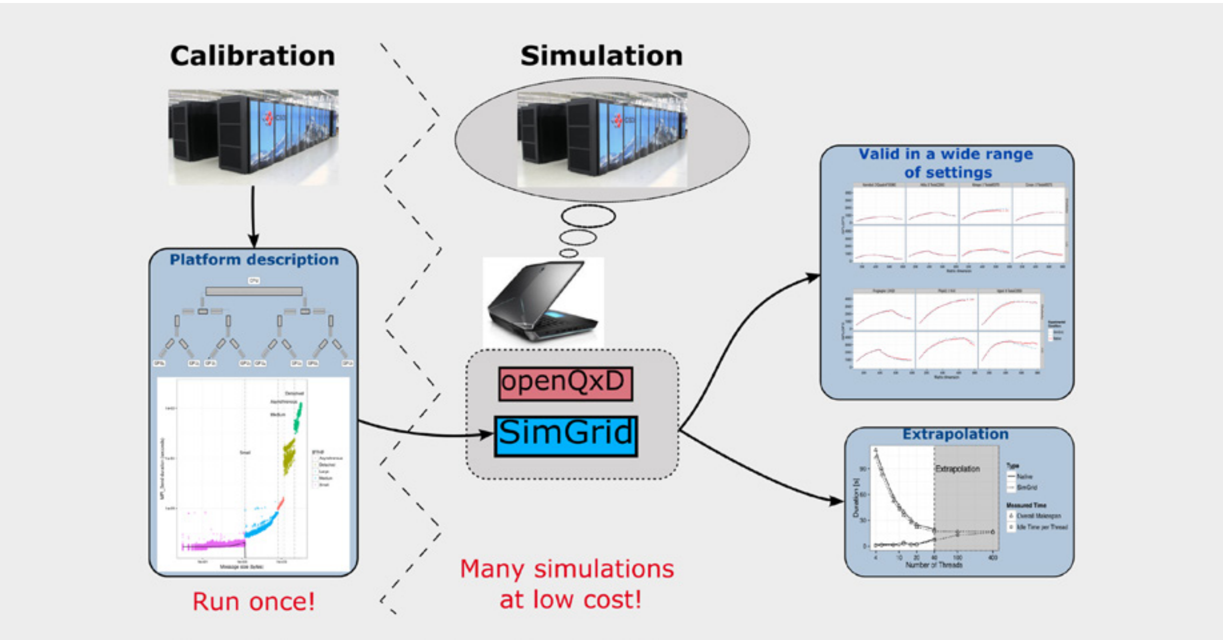
Background

2009-2013	PhD, Humboldt University of Berlin, Germany
2012-2014	Postdoc, University of Southampton, UK
2014-2017	CERN Fellow
2016-2019	Hitachi assistant professor, Trinity College Dublin, Ireland
2020-2021	Junior professor, LMU Munich, Germany
2021-Present	Assistant professor, ETH Zurich

Area of research
Lattice quantum chromodynamics.

Specialised in
QCD+QED, muon g-2, algorithm development and optimisation, machine learning and quantum computing.

HPC means for me
My research would not be possible without HPC. Making predictions and interpreting experiments in particle and nuclear physics is strongly reliant on the recent advances in performance analysis, algorithm and HPC hardware development. I am optimistic about leveraging artificial intelligence to solve long-standing problems in particle physics, as well as applying lessons learned from HPC to the upcoming era of quantum computing.



Researching the theory of strong interaction

Marina Marinkovic and her team are investigating the interplay of the theory of strong interaction — quantum chromodynamics (QCD) — with the quantum theory of electrodynamics (QED). This is important for comprehending the discrepancy between the prediction of the current best theoretical description, the Standard Model of particle physics, and the experiment pertaining to one of the most prominent quantities in the pursuit of new physics beyond the Standard Model: the anomalous magnetic moment of the muon. While working to answer these new physics questions, Marinkovic also works to automatize the adaptations of the existing codes for future HPC machines. Her goal is to enable efficient profiling and optimization of the developed codes on a new platform by developing the profiling procedure through simulation. This will reduce global costs of porting codes and leave more computer and human time for obtaining physics predictions. (Image: M. K. Marinkovic, L. Stanisic)

Neural networks show potential for identifying gamma-rays

A prototype of a CTA telescope at La Palma. (Image: Flickr/CTAO)

The Cherenkov Telescope Array (CTA), currently under construction at La Palma, Canary Islands and in the Atacama Desert in Chile, will be the largest gamma-ray telescope array ever built. It will employ more than 100 telescopes designed to comprehensively record flashes of light induced by gamma rays, which are high-energy photons originating from violent cosmic events such as supernova explosions or mass accretion on a supermassive black hole. Gamma rays are a trillion times more energetic than visible light, so when they hit the Earth's atmosphere, they interact with the atoms and molecules of the air creating a shower of secondary charged particles. These particles move faster than light in the air, emitting ultraviolet light — the Cherenkov light. Flashes of such light are collected by telescopes' mirrors and focused to extremely fast cameras. With this data, astrophysicists can draw conclusions about the physical processes within galactic and extragalactic sources, which act as natural accelerators and produce radiation far beyond even the Large Hadron Collider (LHC).

The photos of these cosmic events show elongated ellipses — a projection of showers of secondary particles. Usually, two kinds of particles cause these events: hadrons (cosmic rays) and gamma rays. There are well established procedures for differentiating between the two; but to be as certain as possible that only gamma rays are detected and evaluated, many ambiguous events are filtered out.

To improve the discrimination procedure and thus the sensitivity of the observatories, Etienne Lyard and his colleagues from the Université de Genève attempted to distinguish them using deep convolutional neural networks (CNNs) trained on "Piz Daint". "Our work is an attempt to use neural networks from computer vision, a kind of machine vision that processes and analyses the images in a variety of ways and adapts them to work on our data," says Lyard. It turns out that, under specific conditions, the CNNs do outperform classical techniques.

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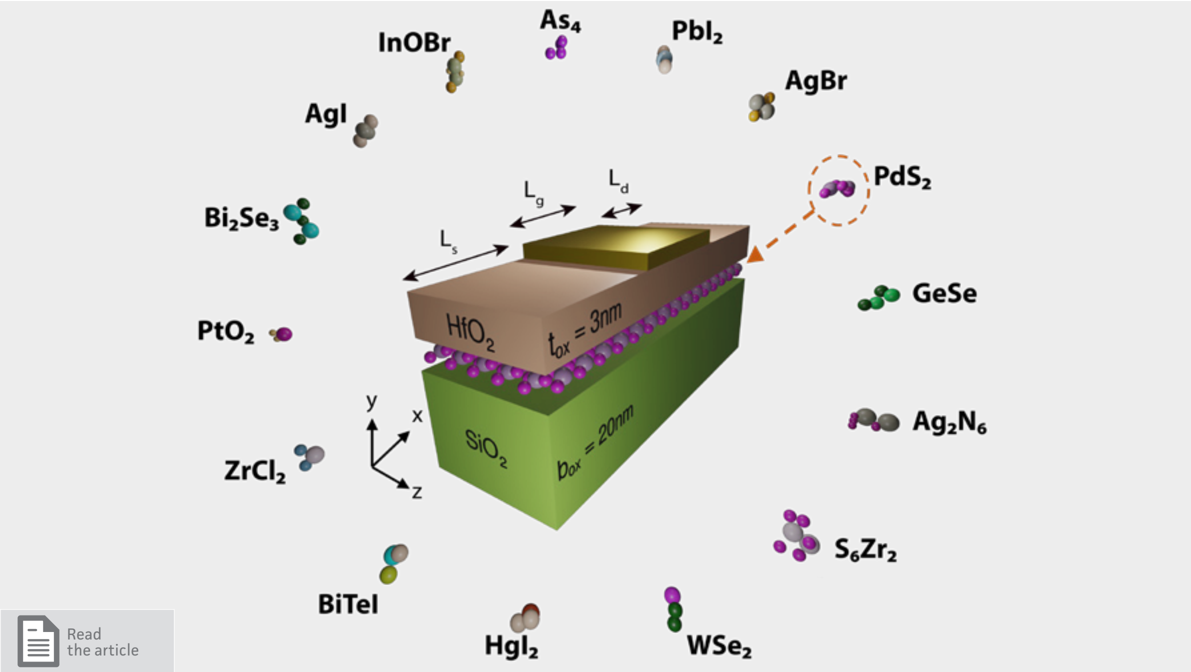
"Simulation microscope" examines transistors of the future



Structure of a single-gate FET with a channel made of a 2-D material. Arranged around it are a selection of 2-D materials that have been investigated. (Image: Mathieu Luisier/ETH Zürich)

After more than 50 years of miniaturizing electronic components, researchers still struggle with several undesirable side effects that impair functionality of nanometre-scale transistors made of silicon, the workhorse of the semiconductor industry. The most detrimental of these effects are increased leakage power, limited ON-state current, slow carriers, and poor scalability. Moore's scaling law, which states that the number of integrated circuits per unit area doubles every 12-18 months, is therefore believed to soon reach its limit. The increasing challenges associated with miniaturisation will ultimately prevent further scaling of the dimensions of currently manufactured silicon-based transistors — called FinFETs — that almost every supercomputer equips.

A recent study by researchers at ETH Zurich and EPF Lausanne showed that this problem could potentially be overcome with novel two-dimensional (2-D) materials. The research groups, led by Mathieu Luisier of ETH Zurich and Nicola Marzari of EPF Lausanne, investigated the properties of 100 promising material candidates under the "ab initio" microscope. In other words, they used "Piz Daint" to first determine the atomic structure of these materials using density functional theory (DFT). They then combined these calculations with a so-called Quantum Transport solver to simulate the electron and hole "current vs. voltage" characteristics of the virtually generated transistors. The study targeted 2-D materials with high carrier velocities that can supply an electron and hole current greater than 3 milliamperes per micrometre and have excellent gate length scalability. "Only when these conditions are met can transistors based on two-dimensional materials surpass conventional Si FinFETs," says Luisier.

The researchers identified 13 possible 2-D materials with which future transistors could be built that could also enable the continuation of Moore's scaling law. Some of these materials are already known, like black phosphorus or HfS2, but Luisier emphasizes that others are completely new — e.g. Ag_2N_6 or O_6Sb_4.

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Is afforestation in any case climate-friendly?

Planting trees to combat climate change might not have the desired effect in every region. (Image: Shutterstock)

Planting trees to combat climate change is a fiercely debated idea in recent times. Trees absorb carbon dioxide (CO_2) trough photosynthesis and could therefore remove this gas from the atmosphere for a limited time. However, when trees die or are used as firewood, the greenhouse gas escapes again. Furthermore, biogeophysical changes resulting from afforestation also have consequences that, until recently, were difficult to quantify. Now, a team of international researchers led by Edouard L. Davin, Senior Scientist at ETH Zurich, have carried out simulations on "Piz Daint" that reveal how the biogeophysical side-effects of afforestation can actually outweigh the benefits. For example, Davin's work shows that afforestation of northern regions could even lead to winter warming.

By comparing model simulations in which Europe is either maximally forested or without any forests at all, the researchers attempted to quantify the biogeophysical effects of land use changes on the regional climate. The ensemble of simulations with varied combinations of land and atmospheric models enabled the researchers to compare the respective influence of atmospheric and land processes. They found that at maximum afforestation, the simulations across all models show temperatures of northern Europe average + 0.2° to +1° Celsius warmer in winter and spring than in a grassland landscape. According to the researchers, this is the direct result of reduced sunlight reflection (albedo) due to afforestation. For summer and autumn, however, the underlying models give a very heterogeneous picture, ranging from large-scale cooling of up to -2° Celsius to a warming of +2° Celsius following afforestation. The researchers suspect that this is due to the fact that models show large differences in the evapotranspiration response to afforestation.

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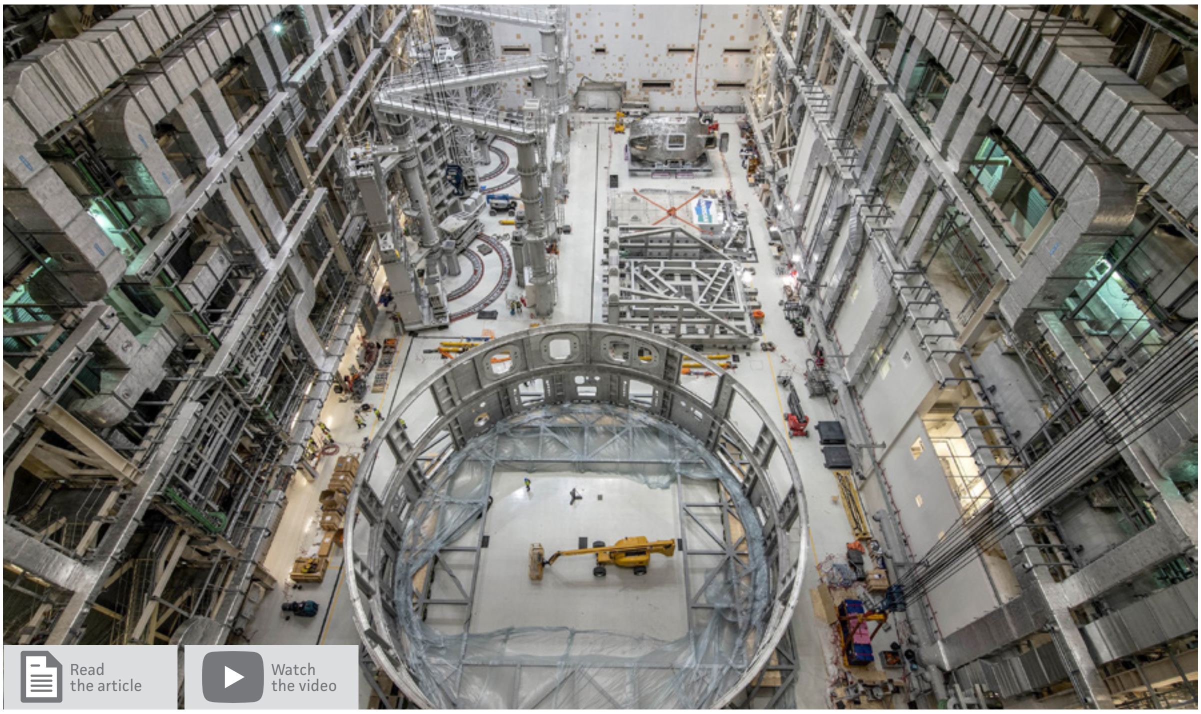
Simulating ITER at CSCS: how scientists aim to control nuclear fusion



ITER construction site in May 2020. (Image: ITER Organization/ EJF Riche)

Construction of the core element of the nuclear fusion reactor ITER — the machine meant to bring a long-sought breakthrough in fusion energy — has begun in southern France. ITER will be the magnetic vessel for ultra-hot hydrogen plasma, designed to fuel fusion reactions to produce energy. Incredibly steep temperature gradients occur within the plasma, between 100 million degrees Celsius in the core and much lower temperatures at the outer rim, which will trigger strong turbulences. "Understanding, predicting and ultimately controlling these turbulences will be crucial for the successful operation of ITER," explains Laurent Villard, adjunct professor at EPF Lausanne. He and his colleague Paolo Ricci, an associate professor at EPF Lausanne, use "Piz Daint" to investigate how heat and particles move within the plasma and affect the reactor wall.

Villard and his team use so-called gyrokinetic modelling to represent the physics of the plasma core, where the particles' velocity and kinetic energy is extremely high. They discovered that turbulence of the plasma core is affected even by small-scale instabilities occurring at the very periphery of the plasma. In addition, the team identified the first-known mechanisms of how large-scale instabilities interact with plasma turbulences — processes that can change the behaviour of the whole reactor.

Complementary to Villard's investigation of the plasma core, Paolo Ricci uses enhanced fluid dynamics to simulate the activity at the edge of the plasma and in the space between the plasma and the reactor wall. "At this interface between plasma and wall, we face the steepest temperature gradient in the system," says Ricci. The simulations enabled his team to understand the dependence of the plasma heat flux on factors like machine size, plasma density and applied heating power, and then to estimate the heat flux in ITER during its start-up phase. Their findings should help to operate the fusion reactor safely and in the most effective way.

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Dominik Obrist – from mechanical engineer to computer salesman to biomedical fluid dynamicist

Dominik Obrist, University of Bern. (Image: Alessandro Della Bella)

Mechanical engineer Dominik Obrist has been enthusiastic about computers for years and working with supercomputers and simulations has become his passion. His work focuses on simulating everything to do with the human circulatory system, particularly the heart. When he was appointed professor at the University of Bern in 2013, he fulfilled a long-held wish: To verify his results on the CSCS supercomputer "Piz Daint" using laboratory experiments.

The delicate valves of the human heart are an impressive anatomical masterpiece: the small, sail-like structures ensure the orderly flow of blood through the heart to the rest of the body. Healthy valves guide the blood so skilfully that it maintains a mostly laminar flow with no turbulence. However, pathological changes or congenital deformities in the heart valves can impair the bloodstream and thus the optimal blood flow. A defective aortic valve, for example, may lead to an aneurysm – a life-threatening event where the misdirected blood broadens and thins out the arterial wall until it eventually ruptures.

In order to prevent an aortic aneurysm, the defective heart valve can be replaced with a biological or mechanical valve. However, biological replacement valves have a limited lifespan of about 10 to 20 years, and it has not yet been possible to develop mechanical heart valves that can regulate blood flow as well as a natural one. Unfortunately, mechanical valves cause turbulence that leads to blood platelets clumping together and forming blood clots on the vessel walls. If these clots detach and move towards the brain, they may obstruct blood vessels and cause a stroke. As a result, patients with mechanical heart valves have to take blood thinners for the rest of their lives.

Turbulence caused by mechanical heart valves

Dominik Obrist, professor and head of the research group for Cardiovascular Engineering at the ARTORG Center for Biomedical Engineering Research at the University of Bern, has been investigating turbulent flow behaviour since 1996 – since working on his master's thesis at ETH Zurich. Supercomputing resources at the CSCS are essential to this research.

Today, Obrist also operates an experimental flow laboratory with cutting-edge measurement technology – a heartfelt wish the researcher was able to fulfil using his professorship funds seven years ago. The Aargau native is proud to show the equipment he and his team constructed themselves to investigate, among other things, the turbulence that occurs when the blood stream hits an artificial heart valve. In this experiment, a mixture of glycerine and water is used to simulate the blood flow. High-speed cameras and laser-based methods for three-dimensional flow quantification show what subsequently happens when the flow encounters the mechanical valve.

What is real?

The combination of simulation and experiment is important, Obrist explains, because running calculations and getting results does not necessarily reflect reality. “We computer people are good at taking partial differential equations, translating them into computer programmes and getting them to run. But we lack an understanding of biological processes.” Afterall, the anatomy of every human is different. This seems trivial at first, says Obrist, but when you build an aeroplane, the blueprint includes tolerances that guarantee that the wing lies within 0.1 mm above or below a specific length. “We know roughly the shape and size of a heart. The word ‘roughly’, however, reflects a mindset with which we as engineers struggle, as we have always learned that things must be precise,” he explains. In biology, everything is suddenly softer and difficult to grasp. Translating this into computer models is difficult, and Obrist is convinced that therefore experiments form a key complementary tool.

On this basis, he and his team were recently able to show what happens when blood meets a mechanical valve – particularly where and how the dangerous turbulence forms. Using this knowledge, heart valves could be optimised in a way that prevents the generation of turbulence altogether. For many people – 250,000 patients around the world receive a new valve every year – this may mean they would no longer need to take blood thinners, which could improve their quality of life.

A research career with detours

At the beginning of his career, it never occurred to Obrist that he would one day use his engineering expertise in medical research, particularly to investigate blood circulation with a special focus on heart valves. He took several professional detours before getting there. One of these initially led him to the University of Washington in Seattle, where he obtained his doctorate on fluid dynamics through research. However, his funding ran out before he could complete his work. Luckily, an internship at Tera Computer (which later became the supercomputer manufacturer Cray) led to a scholarship with which he could continue financing his doctoral thesis.

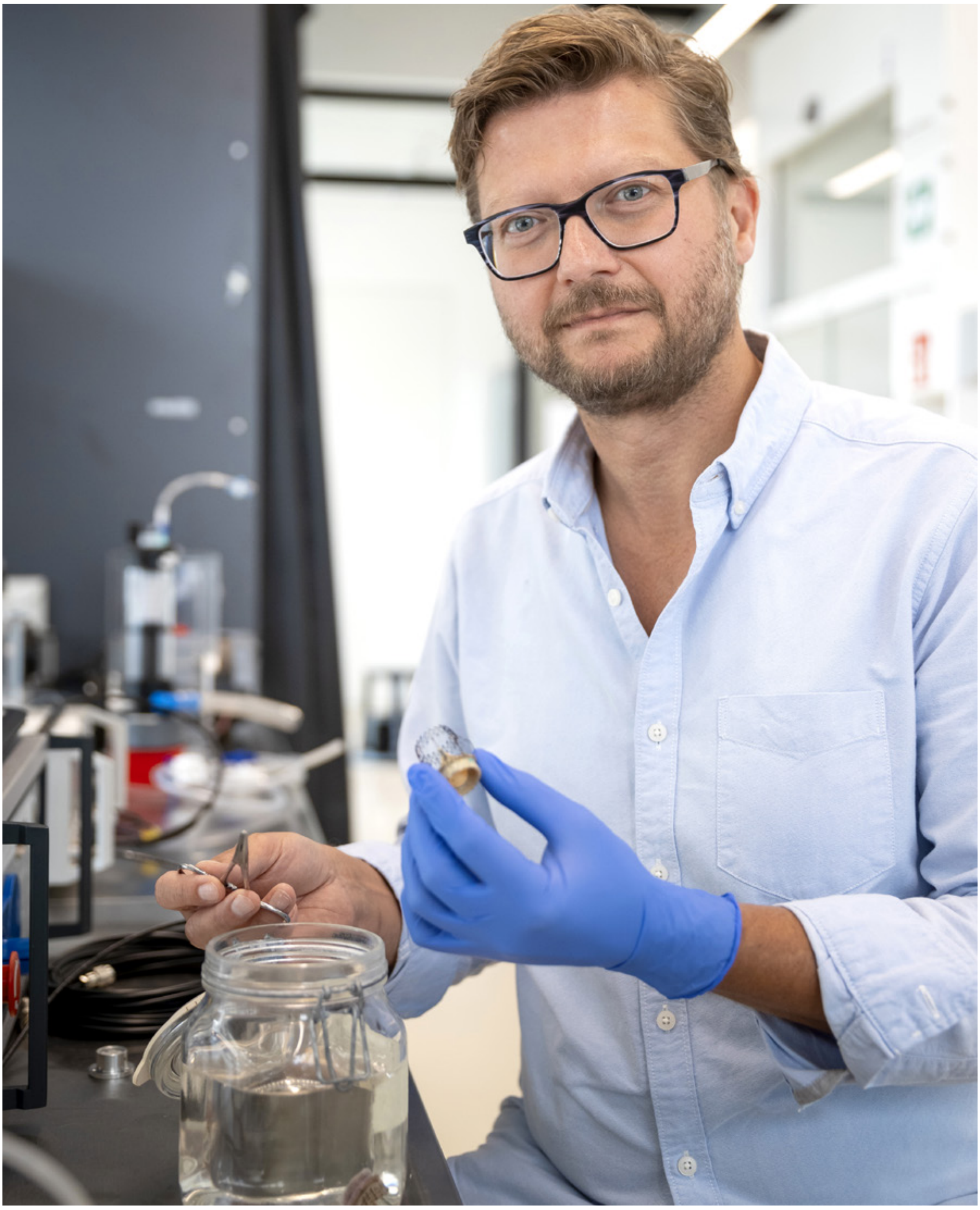
After two years in Seattle, Obrist’s son was born. He and his wife, who moved with him to Seattle, now wanted to return to Europe. “The US is cool for a young couple, but not with children. At the time, I had also had quite enough of the academic world,” he admits openly. “A young family and no money – I wanted to earn a proper salary.”

During his doctoral studies, Obrist had conducted research visits at the Technical University of Munich and the Leibniz Supercomputing Centre in Munich. Cray eventually offered him a steady role in Europe, and at first, he enjoyed the many trips as a pre-sales analyst and then an account manager. However, he eventually began to feel as though he were sitting on the wrong side of the negotiating table when he met researchers. It was therefore a crucial turning point for him when he met a former professor on one of his trips to Munich, who asked Obrist what he now did for a living. At the conference table in his office in Bern, Obrist mimics the way the shaken professor had to sit down under the weight of Obrist's confession that he now sold computers, saying to him half-jokingly: “Mr. Obrist, how low you have fallen.”

When he turned 35, it became clear: “Now is the last opportunity to switch to the other side of the table.” Luckily, ETH Zurich professor Leonhard Kleiser happened to have a vacancy at this time that launched Obrist’s career as a biomedical fluid mechanics engineer. Looking back, he is glad about his naivety – the difficulty he faced in returning to research after five years in industry and living on a senior researcher's salary again only became clear once it was too late to turn back.

Engineers as part of the medical faculty

About 15 years later, Obrist now conducts research in a state-of-the-art building within walking distance of the Inselspital, Bern University Hospital. As his institution is part of the medical faculty, he is convinced that the position he has today is unique in Switzerland, with barely anything similar worldwide. He is proud of his close collaboration with medicine and the direct exchange with doctors, who sometimes take him along to the operating room.



Dominik Obrist in his laboratory at the ARTORG Center for Biomedical Engineering Research at the University of Bern. (Image: Alessandro Della Bella)

There, they can outline specific issues live with a patient, or his team can take measurements and collect data from the patient during surgery. It is also not uncommon for doctors to call him with a question, which then turns into a project. This translation is routine within Obrist's work group, i.e. developing an idea discussed at the operating table or between the doctor and engineer, using it as the basis for a simulation and experiment, and then engineering it into a technical solution – a product. "I always wanted a professorship because I wanted the freedom to test things out," says the professor.

Everything started to fall into place for him in 2005 when he came back to work at ETH Zurich and started a project on the inner ear and the sense of balance. "The inner ear was my ticket to the world of biomedical fluid mechanics," says Obrist. In addition, he took over the biofluid dynamics lecture at ETH Zurich in 2006, a responsibility he still holds today. His research eventually led him to the heart because this is the most prominent area for flows in the body. Still, the flow of blood in the lungs, ear and brain were and remain part of his research portfolio, and a lot of heart research can also be translated to the urinary tract, he says. This is why the 48-year-old recently established a research group and a start-up in the field of urology, with a focus on stents for the ureter between the kidney and bladder. These often become encrusted, leading to problems, and the new team is researching the cause behind this issue.

Although Obrist has moved away from conventional mechanical engineering in the course of his career, he has remained faithful to the simulation of flow processes and thus to supercomputers. Even as a teenager, in addition to his passion for gliding – for which he obtained his license at the age of 17 and subsequently became one of the best glider pilots in Switzerland – he had a strong affinity for computers. At that time, he was not familiar with the term "computational science", but he knew he wanted to study computer science. He is still not entirely sure how he ended up in mechanical engineering – it was a somewhat spontaneous decision when applying for his studies, but one that he has never regretted.

Long-term CSCS user

As a long-term user of supercomputers with a wide range of architectures within the CSCS infrastructure, Obrist now enjoys making the most of interdisciplinary research initiatives such as the Platform for Advanced Scientific Computing (PASC). "The technological changes to CSCS were initially a source of anguish for us, particularly the switch from vector processors to massively parallel computer architectures", admits Obrist. However, when an adjusted code is suddenly able to run 1 000 times faster, he is happy to accept the technological leadership.

In PASC, he is currently working with computer scientists, doctors and medical imaging experts on the project "HPC-PREDICT – High-Performance Computing for the Prognosis of Adverse Aortic Events" to develop software for an innovative prognosis tool for disorders of the ascending aorta, specifically by improving the precision and accuracy of the image data.

Dominik Obrist seemingly never runs out of research ideas. In fact, sometimes he worries that his spectrum is becoming a little too wide – but then he recognises that this variety precisely reflects the freedom he has always wanted.

Ulrike Lohmann - ETH Zurich

“Supercomputers like ‘Piz Daint’ are at the heart of climate modelling. Without such powerful tools, we would not be able to advance weather forecasts and climate projections. Cutting-edge computing technologies enable increased model resolution and improved statistical meaningfulness of the results. They also permit a more detailed treatment of important components of the model, such as clouds and their interactions with aerosol particles. This is crucial for progressing in our understanding of climate change”.

Name
Ulrike Lohmann

Position
Full Professor, Institute for Atmospheric and Climate Science

Institution
ETH Zurich

Background
1993-1996 PhD, University of Hamburg, Germany
1996-1997 Postdoc, Canadian Centre for Climate Modelling and Analysis, Canada
1997-2001 Assistant Professor of atmospheric sciences, Dalhousie University, Canada
2001-2004 Associate Professor of atmospheric sciences, Dalhousie University, Canada
2004-Present Professor, ETH Zurich

Area of research
Atmospheric physics.

Specialised in
Clouds and aerosols in climate, and cloud microphysical processes.

HPC means for me
Being able to study clouds — in the climate system, in their various facets, and on different scales.
This spans from a better understanding on the influence of soot and other aerosol particles on water and ice clouds globally, over investigations about the formation and intensification of Atlantic hurricanes, to hail formation over the Swiss Plateau in summer.

Read
the article

Soot particles influence global warming more than previously assumed

Burning wood, petroleum products or other organic materials releases soot particles into the atmosphere that consist mainly of carbon. This soot is considered the second most important anthropogenic climate forcing agent after carbon dioxide. In the atmosphere or as deposits on snow and ice surfaces, soot particles absorb the short-wave radiation of the sun and thus contribute to global warming. Ulrike Lohmann and her team are the first to use simulations on the CSCS supercomputer "Piz Daint" to investigate how certain ageing mechanisms of soot particles in the atmosphere affect cloud formation. The results show that the influence of ozone and sulfuric acid on soot ageing alters cloud formation and, ultimately, the climate. (Image: Shutterstock)

"We don't just procure a new computer": Thomas Shulthess shares details about planned successor to "Piz Daint"

The flagship supercomputer of the CSCS, "Piz Daint", needs to be replaced. Installation of the successor computer, "Alps", is taking place in three phases and will be completed in 2023. The new machine will provide the CSCS with an innovative supercomputer infrastructure that more directly supports research and helps generate maximum scientific output. CSCS Director Thomas Schulthess explains in an interview with Simone Ulmer why the new computer is so special.

Last year, the first phase of installing the new supercomputer "Alps", the successor to "Piz Daint", started. How has the work been going so far during the Corona crisis?

Thomas Schulthess: We had to change our approach, but we were more or less able to keep to the schedule, even though there were a few minor delays. During the lockdown, it was not possible to bring the first four cabinets of the new computer from the USA to Switzerland as planned. But the manufacturing company HPE still managed to build the hardware, so we had access to our machines in the US in June and July and were able to work on them. Therefore, the acceptance of the computer cabinets in Lugano in autumn went off without any major problems.

The expansion of "Alps" will last until spring 2023. Why is it taking so long?

Because the product we want is not fully developed yet. The central element of the new computer is the Cray Shasta software stack, which we participated in developing with other data centres. This software stack is now operational, but it will take another two years until the desired computer infrastructure will be completely ready.

What is so special about the new computer infrastructure?

With the Cray Shasta software stack, we have opted for a software-defined infrastructure. That is the decisive point for me — without this software stack, the new machine would lose a lot of its value for me. "Alps" would still be the best variant in high-performance computing that will be available on the market in the foreseeable future, but we clearly have higher goals that we would not achieve without the improved infrastructure. That would be a big disappointment.

What does that mean exactly?

At CSCS, we primarily operate a research infrastructure, which we make available to researchers as a User Lab, among other things. That is our core mission. However, in contrast to other

Thomas Schulthess in front of his house. (Image: Alessandro Della Bella) research infrastructures, such as the SwissFEL at PSI, we do practically no research of our own on our instruments. We therefore have to find a creative way to expand our own expertise in order to be able to further develop the research infrastructure. Hence, we collaborate closely with researchers from Swiss universities.

So, the CSCS does not see itself primarily as a service provider?
It does, but not in the sense of an IT company that merely operates computers in order to be able to offer computing time. For us, the computer is the means to an end, and the end is the research infrastructure, which we build and develop together with researchers with funding from the ETH Board; the operation costs are covered by contributions from ETH Zurich. We now want to further develop this research infrastructure with a program with the code name “Kathmandu”.

What exactly is this Kathmandu program about?
The Kathmandu program is an important part of the new procurement mentioned above. We are not simply procuring a new computer that will be integrated into the unchanged computer centre — we are retrofitting the computer centre in several expansion phases. Today, we operate different computer systems for different needs at CSCS, but in the future there will be only one infrastructure. For MeteoSwiss, for example, we have operated a dedicated computer up to now. In the future, MeteoSwiss will compute on one or more partitions of this new infrastructure.

What is the advantage of this solution?
At CSCS, we have always offered various services for researchers, but the system architecture was not service-oriented. Therefore, we always had to expend a lot of human resources to define these services according to the requirements of the users and the architecture of the machines. This process is now easier because we have a software-defined infrastructure.

What does a software-defined infrastructure mean?
If we do everything right together with HPE, our hardware will be very flexible. This means that, in the future, we will define which services we offer via the software, no longer via the hardware. To do this, we combine so-called microservices. In this way, we define the partitions for the various users, which we then make available to them via standardised interfaces. These can be virtual ad-hoc clusters for individual users, but also predefined clusters that research infrastructures such as the PSI put together with us and then operate themselves.

We can also create data platforms with the microservices. For example, we are planning to develop a so-called domain platform for weather and climate simulations with various partners.

You explicitly mention the field of weather and climate. Will "Alps" also be useful for other fields of science?
Yes, with "Alps" we are developing a "general purpose supercomputer". Our goals do not stop at climate simulations at all. However, these are an extremely good means to an end, since the problem is very clearly formulated in climate simulations. In addition, they represent all the requirements of a modern supercomputing and data infrastructure. We respond to these very specific requirements with an infrastructure that we can then also offer to other research areas.

What does this change for the users of the User Lab?
Previous users of "Piz Daint" will be able to use the new system without any adjustments. It should even be easier for them. We will also further develop the HPC platform for the User Lab as a virtual area within the computer system. This will make the resources more powerful, and they will cover larger parts of the workflow. The scientists will not only be able to carry out simulations, but also pre-process or post-process their data. This makes the whole workflow more efficient for them.

So not much will change for the users. What does the conversion mean for the staff at CSCS?
The new strategy will require fundamentally rethinking certain areas. The engineers providing system and user support will have to adjust, for example, because our previous computers that we operated in addition to "Piz Daint" will be virtual clusters in the future. Some staff will develop and maintain microservices, while others will combine these microservices into virtual clusters or applications that are then made available as services to researchers.

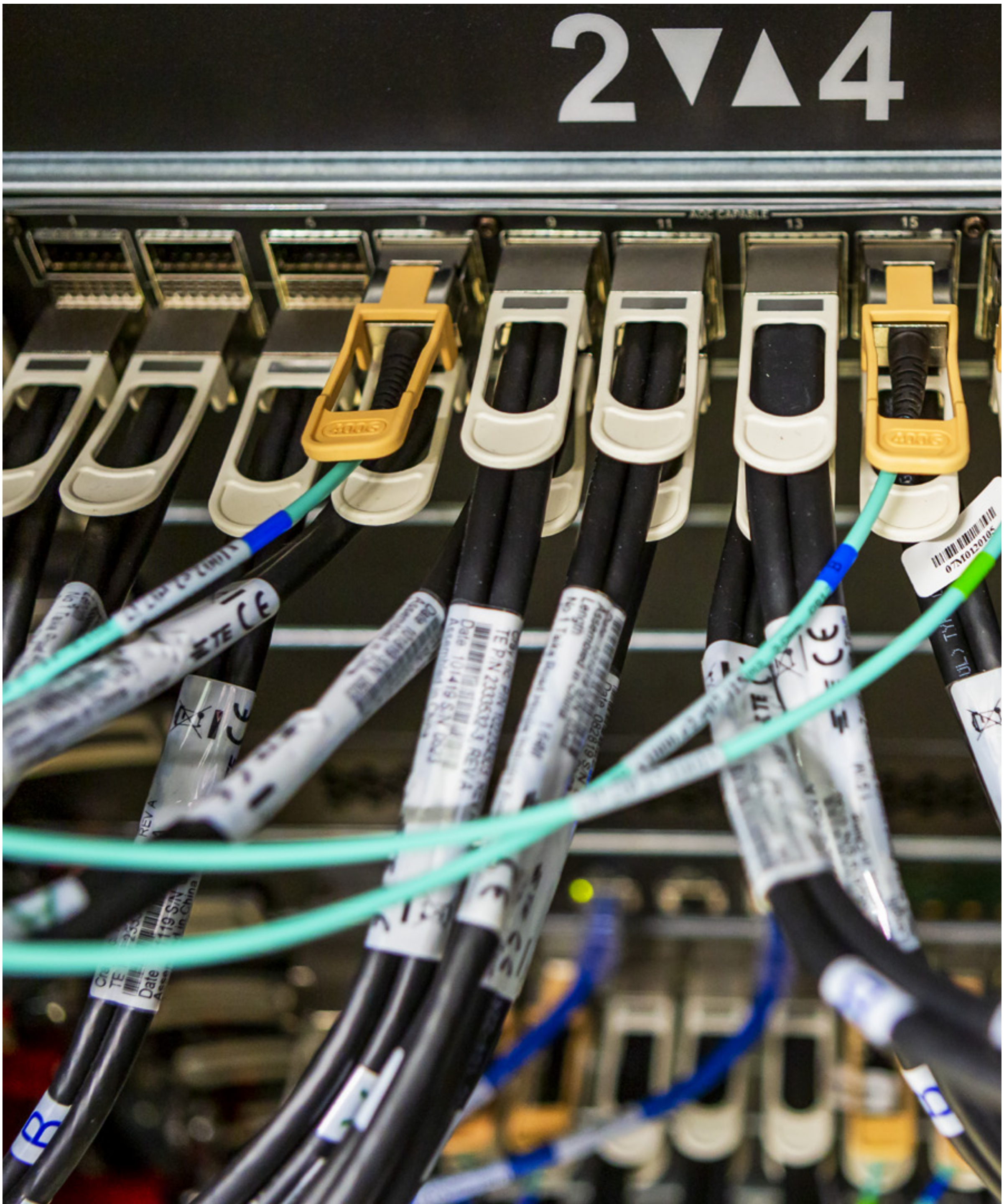
Great efforts are currently being made in Europe to further advance high-performance computing. This includes, in particular, the EU's Pre-Exascale Initiative. How is CSCS involved in these efforts?
CSCS is a member of the LUMI consortium, which is part of the Pre-Exascale Initiative. The acronym stands for "Large Unified Modern Infrastructure". This is a new pre-exascale supercomputer that will be located in Finland. The LUMI consortium has ten member states, including the Scandinavian countries, where the conditions for producing cheap, CO_2-free electricity and cooling the computers are optimal.

Why is this aspect so important?
This can be explained using climate research as an example. Our goal is to develop climate models that can map convective clouds such as thunderclouds. "Alps", the successor to "Piz Daint", will have a connected load of 5 to 10 megawatts. However, a computer infrastructure that is to productively deliver the above-mentioned resolution for climate science must have 50 times the power. Since we can no longer achieve performance gains through Moore's Law, we need a machine 50 times larger than "Alps", which will also increase energy consumption accordingly. It therefore makes sense to build such a computer infrastructure where the required energy can be generated cheaply and in an environmentally friendly way. We do not have such locations in Central Europe, but we do in Northern Europe.

What is the timetable for LUMI?
The LUMI computer is also being built by HPE and is scheduled to reach the pre-exascale performance class in autumn 2021 before going into operation in spring 2022. Our "Alps" system will be installed one and a half years later, at the end of 2022, and will replace "Piz Daint" completely by April 2023. But our new services will already be available this spring and will be expanded later this year during the first expansion phases; and we will try to also integrate LUMI. We will then have a very strong overall infrastructure available, running on two sub-infrastructures, "Alps" and LUMI. We will move faster in this direction than others in Europe.

Does this mean that Swiss computing resources will be relocated abroad in the future?
No, but we must be realistic: We will never operate computers of 100 MW or more in Switzerland. We have to focus the local computing resources in Switzerland on innovative pilot projects and integrate them into a larger network for production. Our intention is to develop software platforms that run on both infrastructures so that users practically don't notice whether their application is running in Finland or in Lugano.

The Swiss National Supercomputing Centre (CSCS) develops and provides the infrastructure and know-how in the field of high-performance computing (HPC) to solve important scientific and societal problems. It implements the national strategy for high-performance computing and networks (HPCN), which was passed by the Swiss parliament in 2009. Since 2011, CSCS has had a dedicated User Lab for supercomputing, and it is part of the Swiss Research Infrastructure Roadmap. Since 2020, it has also been a member of the European LUMI consortium, which is building a European supercomputer of the pre-exascale performance class.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Home office at CSCS

CSCS employees, like many others around the world, had to work from home in 2020 due to COVID-19 public safety measures. During this period, CSCS staff was asked to share their experiences with the home office and their strategies for staying productive.

MICHELE DE LORENZI, deputy director

What are your personal pros and cons of the home office?

In reality, we are not just working from home; we are confined for a longer period of time with our families in our homes. This makes a difference. One of the advantages is that I do not have to commute from Zurich to Ticino, nor from my home in Minusio to Lugano. This makes about 600 km a week. On the other side, I miss the direct contact with my team and work colleagues. I'm not sure if I'm more productive now than I was before.

ALESSANDRO PRATO, IT support

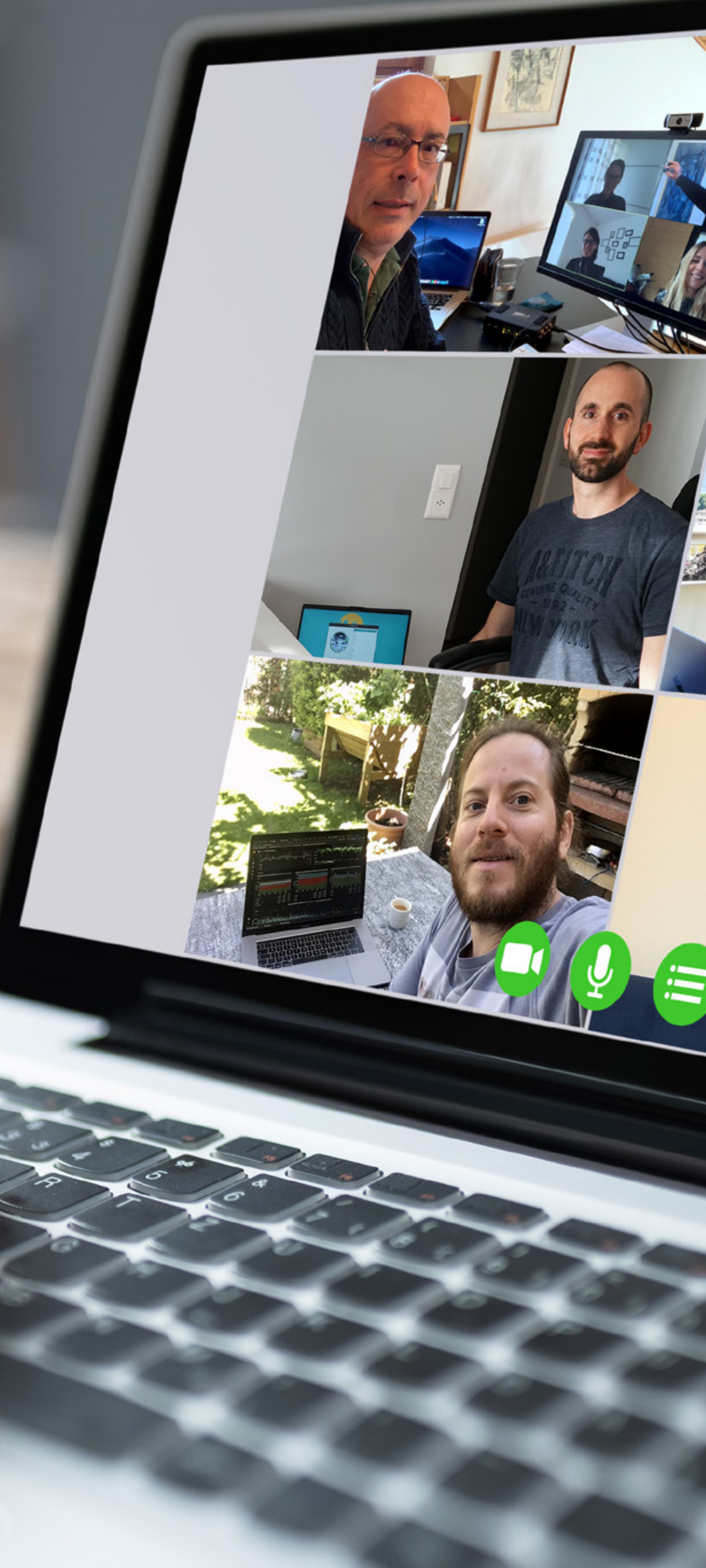
Alessandro, you and your colleagues are providing IT Support to all CSCS staff. What has change since everyone began working from home?

The main challenge is the distance, because I am used to providing IT support in person, where it is easier to investigate and understand a possible issue. Within this situation, I adopted a new approach: I am using remote desktop and video conferencing software. Thanks to these kinds of tools, I can still help all the CSCS staff remotely.

DINO CONCIATORE, system engineer

What are the most common problems with time management (deadline, distraction, overwork)?

I don't have issues with deadlines, personally. Working from home doesn't change my working speed. We are always working with top-of-the-line notebooks, and I was also able to arrange a second monitor screen (my personal iMac). In fact, I have less distraction here, maybe because I don't have children? With fewer interruptions, I can focus more time on topics. On the other hand, I do perhaps overwork, because my laptop is always on. After dinner, I quickly check if the job went fine, if the service is still up, etc. In the morning, I wake up and always take a look at the dashboards to see if something went wrong, and I already start thinking about solutions while brushing my teeth.



PABLO FERNANDEZ, service/business manager

How do you manage to combine family and work?

Both actually take a hit. My kids don't really understand that I'm at home without actually being at home; and, even if I put a sign at the door when there's a meeting happening, they still storm in from time to time. Be it a question, needing help with something, or just wanting to share a drawing, they count on me. I can't blame them — this is difficult for them, too. My wife carries much more extra load than me and is also working part-time… I could not do this without her!

MAXIME MARTINASSO, computer scientist

As a portfolio manager, what are the main challenges you're facing at work, having to meet virtually with so many people every day?

My role as a portfolio manager is to ensure that developments of initiatives continue in the right direction. Like everybody else, I use videoconference tools or chats to talk with the team leaders and organize planning meetings. I find these tools both useful and sufficient to do my work. Sometimes it is even better than starting a discussion in person by entering an office, as it allows your interlocuter to select a time that suits his/her workload better.

NORA ABI AKAR, software engineer

Having worked now for several months exclusively from home, what kind of advice would you give to someone starting full-time home office tomorrow?

I would advise them to get a comfortable work setup with good lighting and to have regularly scheduled work hours. It's easy to slip into the habit of skipping breaks and working late, but my experience is that it's often detrimental to both one's mental state and to the quality of the work. I would also recommend going outside at the end of the workday — it really helps with the transition from work time to personal time.

Finances

Expenditures in CHF

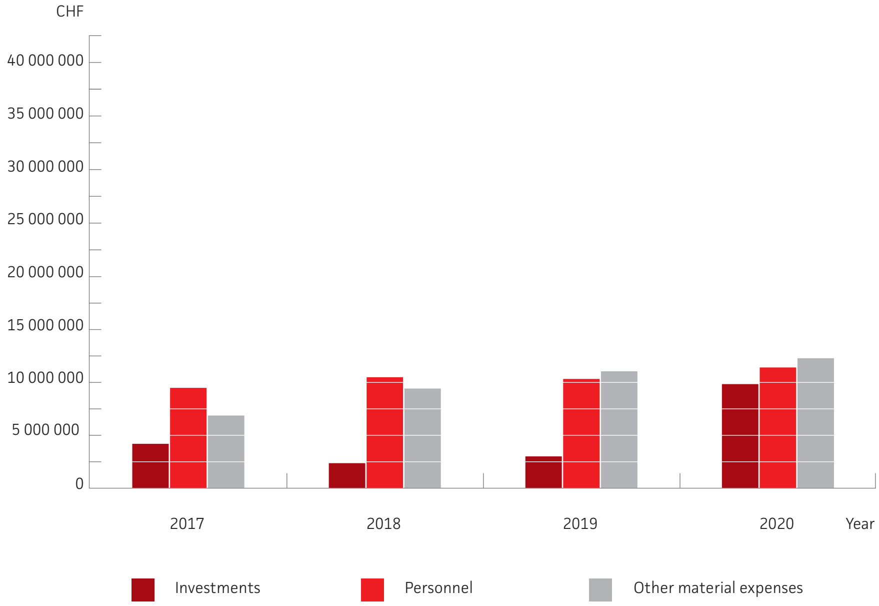
Expenditures in CHF	User Lab	Third Party	Total
IT Investments	**9 840 366.00**	**1 807 245.00**	**11 647 611.00**
Personnel	**11 378 508.00**	**5 019 609.00**	**16 398 117.00**
Payroll	11 171 549.00	5 018 353.00	16 189 902.00
Further education, Recruitment	206 959.00	1 256.00	208 215.00
Material expenses	**12 261 041.00**	**2 666 771.00**	**14 927 812.00**
Maintenance building & technical infrastructure	1 193 233.00	85 157.00	1 278 390.00
Energy	2 774 192.00	773 723.00	3 547 915.00
Backup connection power supply	1 615 000.00		1 615 000.00
Maintenance hardware & licenses	4 131 783.00	384 634.00	4 516 417.00
Remunerations, Marketing, Workshops, Services, Travel, Membership fees	903 236.00	114 057.00	1 017 293.00
Granting of funds for PASC projects	1 643 597.00		1 643 597.00
Granting of funds for EuroHPC LUMI		1 309 200.00	1 309 200.00
Total expenditures	**33 479 915.00**	**9 493 625.00**	**42 973 540.00**

Income in CHF

Income in CHF	User Lab	Third Party	Total
Contribution ETH Zurich	20 483 380.51		20 483 380.51
Contribution ETH-Rat - HPCN Investments	11 700 000.00		11 700 000.00
Contribution ETH-Rat - PASC Initiative	3 000 000.00		3 000 000.00
Contribution SERI - EuroHPC LUMI		1 309 200.00	1 309 200.00
Research collaboration projects		2 857 948.51	2 857 948.51
Services for paying customers		3 799 882.14	3 799 882.14
Other income	38 858.94	96 171.00	135 029.94
Total income	**35 222 239.45**	**8 063 201.65**	**43 285 441.10**

User Lab Expenses Development (CHF)

	2017	2018	2019	2020
Investments	4 218 973	2 472 847	2 998 292	9 840 366
Personnel	9 478 260	10 479 422	10 286 088	11 378 508
Other material expenses	6 877 461	9 414 401	11 006 943	12 261 041



“Our thinking is often far too linear to grasp and correctly dissect complex phenomena”.

Name
Viola Vogel

Position
Full Professor, Laboratory of Applied Mechanobiology

Institution
ETH Zurich

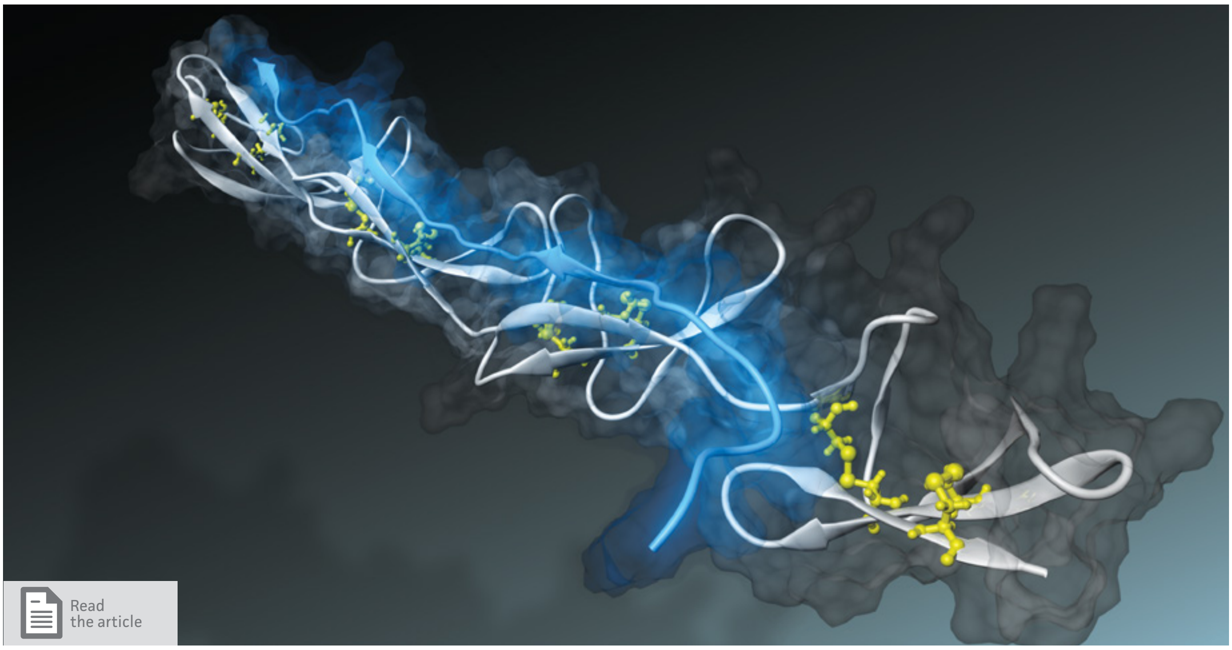
Background

1984-1987	PhD in physics, University of Frankfurt am Main, Germany
1988-1990	Postdoc in physics, UC Berkeley, USA
1990-2004	Professor in bioengineering, University of Washington in Seattle, USA
2004-Present	Professor, ETH Zurich
2012	Honorary Doctor of Philosophy from Tampere University, Finland

Area of research
Applied mechanobiology, bioengineering and regenerative medicine.

Specialised in
Researching the impact of mechanical forces on protein function and in tissues fibres. Forces drive essential life processes, from the first steps in fertilization all the way to shaping growing clumps of cells into organisms.

HPC means for me
Since only protein equilibrium structures can be experimentally resolved at atomistic detail, even today, HPC is crucial to derive their mechanically-stabilized, non-equilibration structures at atomistic resolution. This in turn serves as an essential foundation for the rapidly growing field of mechanobiology.
We simulate how protein stretching alters their equilibrium structures and try to develop novel hypotheses for how forces regulate protein, cell and tissue functions.


Read
the article

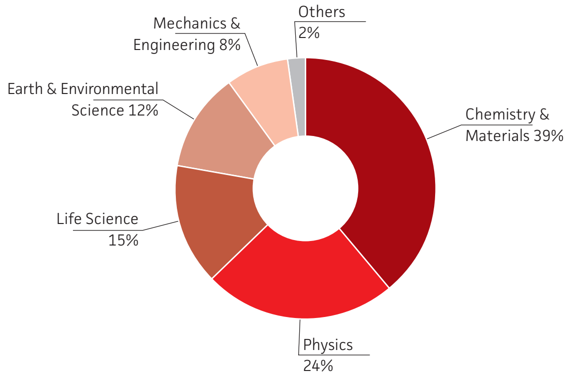
Nano-sensor measures tension of tissue fibres

As later verified experimentally, Viola Vogel and her team used computer simulations to discover a peptide that is able to detect the tensional state of tissue fibres. This paves the way for completely novel research approaches in medicine and pharmacology. External and cell-generated forces also orchestrate tissue homeostasis in healthy organs, but misbalanced forces may result in a range of degenerative diseases. With state-of-the-art experimental and computational tools, their goals are to decipher how cells sense mechanical forces and convert them into biochemical signals, ultimately altering molecular transcription processes. Even though most of our knowledge in biology, medicine and pharmacy is rooted in the structure-function relationships of proteins under equilibrium, many proteins get stretched by mechanical forces. They have revealed various mechanisms for how forces can alter their structure-function relationships.
(Image: Samuel Hertig)

Usage Statistics

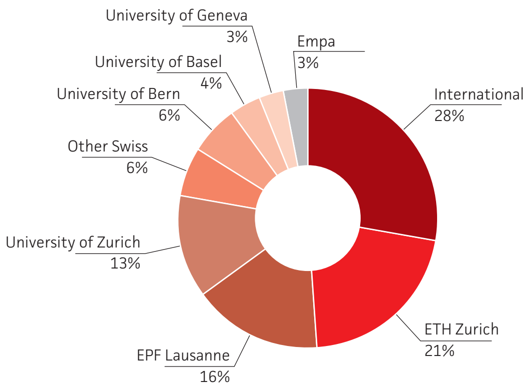
User Lab Usage by Research Field

Research Field	Node h	%
Chemistry & Materials	16 252 868	39
Physics	10 082 500	24
Life Science	6 072 597	15
Earth & Environmental Science	5 120 020	12
Mechanics & Engineering	3 511 543	8
Others	725 232	2
Total Usage	**41 764 760**	**100**



User Lab Usage by Institution

Institution	Node h	%
International	11 907 049	28
ETH Zurich	8 834 857	21
EPF Lausanne	6 558 708	16
University of Zurich	5 360 017	13
Other Swiss	2 485 546	6
University of Bern	2 572 587	6
University of Basel	1 500 656	4
University of Geneva	1 335 542	3
Empa	1 209 798	3
Total Usage	**41 764 760**	**100**



Compute Infrastructure

Computing Systems Overview

Name	Model	Installation/Upgrades	User	TFlops
Piz Daint	Cray XC50/Cray XC40	2012 / 13 / 16 / 17	User Lab, UZH, NCCR Marvel, CHIPP	27 154 + 2 193
Grand Tavé	Cray X40	2017	Research & Development	437
Tsa/Arolla	Cray CS-Storm 500	2020	MeteoSwiss	1 126
Alps	HPE Cray EX	2020	User Lab, Research & Development	4 719

Computing Systems Specifications

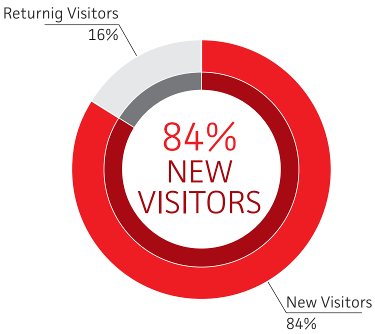
Name	Interconnect Type	CPU Type	Cores	Sockets	GPUs	Nodes
Piz Daint	Cray Aries	Intel Xeon E5-2690 v3/Nvidia Tesla P100	12	1	1	5 704
		Intel Xeon E5-2695 v4	18	2		1 813
Grand Tavé	Cray Aries	Intel Xeon Phi CPU 7230	64	1	0	164
Tsa/Arolla	100 Gb Ethernet	Intel Xeon Skylake 6143 Nvidia Tesla V100	8	2	8	18
		Intel Xeon Skylake 6148	20	2	0	6
Alps	HPE Cray Slingshot	AMD EPYC 7742	64	2	0	1 024

Communications Statistics

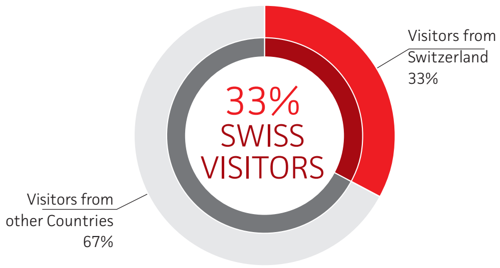
Website cscs.ch

	2019	2020
Total Website Visitors	76 986	67 360
Average Website Visits (Minutes)	2:17	1:99

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. Internships www.cscs.ch/about/internships/
4. Staff www.cscs.ch/about/staff/
5. Working at CSCS www.cscs.ch/about/working-at-cscs/

Twitter

	2019	2020
Followers	1 480	1 735

LinkedIn

	2019	2020
Followers	7 880	8 678

YouTube

	2019	2020
Watch Time (Minutes)	456 815	553 764
Average View Duration (Minutes)	4:33	4:00
Number of Views	105 500	138 234

Facebook

	2019	2020
Followers	220	236

CSCS in the News

	2019	2020
News Websites	304	166
Print	254	97
Radio & TV	10	5

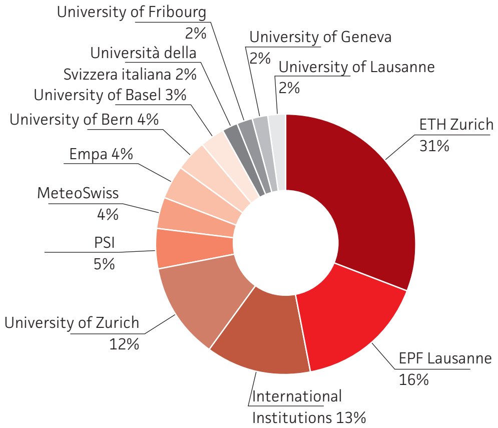
Word Cloud of News Related to CSCS

User Satisfaction

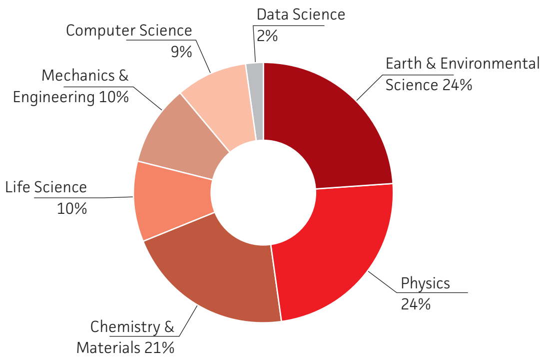
A user satisfaction survey was submitted to 1 375 users in January 2021. The response rate was of 18.3% (251 answers).

User Profile

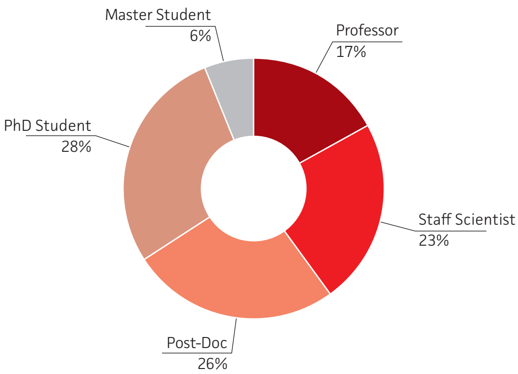
Your institution



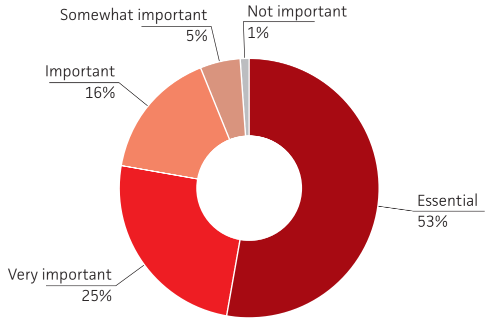
Your scientific field



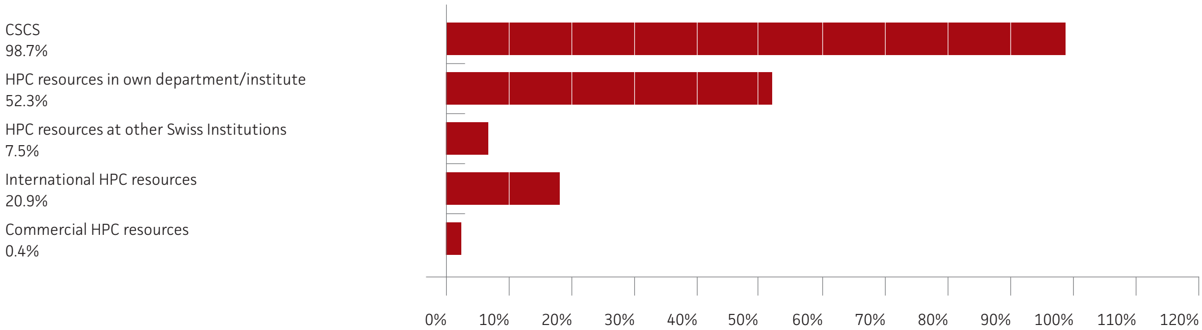
Your position



resources are

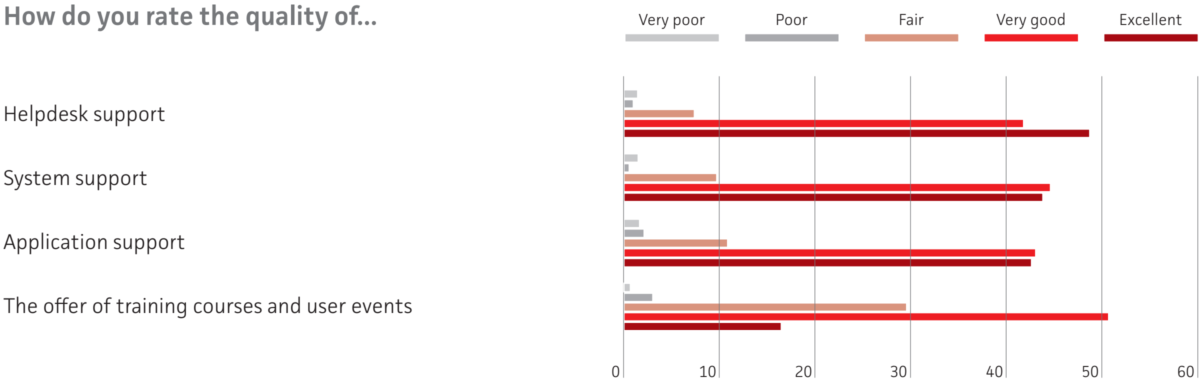


Which HPC resources are you using?

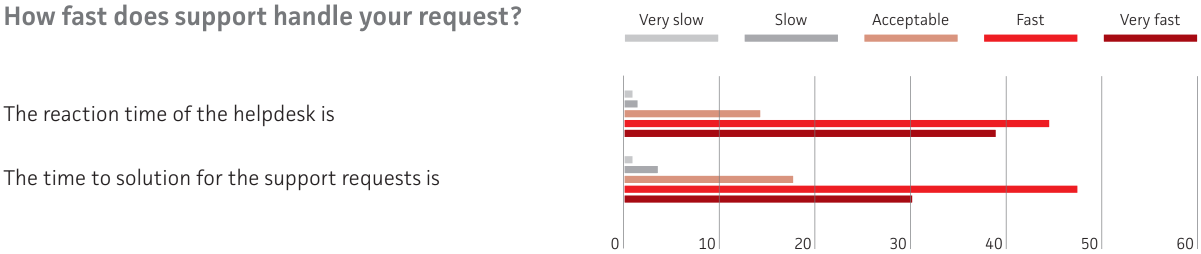


User Support

How do you rate the quality of...

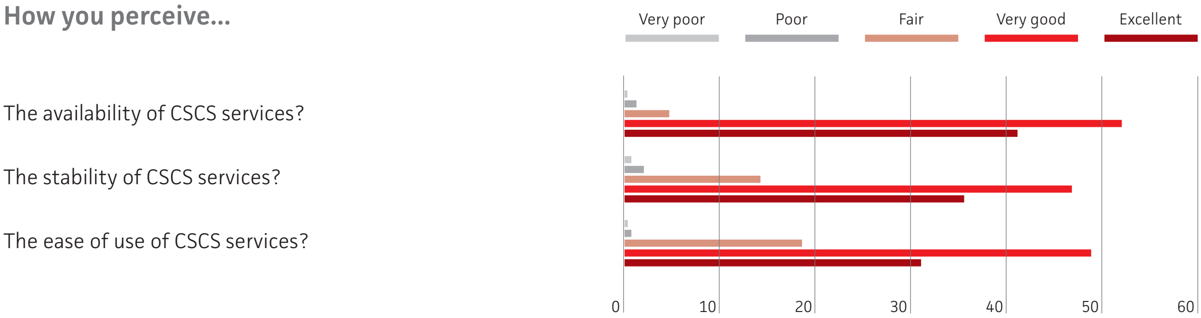


How fast does support handle your request?

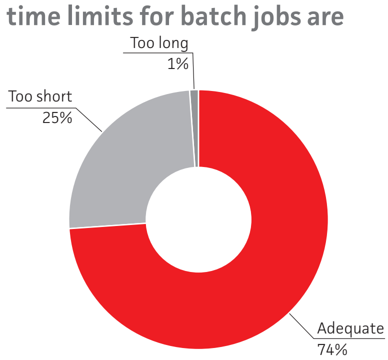


Service Availability, Stability and Usability

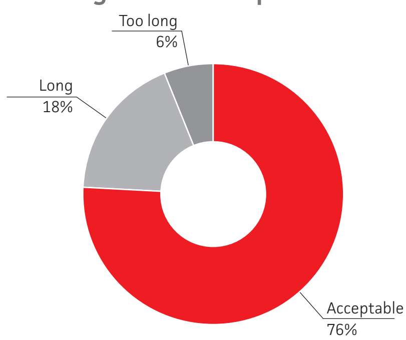
How you perceive...



The run time limits for batch jobs are

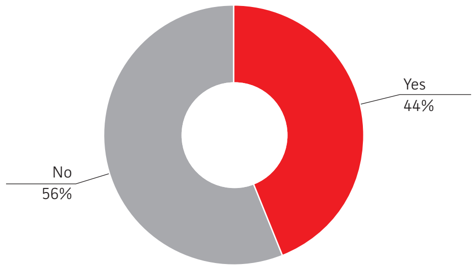


The job waiting time in the queue is

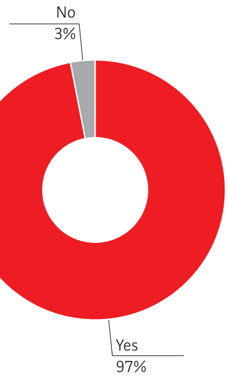


Project Proposal Process

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?

The submission portal is

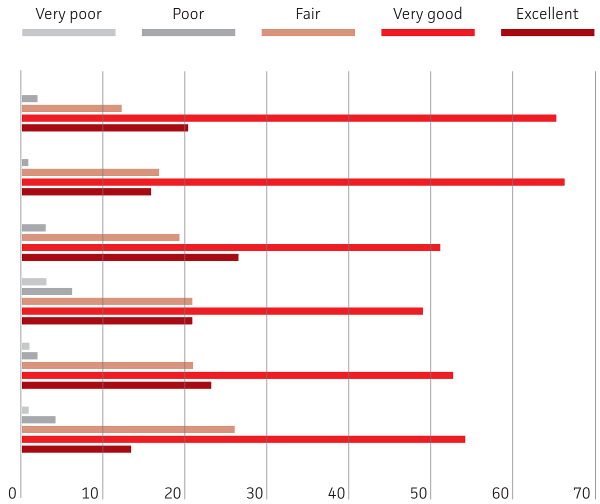
The quality of the submission form is

The support provided during the call is

The feedback from scientific reviewers is

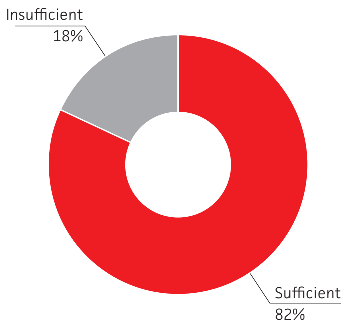
The feedback from technical reviewers is (when given)

The information provided by the panel committee is

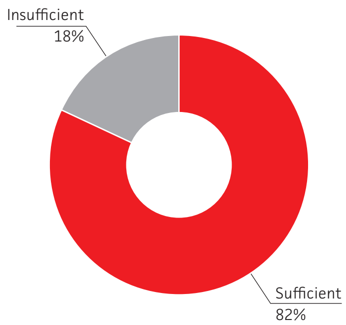


Adequacy of Allocated Resources

The resources assigned to my project are

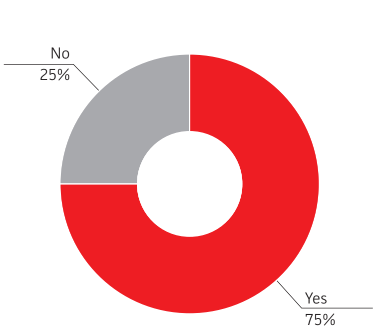


My storage allocation on “project” is

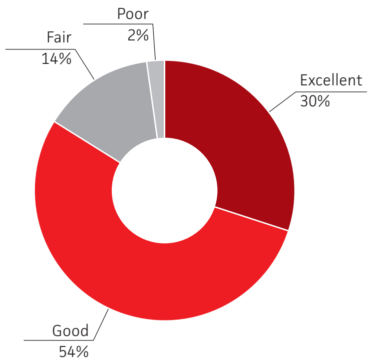


Application Development

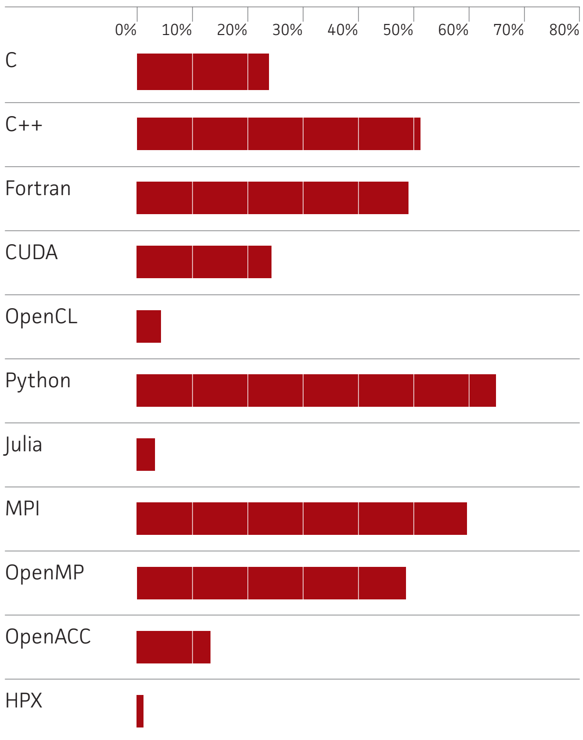
Do you develop and maintain application codes?



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

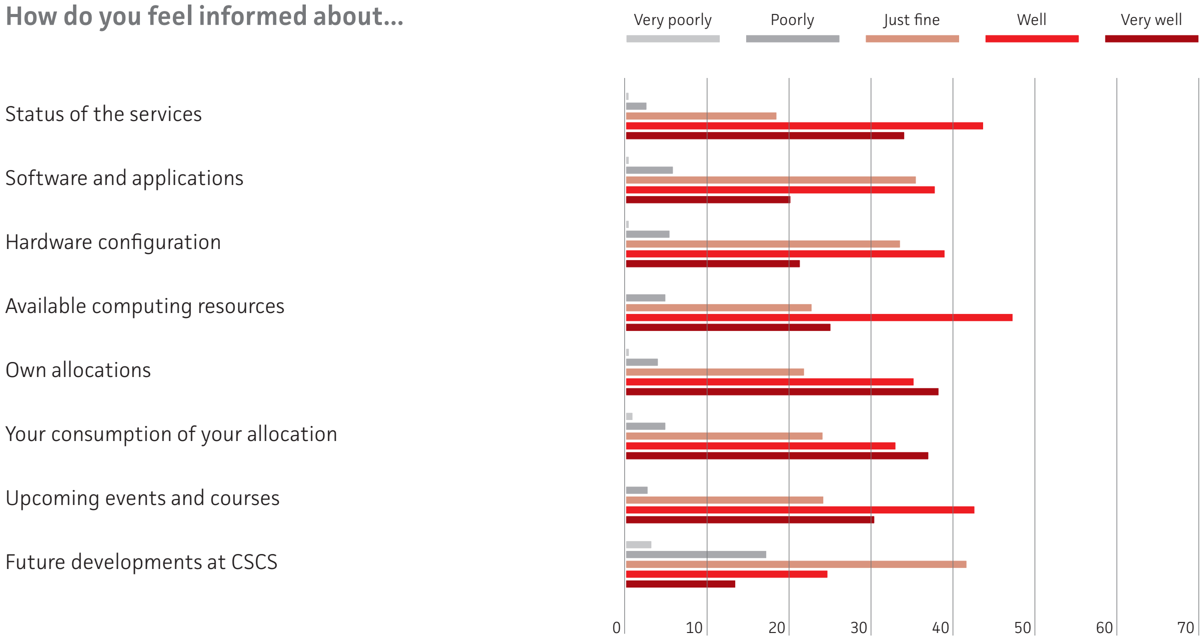


Which programming languages and parallelization paradigms are you using primarily?



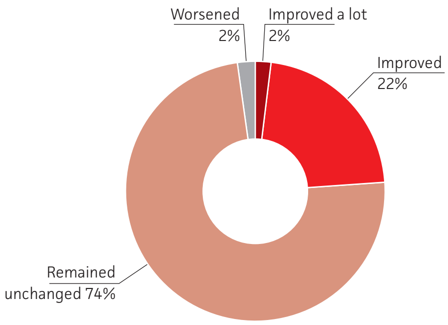
Information & Communication

How do you feel informed about...

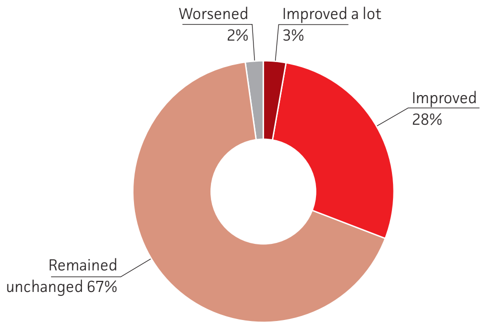


Perception of CSCS

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



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



Impressum

CSCS Swiss National Supercomputing Centre
Via Trevano 131
6900 Lugano
Switzerland

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

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