CSCS

Annual Report
2022

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

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Photographer Marco Abram took photos featured on the cover and inside the annual report in the new CSCS offices located at Via Chiosso 7A in Porza.

The photographer Alessandro Della Bella has portrayed seven staff members of CSCS: Tomas Aliaga, Tiziano Belotti, Monica Frisoni, Maria Grazia Giuffreda, Matthias Kraushaar, Angela Schneebeli, Stefano Schuppli, Mikael Simberg.

Welcome from the Director

Thomas Schulthess, Director of CSCS

Welcome to this year's edition of the CSCS annual report. The close of 2022 saw a wave of change for our organization. Because Swiss researchers and research infrastructures, like ours at CSCS, face exclusion from European research programmes, we are actively looking for new ways to shape collaborations in Europe and globally. Despite these new challenges, we feel confident that we can live up to our worldwide reputation of being at the forefront high-performance computing.

Of course, there are new perspectives as well as new challenges emerging at the international level. For example, in January 2022 Switzerland became a member of the Square Kilometre Array Observatory. CSCS staff are now taking a leading role in SKAO and the SKACH (the SKA Switzerland Consortium) by building a robust platform to analyse the data collected by the gigantic radio telescope. With our new "Alps" infrastructure at CSCS, we will build the competencies and workflows needed to turn this data into valuable scientific information.

Furthermore, SKA is directly supported by two of the 15 PASC projects I had the pleasure of presenting to you here a year ago. In these two projects, CSCS research software and HPC application engineers engage with the academic teams to contribute both code developments and software engineering expertise, making the simulations more detailed and at the same time faster (read more about this on page 20 of this report).

Additionally, I would like to note that it is gratifying to see the pieces of the puzzle from past years gradually coming together to form a picture: Large-scale projects like SKA are benefiting from the PASC initiative, which was launched over ten years ago as part of the Swiss initiative for HPC and Networking (HPCN). This confirms us once again that we are on the right track with our strategy.

The development of our new “Alps” infrastructure is progressing well and I am confident that in a year's time we will be reporting on new collaborations this next generation flagship system will have enabled with research institutions in Switzerland and Europe.

I would like to thank all those who make this possible, starting with the State Secretariat for Education, Research and Innovation; ETH Zurich; our users, as well as our European and international partners in high-performance computing and research; and my staff, who work tirelessly to make all these ideas and plans come to fruition.

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Founded in 1991, CSCS develops and provides the key supercomputing capabilities required to solve challenging problems in science and 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
2022: 57 226 000 node h
2021: 56 321 000 node h

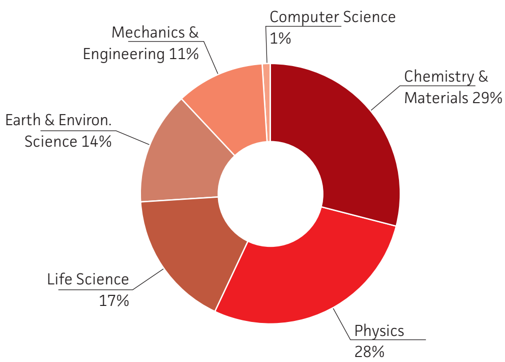
User Community
2022: 139 projects, 2 430 users
2021: 153 projects, 2 318 users

Employees
2022: 119
2021: 118

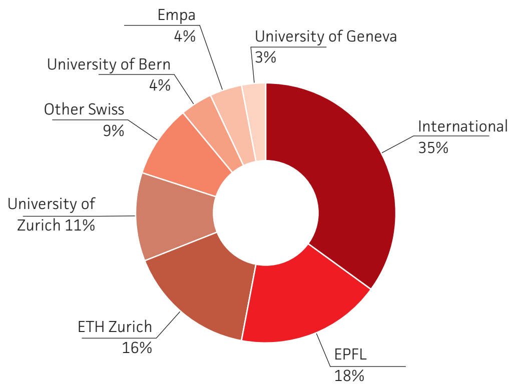
Investments
2022: 12.6 Mio. CHF
2021: 21.45 Mio. CHF

Operational Costs
2022: 29.9 Mio. CHF
2021: 26.2 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, CHIPP	27 154 + 2 193
Tsa / Arolla	Cray CS-Storm 500	2020	MeteoSwiss	1 169
Alps	HPE Cray EX	2020	User Lab, Research & Development, UZH, CHIPP	4 719

Name
Tomas Aliaga

Nationality
Argentinian and Italian

Position
Senior Software Engineer

Working at CSCS since
October 2019

Background

2006-2012	Engineering degree Informatics, Universidad Blas Pascal, Argentina and TU Graz, Austria
2012-2016	Scientific applications developer, ESSS , Brazil
2015-2018	MSc computer science, Computing Systems, Georgia Tech, USA
2016-2019	Cloud software engineer, Martel Innovate, Switzerland
2019-Present	Software Engineer for HPC Platform Services, CSCS

Specialisation

Back-end software engineering for cloud and HPC systems, particularly focused on Linux systems, DevOps, and containers. I design, develop, consult, and maintain software solutions in collaboration with varied HPC engineering teams. This covers varied aspects ranging from conception to orchestration of the distributed (Linux) processes that give life to scientific applications on supercomputers.

What working at CSCS means to me

Joining CSCS allowed me to gain first-hand experience with the world of HPC, something I aspired to in my early career. At CSCS I can work at the intersection of three elements I'm passionately interested in: software, science, and education.

What I like most about my work

Working at an HPC centre offers me the chance to not only discover antique software underlying Linux sytems, but also to explore, develop and introduce new technologies and mechanisms to change the status quo of our offerings. It's a fascinating continuous gain and application of old and new knowledge. I also enjoy working with colleagues and partners of diverse technical and cultural backgrounds. Solving problems for them or learning from their experiences also brings me job satisfaction.

What challenges me at my work

One of my biggest challenges these days is balancing ways to amplify my individual contribution and ways to curb natural factors hindering engineering synergies. By that, I mean finding new approaches to exploiting software automation, connecting and empowering teams, and ensuring feasibility, compatibility, and longevity of technical solutions — all while tackling dysfunctional documentation, preventing duplicated efforts, or responding to shifting priorities. I believe this balance is of critical importance, particularly in a multicultural centre with such a wide range of services and know-how that develops and operates a world-class research infrastructure.

January

10 Read the article

The shutdown of "Grand Tavé"

Five years after its installation, the Cray XC40 KNL, "Grand Tavé", is shut down for the very last time. "Grand Tavé" is the name of a Swiss mountain of 3158 m in the canton Valais. "Grand Tave", a reasearch and development (R&D) system installed in 2017, was a Cray XC40 featuring Intel Knights Landing (KNL) compute nodes.

March

08 / 09

2022 Swiss Conference and HPCXXL User Group meet online

Encouraging shared knowledge for over a decade, the 2022 Swiss Conference and HPCXXL User Group is again organised online. From thought leadership to practical application, each expert-led session provides a sampling of topical works, usage models, and best practices addressing a range of interests, including artificial intelligence, cloud data science, high-performance computing, and much more.

11 Read the article

Webinar: "User Lab: Getting started at CSCS"

This webinar focuses on presenting the CSCS User Lab. CSCS staff gives instructions on how to access CSCS systems, adhere to best practices, use different filesystems, manage computing resources, and submit and monitor batch jobs.

16 Read the article

Construction of 6 MW thermal power plant begins next to CSCS

Lugano Industrial Companies (AIL), a partner of CSCS for electricity supply, announces the construction of a 6 MW thermal power plant next to CSCS's main building. Thanks to the residual heat produced by CSCS's supercomputers and the heat pumps planned for various facilities, a great deal of energy will be saved. Construction work starts in May 2022 and last about six months.

April

01

Node hours distributed in User Lab and PRACE Calls

A total of 21 million node hours are distributed in the first national call for proposals and in the PRACE Tier-0 Call 24. The allocation period is between April 1, 2022, and March 30, 2023.

06

CSCS meets students from USI at Long Night of Careers

CSCS staff attends the Long Night of Careers at Università della Svizzera italiana (USI) to present a general overview of the Centre and its offerings, such as internships, training courses, and self-development. Moreover, student participants have the opportunity to meet CSCS representatives in one-to-one sessions to learn about possible careers at the Centre.

12

Read the article | Watch the video

Webinar: "How to prepare the technical report for proposal submission"

This webinar is for applicants to the CHRONOS Tier-0 Call and the national calls for proposals at CSCS. It provides guidelines for the submission and practical information on how to prepare the needed technical reports.

May

05

Read the article | Watch the video

Webinar: Information about calls for proposals

This is a recurrent webinar that CSCS organises twice a year to give applicants the necessary details on the CHRONOS, national, and European calls for proposals. It also focuses on what is new and different from previous calls and provides information about the resources available in each call.

10

Read the article | Watch the video

In-person course: "In Situ Analysis and Visualization with ParaView Catalyst and Ascent"

This half-day tutorial introduces ParaView Catalyst and Ascent, two open-source implementations enabling in-situ processing. Both packages share a joint project called Conduit, which provides an intuitive model for describing hierarchical scientific data in C++, C, Fortran, and Python. The course covers how to describe simulation data with Conduit; how Ascent or Catalyst can transform data, render images, and export results; and the pros and cons of both implementations.

19

Empa hosts hpc-ch Forum on Configuration Management

The Swiss Federal Laboratories for Materials Science and Technology (Empa) hosts the Spring hpc-ch Community Forum on Configuration Management. Representatives of the Swiss HPC Service Provider Community meet to discuss how to manage both small and large HPC systems.

25

Read the article

CSCS becomes Swiss provider of data infrastructure for Square Kilometre Array Observatory (SKAO)

CSCS announces its support for scientists of the Square Kilometre Array Observatory (SKAO) consortium, which aims to shed light on the universe's first billion years. Along with other centres around the world, CSCS will receive a portion of the expected 700 petabytes of data generated annually by SKAO – data waiting to be processed and analysed by the scientists.

25

New CSCS offices open in Lugano

To support the staff growth in Lugano, new offices are rented by ETH Zurich in a building 450 meters from CSCS headquarters. The new offices include a total of 54 workplaces as well as a kitchen, meeting rooms, collaborative rooms, and a room designed to host hackathons.

30/01

CSCS booth featured at ISC22

After a two-year break due to the pandemic, CSCS and the Swiss HPC community are again present at the high-performance computing conference and exhibition, ISC22, in Hamburg, Germany. Attendees discover the latest news about CSCS and HPC in Switzerland while enjoying a cup of coffee and some world-famous Swiss Chocolate.

June

13

Read the article

Inauguration of supercomputer LUMI

The supercomputer LUMI, owned by the EuroHPC Joint Undertaking and operated by a consortium of 10 countries, is inaugurated. As a member of this consortium, CSCS celebrates this milestone with its colleagues in Kaajani, Finland.

21

Read the article

Watch the video

Webinar: High-performance computing with Python

This three-day online course includes lectures and hands-on sessions aiming to show how the programming language Python can be used on parallel computer architectures and how to optimise critical parts of the kernel using various tools.

20/27

Read the article

PASC22 Conference in Basel

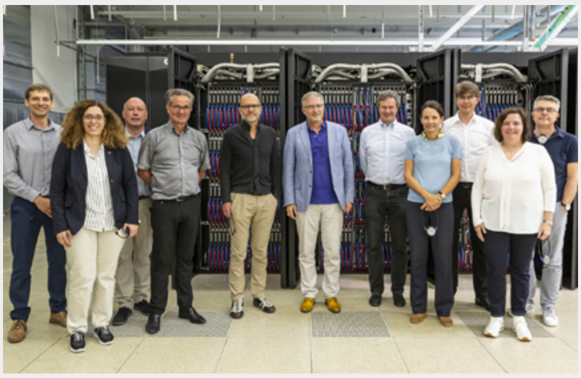
The PASC22 Conference – with the theme "Computing and Data… For All Humankind" – takes place at the Congress Center in Basel. More than half of the 400 attendees come from abroad, continuing the conference's growth in attendee numbers every year since its inception. The technical program includes keynote talks, mini-symposia, a peer-reviewed paper track, poster sessions, and panel-style discussions.

July

03

Secretary generals of departments visiting CSCS

CSCS Director Thomas Schulthess welcomes the secretaries general of the seven departments of the Swiss Confederation and introduces them to the HPC and data challenges of the upcoming years. Then the delegation had the opportunity to visit the whole data centre infrastructure



11/21

Summer University 2022 on hybrid computing systems

CSCS and Università della Svizzera italiana (USI) host their annual Summer University on effective high-performance computing and data analytics both online and in-person. 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. Twenty-two of the participants also attended the three on-site days, from July 23-25, to enjoy the social program and to meet colleagues and experts in person for more in-depth networking.

August

29 Read the article Watch the video

Webinar: "ReFrame – Efficient System and Application Performance Testing"

This webinar presents ReFrame, a tool for writing portable systems and application performance and validation tests, to the scientific community. It focuses on the basic concepts of the tool through examples.

September

02

User Lab Day held in Bern

CSCS welcome current and possible future users to a one-day, in-person event at the Kongresszentrum Kreuz in Bern. Attended by 81 researchers, the event provides ample time for presenting CSCS roadmaps and plans, as well as conversation with CSCS staff about the current infrastructure and new services already on the horizon.

17 Read the article

CSCS supports Corsa della Speranza (Run for Hope)

A group of 20 staff members and their families participate in the Corsa della Speranza (Run for Hope) in Lugano. Celebrated in more than fifty countries around the world, the event raises awareness of cancer and raises funds for scientific cancer research. The funds raised, consisting of both registrations and donations, will be paid in full to the Ticino Cancer Research Foundation, which supports international research projects in Ticino.

27 / 29

EuroHack22: GPU programming hackathon

The eighth GPU-programming hackathon takes place again, finally in person, at the Hotel De La Paix in Lugano. EuroHack22 engages a total of 8 teams comprised of 35 participants from Switzerland and around the world. With the support of expert mentors, the hackathon is designed to help researchers port their codes to a GPU-hybrid supercomputing environment.

October

01

Node hours distributed in User Lab Calls for Proposals

A total of 20 million node hours are distributed in the second national call for proposals. As of this year, CSCS has also reopened the CHRONOS Tier-0 annual call to distribute resources larger than 1 million node hours on CSCS's "Piz Daint" and the LUMI system in Finland.

03 / 04

Swiss SKA Days held in Lugano

Università della Svizzera italiana (USI), with the support of CSCS, hosts the Swiss SKA Days conference with 106 participants. In this sixth edition of the meeting, the Swiss participants in the ambitious Square Kilometer Array (SKA) radio astronomy project get together to present their activities and discuss the challenges of this ambitious project, which is at the forefront of technologies and calculations.

06

Autumn hpc-ch Community Forum focuses on user-centric view of HPC

Campus Biotech in Geneva hosts the Autumn hpc-ch Community Forum on the user-centric view of HPC. Representatives of the Swiss HPC Service Provider Community discuss the efforts of placing users at the center of the HPC infrastructure design.

12 Read the article

Students from USI and ETH Zurich visit CSCS

Professor Olaf Schenk and the Institute of Computing (CI) welcome 80 bachelor's and master's students from Università della Svizzera italiana (USI) and ETH Zurich for a tour of CSCS headquarters.

12 Read the article

Open public visits back on schedule

Visits open to the public were interrupted in 2020 due to Covid-19. This year, CSCS opens its doors once again and welcomes visitors interested in learning about our Centre. Every three months, people can register for a presentation of the Centre that includes a viewing of the technical infrastructure and machine room.

November

10

CSCS attends "Notte bianca delle carriere"

Through interactive stands, bilateral meetings, workshops, and playful activities, the event promotes interaction and exchange between SUPSI students and companies in the Ticino area. CSCS participates in the event to encourage students to learn about the Centre and job opportunities there.

10

Nuovo Futuro - Day to discover professions in the IT sector

CSCS participates in a day organized by the Canton of Ticino to help students discover professions in the IT sector. The attending middle school boys and girls learn about the different jobs in the IT field at CSCS and get a glimpse of the world of HPC.

13/17

CSCS attends Supercomputing Conference 2022

CSCS presents its activities at the world's largest supercomputing conference, SC22, in Dallas, Texas, USA. In a friendly and inviting booth, visitors have the opportunity to ask about the latest HPC developments in Switzerland and to have open discussions with CSCS technical staff attending the conference.

15

Read the article

Torsten Hoefler receives Sidney Fernbach Award 2022

The IEEE Computer Society honours ETH Zurich professor Torsten Hoefler with the Sidney Fernbach Memorial Award for his pioneering contributions to large-scale parallel processing systems and supercomputers. The ideas and software professor Hoefler and his group developed are actively used by tens of thousands of scientists today to power large-scale scientific simulations and artificial intelligence systems.

28/02

Read the article

CSCS hosts EuroCC Kubernetes Hackathon

The EuroCC/CSCS Kubernetes Hackathon is held in Lugano. A total of 46 participants work closely with experienced mentors throughout the immersive coding session to work on tasks from their home institutions. The teams come from CSCS and other institutions in Switzerland, as well as from NCCs of other European countries like Austria, Norway, and Portugal.

Name
Tiziano Belotti

Nationality
Swiss

Position
Associate Director

Working at CSCS since
October 2010

Background

1981-1987	Swiss Federal Diploma in precision mechanics & electronic engineering
1987-1990	Train driver, Swiss Federal Railways
1990-1994	Building automation project manager, Honeywell Zurich
1994-2008	HVAC and electric project manager, SSR SRG Idee Suisse
2001-2004	Swiss Federal Diploma in HVAC engineering

2009-2012	Diploma CECE / Minergie Expert, University of Applied Sciences and Arts of Southern Switzerland
2015-2016	Federal diploma in Advanced Studies in Real Estate Management, University of Applied Sciences and Arts of Southern Switzerland
2010-2022	Facility Management Group Leader, CSCS
2022-Present	Associate Director, Head of Facility Management, CSCS

Specialisation

Technical installations. In particular, I am responsible for supporting the management in the Centre's development strategy and in managing the maintenance, renovation, and extension of the CSCS installations and buildings. I collaborate closely with the COO on business continuity, risk management, and energy procurement. I also represent CSCS in the cooperation with the buildings department of ETH Zurich for the planning and execution of new projects and renovations. A further strategic part of my job is to define the CSCS facility requirements for IT procurement projects. I am responsible for and lead the Facility Management Working Structure and its members.

What working at CSCS means for me

I have the opportunity to work in an international environment whilst enjoying the beauty of an idyllic location such as Ticino. The melting pot of people with completely different experiences, habits, languages, and social backgrounds allows each and every one to grow and widen their horizons.

What I like most about my work at CSCS

For a job to be interesting to me, it needs to be dynamic, innovative, challenging, and give me the opportunity to learn and grow continuously. My current position at CSCS satisfies all the above on a daily basis!

What challenges me at my work

Because timelines for construction projects are significantly longer than those for the procurement of supercomputers, one of my greatest challenges is to try to anticipate the needs of future systems in order to prepare the building to accommodate them when they arrive.

A New European HPC Landscape

2022 marked the end of PRACE, the *Partnership for Advanced Computing in Europe*, as a European platform to share supercomputing infrastructure of all member states among their scientists. Call 24 was the last of the biannually organized calls for proposals, and CSCS successfully completed its commitment as a PRACE hosting member, distributing 7.96 million node hours to 5 Tier-0 proposals.

As a hosting member, Switzerland had agreed to have "Piz Daint" supercomputer available for cutting-edge PRACE research. Back in 2017, CSCS was the only PRACE computing centre with a scalable hybrid system that utilizes both graphics and conventional processors, offering a peak performance of around 20 petaflops. Researchers in all PRACE member states were able to apply for compute time on "Piz Daint", while researchers in Switzerland gained access to infrastructure supplied by other hosting member states. Applications for compute time from CHRONOS (***C**omputationally-Intensive, **H**igh-Impact **R**esearch **O**n **N**ovel **O**utstanding **S**cience*) proposals, already established at CSCS since 2014, were routed through PRACE instead.

The establishment of EuroHPC JU (*European High Performance Computing Joint Undertaking*) has made PRACE change its focus to function as a link between users (Association of Users) and HPC Centres in Europe. The core business of the new PRACE Association encompasses user representation, communication and dissemination, networking and cooperation of HPC Centres and users in Europe.

Swiss computational and computer scientists in need of computing and data resources can continue to apply for up to 1 million node hours in the national Tier-1 calls, open twice a year, with projects starting on April 1 and October 1. Larger Tier-0 proposals can be submitted in the annual CHRONOS calls, which have a deadline in May and start allocation on October 1, either on CSCS research infrastructure or on the Swiss share of LUMI in Finland. EuroHPC JU runs Extreme Scale Calls for Proposals on LUMI, and Swiss scientists are encouraged to apply there if they need very large resources.

Resources allocated in 2022

Usage statistics indicate some relevant changes with respect to 2021. Chemistry & Materials allocations drop from 35% to 29% of available resources, and are now closely followed by Physics at 28% (+11%). Life Science and Earth & Environmental Science follow with 17% and 14% of the total allocation, respectively, only 1% less than last year. Mechanics & Engineering and Computer Science complete the statistics with 11% and 1%, respectively.

EPFL and ETH Zurich are the largest users among institutions with 18 and 16%, respectively. The Universities of Zurich, Bern, and Geneva (11, 4, 3%), Empa (4%), and other Swiss institutions (9%) are sharing the remainder of the resources, as are international users whose utilization remains high at about 35%. Like in previous years, the User Lab calls are still the primary path to resource allocation for domestic research institutions, but most of the international allocation has been granted in PRACE Tier-0 and CHRONOS calls.

List of PRACE Tier-0 Projects

Principal Investigator	Organisation	Research Field	Project Title	Node h
David Wilson	University of Cambridge	Physics	Scattering amplitudes and charmonium resonances with physical light quarks	2 000 000
Savvas Zafeiropoulos	Aix Marseille University	Physics	Neutron electric dipole moment with stabilized Wilson fermions: The theta term	1 970 600
Olaf Kaczmarek	University of Bielefeld	Physics	Curvature of the chiral phase transition line	1 953 000
Nikolina Ban	University of Innsbruck	Earth & Environ. Science	Mountain climate at the kilometre-scale resolution: Phase 2 (kmMountains)	1 498 000
Lucie Delemotte	Royal Institute of Technology in Stockholm	Life Science	Structure and dynamics of ion-channel modulation by lipophilic drugs	1 037 800
Christoph Schär	ETH Zurich	Earth & Environ. Science	Kilometer-resolution climate modeling on GPUs (kmCLIM3)	1 000 000
Raffaela Cabriolu	EPFL	Chemistry & Materials	Thermal conductivity of metal-organic-frameworks (TC_MOFs)	582 000

Largest Projects (> 600 000 Node h)

Principal Investigator	Organisation	Research Field	Project Title	Node h
Nicola A. Spaldin	ETH Zurich	Chemistry & Materials	Coupled and competing instabilities in complex oxides	990 000
Urs Wenger	University of Bern	Physics	Hadronic light-by-light scattering: the muon anomaly at next-to-leading order	920 000
Ursula Röthlisberger	EPFL	Chemistry & Materials	Assessing the impact of defects and interfaces in lead halide perovskite based solar cells	900 000
Ben Schuler	University of Zurich	Life Science	Interactions and dynamics of highly charged disordered proteins inliquid-liquid phase separation	900 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	Ab initio modeling of three-terminal valence change memory cells for neuromorphic computing applications	880 000
Paolo Ricci	EPFL	Physics	Simulation of the tokamak boundary in reactor-relevant conditions	880 000
Sandra Luber	University of Zurich	Chemistry & Materials	Guiding the design of novel and highly efficient water reduction catalysts by ab initio methods	840 000
Peter Vincent	Imperial College London	Mechanics & Engineering	Investigating the effects of free-stream turbulence and non-sharp leading and trailing edges on flow over a triangular airfoil under Martian aerodynamic conditions	804 400
Daniele Passerone	Empa	Chemistry & Materials	Effects of non-local electronic correlation in enantioselective properties of DBBA and 9-PBA on PdGa-surfaces	800 000
Nicola Marzari	EPFL	Chemistry & Materials	Materials for energy	768 000
Laurent Villard	EPFL	Physics	ORB5TCVHEAT	763 400
Sandra Luber	University of Zurich	Chemistry & Materials	Advancing real-time propagation methods for spectroscopy in the condensed phase	750 000
Constantia Alexandrou	Cyprus Institute & University of Cyprus	Physics	Nucleon electroweak matrix elements controlling two-particle states - towards a new frontier within lattice QCD	700 000
Andreas Fichtner	ETH Zurich	Earth & Environ. Science	Hamiltonian Monte Carlo full-waveform inversion	700 000
Carlo A. Pignedoli	Empa	Chemistry & Materials	Fabrication and characterization of magnetic carbon based nanomaterials	700 000
Ursula Röthlisberger	EPFL	Life Science	Multiscale simulations of biological systems: From simulations of DNA damage and repair to the design of new metallodrugs and metalloproteins	700 000
Ursula Röthlisberger	EPFL	Chemistry & Materials	Mechanisms of passivation: A route towards more efficient and stable lead halide perovskite based solar cells	664 000
Francesco L. Gervasio	University of Geneva	Life Science	Understanding the effect of pressure and lipids on the conformational equilibria of B1AR	600 000
Ulrike Lohmann	ETH Zurich	Earth & Environ. Science	Understanding the role of aerosols and internal variability in climate and understanding drivers of weather extremes	600 000
Franco Vazza	University of Bologna	Physics	The Radio Cosmic Web2: The network of radio shocks and radio galaxies	600 000

What’s Next for PASC: Next-Generation Radio Interferometry and the SPH-EXA2 projects bring the stars into focus for SKAO

The programme of the Platform for Advanced Scientific Computing (PASC) is currently in its third cycle: From 2021-2024, a total of 15 projects are underway. The overarching goal for this period is both to position Swiss computational sciences in the emerging exascale era and also to ensure application readiness on CSCS's infrastructure.

Switzerland has been a member of the Square Kilometre Array Observatory (SKAO) project since January 2022. Therefore, two projects from the PASC programme that play an important role in this ambitious collaboration are presented here: "SPH-EXA2", led by Florina Ciorba, professor at University of Basel; and "Next-Generation Radio Interferometry", led by Jean-Paul Kneib, professor at EPFL.

The declared goal of the Square Kilometre Array (SKA) is nothing less than revolutionising our understanding of the universe and its fundamental physical laws. Furthermore, the SKA Switzerland Consortium (SKACH) is intended to benefit both research and industry.

The radio telescope — which, according to the consortium, will be one of the largest scientific facilities ever built — is being constructed at two locations: Australia and South Africa. In Australia, about 131,000 stationary antennas will collect low-frequency radio signals; and in South Africa, 197 dish antennas will collect medium to high radio frequencies. All these antennas combined will generate 600 petabytes of astronomical data annually once operational. Both sites will have a high-performance computing (HPC) data centre to collect and correlate the data and to make it available to other data centres. With the "Alps" infrastructure, CSCS will provide the platform to analyse the data, as well as build the competencies and workflows needed to turn the data into scientific information. In SKA and SKACH, CSCS staff are taking a leading role in building the desired data platform.

In the two correlating PASC projects — as in all other PASC projects — CSCS research software and HPC application engineers are engaging with the academic teams and contributing code developments, software engineering expertise, and more.

SPH-EXA2: High-performance simulation software made in Switzerland

To simulate planet formation with high-resolution models or the core collapse of dying stars and their subsequent explosion (supernovae), ’is challenging. These numerical simulations performed in astrophysics and computational fluid dynamics that reproduce the behaviour of a fluid or plasma are among the most computationally intensive calculations in HPC. This is because of the complex physics of the non-linear systems, as well as the different size scales that need to be modelled. With the computational resources currently available, either the computational scale, i.e. the resolution of the simulation and/or the dimension, must be reduced; or, the physics involved must be mapped using approximation methods, write Florina Ciorba, head of the High Performance Computing research group at the University of Basel, along with her two co-initiators of SPH-EXA2 Lucio Mayer, professor of astrophysics at the University of Zurich and Rubén Cabezón, senior scientist at University of Basel, in their PASC project proposal. However, how these limitations influence the results is not yet sufficiently understood.

The researchers aim to eventually achieve realistic simulations with up to a trillion particles using new optimised codes and the future exascale computer architectures, which will be able to perform 1,018 computational operations per second. For the SPH-EXA2 project, the researchers are using the smoothed particle hydrodynamics (SPH) technique to solve the hydrodynamic equations. With this empirical method, there is no fixed grid point, so the coordinates move with the fluid being calculated. Although this simplifies the simulation of the system, it also makes the calculations less efficient: since the coordinates are not fixed, the system to be simulated is subject to constant changes, which makes it is difficult to parallelise the calculations on the computer architectures.

Simulating subsonic turbulence with SPH-EXA2 on LUMI

In 2022, the SPH-EXA2 project, also financed by PASC, was selected as a Swiss pilot project to run on the LUMI system. This is an important milestone, as enabling Swiss codes on this pre-exascale system is an explicit goal of the PASC programme. Scientifically, the goal is to perform the most detailed simulation yet of subsonic turbulence, which occurs when gas particles are moving slower than the speed of sound.

It manifests as large eddies that become smaller and smaller until all their energy has been thermally dissipated by viscosity.

Turbulent flows are recurrent phenomena in the interstellar medium, and their importance is paramount in star and planet formation as well as in stellar explosive scenarios, such as supernovas. While supersonic turbulence and the accompanying shock waves are reasonably captured by SPH methods, subsonic turbulence is more difficult to model without static or moving meshes. Improved SPH solvers, such as those implemented in SPH-EXA2, allow scientists to overcome the underlying numerical issues of not having a mesh. However, discreteness noise is an additional problem plaguing subsonic turbulence simulations using particle-based methods. Nevertheless, owing to its superior scalability, SPH-EXA2 can simulate turbulence with a much higher number of particles and will provide highly relevant results in many areas. In astrophysical and cosmological applications, for example, an accurate description of subsonic turbulence will capture the diffusion of newly formed heavier elements based on first principles and eliminate the need for semi-empirical corrections.

In order to demonstrate the accuracy and performance of the SPH solver in SPH-EXA2, the LUMI system was employed to simulate a gas cloud in which subsonic turbulence was artificially induced. Compared to previous results obtained on CSCS's "Piz Daint", which themselves achieved unprecedented accuracy, the SPH-EXA2 team was able to improve the resolution of the turbulent fine-structure by another factor of 27. In a separate sub-project of this pilot allocation, SPH-EXA2 was selected to participate in the LUMI hero-run program that provided the team with 12 hours of exclusive access to the entire LUMI system. Aside from examining subsonic turbulence, this opportunity was used to test the limits of the gravitational solver of SPH-EXA2, another component that will work in tandem with the SPH technique. Running on all the available hardware, SPH-EXA2 sustained a processing rate in excess of 100 petaflops and simulated eight trillion particles — eight times more than what will be needed for the planned ExaPHOEBOS flagship scientific application.

The team is convinced that its new simulation code underpins Switzerland's outstanding position in experimental physics and observational astronomy, and it's why they are an integral part of the Swiss consortium for the SKAO.

Picture the Universe: Next-Generation Radio Interferometry

Converting the data collected by SKA into images is also a particular challenge, because the received signals are incomplete due to the gaps between the antennas. These gaps create artificial noise artefacts that result in a "dirty image", explains Shreyam Krishna, a PhD student at the Laboratory of Astrophysics at EPFL. Krishna is part of the research group led by Professor Kneib of EPFL and Emma Tolley, group leader at EPFL's Scientific IT & Application Support (SCITAS) platform, who are both spearheading the Next-Generation Radio Interferometry project through PASC. One of the goals of the PASC project "Next-Generation Radio Interferometry" is to develop algorithms that quickly and reliably process the enormous amounts of SKA data and calculate a clearer picture of the received signals from these dirty images.

A mathematical method known as the Fourier Transform makes it possible to convert the registered signals into complete images. To put it simply, the Fourier Transform does the same work as a prism does when it converts white light into its constituent colours. The challenge with SKA, though, is how to get from the incomplete signal recording to the actual image. Unlike with optical telescopes, for example, where it is the diffraction of light that blurs the image, with SKA there are also the artificial noise artefacts that make it difficult to calculate and reconstruct the image, even with the help of supercomputers like CSCS's "Piz Daint" or its successor "Alps".

To calculate a single image from the thousands of antennas, researchers use a method called interferometry, which employs algorithms of the so-called CLEAN family that have been used for about 30 years. The algorithms calculate out the blurs and produce a sharp image by assuming that the intensity distribution of radio sources in the sky is a collection of so-called point sources. In order to obtain a cleaned-up image from the dirty image, the distortions of the point sources are repeatedly recalculated and subtracted from the dirty image until it, or the point source, is sharp. Depending on the telescope, this has typically required 1,000 to several thousand iterations. However, telescopes as large as the SKA and its much larger data rates increase the iterations per image to at least tens of thousands and up to a few million iterations. After all, if SKAO is fully operational by 2030, as planned, the researchers expect a terabyte of data per second. This deluge of data can no longer be handled by conventional algorithms within a reasonable period of time, the researchers say.

To handle this volume of data, the EPFL Center for Imaging has developed a new algorithm called Bluebild, which can image the sky more accurately and more efficiently than CLEAN. To this end, the EPFL researchers in PASC are working together in an interdisciplinary manner with specialists from the fields of image processing, astronomy and radio astronomy, as well as Big Data. The aim of the collaboration is, first, to optimise the Bluebild algorithm so that it efficiently solves the problem of the incomplete yet enormous data collection, and second, to one day convert the received data into images in real time. As a result of the collaboration, the optimised algorithm already performs up to 600 times better on CSCS' accelerated hardware than on pre-existing code on CPUs.

"The trick with Bluebild is what's called eigenvalue decomposition," says Tolley, "which means, even before you do any imaging, you split up all your signals according to brightness of the different sources in the sky." In other words, all the light sources are sorted from very bright to medium to low intensity. "The eigenvalue decomposition allows us to isolate these different sources in different flux levels, all in one go. Just by tuning the signal a little bit, we remove 5 percent of the data, so we automatically filter out the noise," Krishna adds.

But the method has another advantage: By sorting the light sources according to strength, it is possible to see very weak sources that were previously covered by strong light sources. "This eigenvalue decomposition gives us access to scientific cases that were previously inaccessible," Tolley explains.

Astronomical amounts of data

When the SKAO goes into full operation around 2030, it is expected that over a period of about 50 years, roughly 10 exabytes of data will be generated. For comparison, one exabyte is equal to ten to the power of 18 — 1,000,000,000,000,000,000 bytes to be exact. Processing and storing the data is a challenge that Bluebild aims to better address. While researchers in PASC are optimising Bluebild with the support of CSCS software developers, CSCS is also preparing everything to make portions of the generated data available for independent research as soon as possible.

The PASC Conference

The PASC Conference is an interdisciplinary meeting in large-scale scientific computing, which has been held annually since 2014. The conference fosters the exchange of competence in scientific computing and computational science, focusing on methods, tools, algorithms, application challenges, and novel techniques and usage of high-performance computing across various areas of computational science and engineering. The conference program is organized around seven scientific fields: physics; life sciences; chemistry and materials; climate, weather and earth sciences; engineering; humanities and social sciences; and computer science and applied mathematics.

The conference has grown in attendee numbers every year since its inception – and last year had almost 500 participants from 28 countries. The technical program includes keynote talks, minisymposium sessions, a peer-reviewed paper track, poster sessions, and panel-style discussions.

The PASC Program

The Platform for Advanced Scientific Computing (PASC) funds HPC software development projects that address the broad availability, quality, and performance of software on GPU-accelerated supercomputing platforms. Motivated by an important science case, these projects develop the necessary software to enable large scale calculations and lead to Tier-0 applications. Furthermore, the PASC program plays a crucial role in the evaluation and the co-design of the supercomputing infrastructure that serves the User Lab.

PASC projects cover a wide range of scientific domains, and the teams are interdisciplinary, including domain scientists, computational scientists, mathematicians, computer scientists and software engineers. The academic PIs collaborate closely with the PASC core team at CSCS that supports these projects with code development and software engineering expertise.

List of PASC Projects

Principal Investigator	Organisation	Research Field	Project Title	Approved funding (in CHF)
Paul Tackley	ETH Zurich	Earth & Environ. Science	GPU4GEO: Frontier GPU multi-physics solvers	543 658.00
Thomas Driesner	ETH Zurich	Earth & Environ. Science	FraNetG - Fracture Network Growth	489 771.00
Nicola Marzari	EPFL	Chemistry & Materials	Spectral properties of materials on accelerated architectures	488 320.00
Juerg Hutter	University of Zurich	Chemistry & Materials	Ab initio Molecular Dynamics at the Exa-Scale	448 930.00
Dominik Brunner	Empa	Earth & Environ. Science	HAMAM (HAM and ART Acceleration for Many-Core Architectures)	441 400.00
Torsten Hoefler	ETH Zurich	Computer Science & High-Performance Computing	DaCeMI - Harnessing future hardware using Data-Centric ML Integration	440 986.00
Florina Ciorba	University of Basel	Astrophysics/Cosmology	SPH-EXA2: Smoothed Particle Hydrodynamics at Exascale	440 000.00
Marina Marinkovic	ETH Zurich	Physics	Efficient QCD+QED Simulations with openQ*D software	440 000.00
Dominik Obrist	University of Bern	Life Sciences	MitrAccel – accelerated simulation of mitral heart valve biomechanics	440 000.00
Heini Wernli	ETH Zurich	Earth & Environ. Science	KILOS – Kilometer-scale nonhydrostatic global weather forecasting with IFS-FVM	440 000.00
Andreas Fichtner	ETH Zurich	Earth & Environ. Science	Bayesian Waveform Inversion	428 955.00
Andrew Jackson	ETH Zurich	Earth & Environ. Science	AQUA-D: Accelerated QuICC Application - Dynamo	401 500.00
Jean-Paul Kneib	EPFL	Astrophysics/Cosmology	Next-Generation Radio Interferometry	386 713.00
Rolf Krause	Università della Svizzera italiana	Computer Science & High-Performance Computing	ExaTrain - towards Exascale training for Machine Learning	330 000.00
Michele Ceriotti	EPFL	Chemistry & Materials	Machine learning for materials and molecules: toward the exascale	313 525.00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List of Projects by Institution

Dalle Molle Institute for Artificial Intelligence Research IDSIA

Advancing general purpose sequence processing neural networks, Kazuki Irie (Computer Science, 40 000 node h)

Improving systematic generalization of neural networks, Jürgen Schmidhuber (Computer Science, 250 000 node h)

EPFL

Basic local gyrokinetic study of internal transport barriers, Justin Ball (Physics, 277 000 node h)

Supporting Europe's path to net zero greenhouse gas emissions, Stephan Brunner (Physics, 99 500 node h)

Modulation of protein/membrane structure and dynamics by S-acylation, Matteo Dal Peraro (Life Science, 260 000 node h)

Effect of nanoparticles on shear-induced alignment of block copolymer thin films, Javier Diaz Brañas (Chemistry & Materials, 70 000 node h)

Shape-induced alignment in self-propelled dimers, Pasquale Digregorio (Chemistry & Materials, 160 000 node h)

Stationary and dynamical properties of topological defects in the active Brownian particles model, Pasquale Digregorio (Chemistry & Materials, 150 000 node h)

Modeling of turbulence measurements with gyrokinetic simulations and synthetic diagnostics, Oleg Krutkin (Physics, 250 000 node h)

Engineering the stability of metal halides: The route to eco-friendly perovskite solar cells, Lorenzo Monacelli (Chemistry & Materials, 200 000 node h)

Fluid simulations of plasma turbulence in the TJ-K stellarator, Joaquim Loizu (Physics, 40 000 node h)

CO-induced restructuring of Cu nanocrystal, Kevin Rossi (Chemistry & Materials, 36 000 node h)

Assessment of the importance of fluctuations and turbulence in the divertor region of magnetically confined fusion plasmas, Christian Theiler (Physics, 300 000 node h)

Novel electronic phases in condensed matter systems, Oleg Yazyev (Chemistry & Materials, 213 800 node h)

ETH Zurich

Architected materials for tailored elastic wave control: From lattice-like to shell and bio-inspired structures, Andrea Colombi (Mechanics & Engineering, 70 000 node h)

Extreme scale computing and data platform for cloud resolving weather and climate modelling, Anurag Dipankar (Earth & Environmental Science, 500 000 node h)

Modeling seismic waveforms of induced earthquakes, Laura Ermert (Earth & Environmental Science, 35 000 node h)

Simulations with quantified uncertainties and control of complex systems across scales through learning their effective dynamics, Petros Koumoutsakos (Computer Science, 403 000 node h)

Leading hadronic contribution to the muon magnetic moment with C* boundary conditions, Marina Marinkovic (Physics, 300 000 node h)

Large Eddy simulation of sequential combustors, Nicolas Noiray (Mechanics & Engineering, 278 000 node h)

Institute for Snow and Avalanche Research SLF

Representation of land-atmosphere interactions in complex terrain: Applying HICAR to study snow-atmosphere processes and characterization of meteorological forcings for cascading processes in a changing climate, Rebecca Mott (Earth & Environmental Science, 60 000 node h)

Istituto Ricerche Solari IRSOL

Realistic magneto-hydrodynamic simulations of solar and stellar atmospheres, Fabio Riva (Physics, 220 000 node h)

Italian Institute of Technology Genoa

First principles study of the ammonia decomposition reaction in lithium imide catalyst: combining machine learning with enhanced sampling, Manyi Yang (Chemistry & Materials, 300 000 node h)

Paul Scherrer Institute

Mechanism of gas transport in argillaceous rocks at saturated and partially condition from molecular dynamics simulations and pore scale modelling, Sergey Churakov (Earth & Environmental Science, 50 000 node h)

Molecular mechanism of Tc and Pu adsorption on magnetite by ab initio simulations and spectroscopy, Sergey Churakov (Earth & Environmental Science, 255 000 node h)

Thermodynamic model for competitive adsorption of cations on clays by ab initio simulation and X-ray spectroscopy, Sergey Churakov (Earth & Environmental Science, 266 000 node h)

Multiphase simulation of flow within porous mineral deposit layers (CRUDS) formed on top of zirconium alloy nuclear reactor fuel cladding using lattice Boltzmann framework, Nikolaos Prasianakis (Earth & Environmental Science, 100 000 node h)

Mesoscopic modeling of counter-diffusion experiments co-precipitation of metal with carbonates in porous media, Nikolaos Prasianakis (Earth & Environmental Science, 100 000 node h)

Recycling of iodine in the upper troposphere, Antoine Roose (Chemistry & Materials, 312 000 node h)

Physical Meteorological Observatory Davos / World Radiation Centre

Exploring future dangers for the ozone layer and its connection to climate, Timofei Sukhodolov (Earth & Environmental Science, 209 000 node h)

SUPSI

Understanding the impact of trodusquemine on the dynamic formation of lipid raft, Gianvito Grasso (Life Science, 35 000 node h)

Università della Svizzera italiana

Computational investigations on innovative NMDA channel blockers, Andrea Cavalli (Life Science, 35 000 node h)

Massively parallel global sensitivity analysis for power systems, Juraj Kardos (Computer Science, 60 000 node h)

Unraveling G-protein coupled receptor activation mechanism through µs-long atomistic molecular dynamics calculations, Vittorio Limongelli (Life Science, 190 000 node h)

In-silico ligand competitive binding assay using coarse-grained molecular dynamics simulations, Vittorio Limongelli (Life Science, 141 000 node h)

University Hospital Zurich

Self-supervised algorithms for skin lesion and management (Salesman), Javier Garcia Barranco (Life Science, 12 000 node h)

University of Basel

Density functional and machine learning schemes for structure predictions and free energy calculations, Stefan Goedecker (Chemistry & Materials, 400 000 node h)

University of Bern

Design-based computational study of the leaflet motion and flow characteristics of 3D-printed fibre-reinforced aortic valves, Pascal Corso (Life Science, 62 500 node h)

OVERSHOOT: Ocean impacts of temporarily overshooting the Paris Agreement, Thomas Frölicher (Earth & Environmental Science, 140 000 node h)

Dissolution mechanism of alkali-silica-reaction (ASR) by ab initio metadynamics, Kostantinos Karalis (Chemistry & Materials, 224 000 node h)

Influence of geometrical aortic wall parameters on three-dimensional laminar-turbulent transition mechanisms past bioprosthetic aortic valves, Dominik Obrist (Life Science, 200 000 node h)

Characterization and process understanding of extreme cyclones in the Mediterranean during the late Holocene (HARPYIE), Christoph Raible (Earth & Environmental Science, 180 000 node h)

University of Fribourg

Structural and dynamical characterization of canonical and non-canonical binders TCRs in a lipid environment, Josephine Alba (Life Science, 150 000 node h)

Molecular insights on the mode of action of Re(I) antibacterial complexes, Pablo Campomanes (Life Science, 145 000 node h)

Let there be fat: the molecular mechanism of neutral lipid synthesis by the acyltransferases DGAT1 and ACAT1/2, Stefano Vanni (Life Science, 400 000 node h)

University of Geneva

Monte Carlo Simulations of the medium mass nuclei for the DArk Matter Particle Explorer (DAMPE), Maksym Deliyergiyev (Physics, 215 000 node h)

University of Rome 2

Effect of mutations on the electroosmotic flow in biological and de novo designed b-barrel nanopores, Mauro Chinappi (Chemistry & Materials, 90 000 node h)

University of Zurich

Trapping noble gases in metal-organic frameworks, Jürg Hutter (Chemistry & Materials, 300 000 node h)

Catalysis under cover: The case of the hybrid hBN/Cu2O/Cu heterostructure, Marcella Iannuzzi (Chemistry & Materials, 300 000 node h)

Renewals

Dalle Molle Institute for Artificial Intelligence Research IDSIA

Meta learning general purpose reinforcement learning algorithms, Jürgen Schmidhuber (Computer Science, 100 000 node h)

EPFL

A single-cell atlas of spinal cord injury, Quentin Barraud (Life Science, 200 000 node h)

Dynamics of minority species in 3D fusion plasmas: Unconventional fast ion heating, Jonathan Graves (Physics, 100 000 node h)

Accurate determination of energy levels in advanced electronic-structure calculations, Alfredo Pasquarello (Chemistry & Materials, 200 000 node h)

Photocatalytic and photovoltaic applications for energy harvesting from sunlight, Alfredo Pasquarello (Chemistry & Materials, 277 000 node h)

Large-eddy simulation of large-scale wind-farm flows, Fernando Porté-Agel (Mechanics & Engineering, 156 000 node h)

ETH Zurich

Simulation of drying and deposition processes in deforming porous materials at pore scale using innovative hybrid LBM approaches, Jan Carmeliet (Mechanics & Engineering, 50 000 node h)

Simulating the dynamics of marine extreme events and their impact on ocean biogeochemistry, Nicolas Gruber (Earth & Environmental Science, 200 000 node h)

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

The origin of magnetism in planets and stars, Andrew Jackson (Earth & Environmental Science, 494 500 node h)

Lattice Boltzmann simulation of compressible and reactive flows, Ilia Karlin (Mechanics & Engineering, 150 000 node h)

Computation of forward and inverse problems for statistical solutions of compressible fluid flow, Siddhartha Mishra (Computer Science, 314 880 node h)

Climate, extremes, and land-climate dynamics, Sonia Seneviratne (Earth & Environmental Science, 36 000 node h)

Agent-based multiphysics modelling of bone turnover: Establishing preclinical and clinical tools for exploring the pathophysiology of aging, Harry van Lenthe (Life Science, 68 000 node h)

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

Institute for Snow and Avalanche Research SLF

Blowing snow dynamics and its impact on snow cover and theatmospheric boundary layer, Michael Lehning (Earth & Environmental Science, 215 000 node h)

Paul Scherrer Institute

Dynamics of porous catalytic particles in fluidized beds for biogas methanation, John Mantzaras (Mechanics & Engineering, 40 000 node h)

Stanford University

Scaling the Legion programming system, Alex Aiken (Computer Science, 36 000 node h)

Università della Svizzera italiana

LongAF: in silico study of the combined effect of structural and electrical heterogeneities in long episodes of atrial fibrillation, Simone Pezzuto (Life Science, 180 000 node h)

University of Bern

Climate, land use and biodiversity pathways for sustainable futures, Edouard Davin (Earth & Environmental Science, 36 000 node h)

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

University of Geneva

Digital blood: A study of platelet transport in blood, Bastien Chopard (Life Science, 235 000 node h)

University of Lausanne

Study of the TWIK1 channel ion selectivity modulation by the pH, Olivier Bignucolo (Life Science, 137 000 node h)

Analysis of the activation pathway of acid-sensing ion channels, Stefan Kellenberger (Life Science, 112 000 node h)

University of Zurich

Outflows in simulated massive galaxies at high redshift, Luigi Bassini (Physics, 100 000 node h)

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

Vulcan Inc.

Enabling a global storm-resolving climate model on hybrid supercomputing infrastructures for machine learning of physical parametrizations, Oliver Fuhrer (Earth & Environmental Science, 120 000 node h)

Name
Monica Frisoni

Nationality
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Position
Software and Database Engineer

Working at CSCS since
September 2015

Background

2005-2008	Master's in Computer Science, ETH Zurich
2008-2009	Assistant at the University of Lugano, Faculty of Informatics
2010-2012	Application Architect at UNIC, Zurich
2012	Senior Software Engineer at uFirst Group, Zurich
2012-2015	Senior Software Engineer at Ente Ospedaliero Cantonale (EOC), Bellinzona
2015-Present	Software and Database Engineer, CSCS

Specialisation

I am focused on working and dealing with various types and amounts of data, from which we need to extract useful and strategic information for the Centre. The quality and completeness of the data allows us to have the means to verify what is happening, anticipate and prevent any errors, and analyse the trends in order to better define future goals.

What working at CSCS means to me

Working in an academic environment of national importance is very enriching and motivating. CSCS gives me the opportunity to continue to grow, train, and improve my skills.

What I like most about my work

I like being surrounded by people with both different and common interests. This allows me to gain knowledge and understanding every day, and it is always a stimulus to continue to differentiate and explore fields other than mine during my daily work.

What challenges me at my work

Data has and is becoming increasingly important, and this allows us to be creative and open to new ideas, technologies, and solutions. I find it interesting — and challenging — to be able to extract useful and important information starting from simple raw data. By combining this data together with technical knowledge and business needs, we can structure the information in a way that better guides the Centre in making decisions.

Papers with Highest Journal Impact Factor[1)]

Nature

Impact Factor: 69.50

C. Kathe, M. A. Skinnider, T. H. Hutson, N. Regazzi, M. Gautier, R. Demesmaeker, S. Komi, S. Ceto, N. D. James, N. Cho, L. Baud, K. Galan, K. J. E. Matson, A. Rowald, K. Kim, R. Wang, K. Minassian, J. O. Prior, L. Asboth, Q. Barraud, S. P. Lacour, A. J. Levine, F. Wagner, J. Bloch, J. W. Squair, G. Courtine, The neurons that restore walking after paralysis, Nature, DOI 10.1038/s41586-022-05385-7.

V. Kapil, C. Schran, A. Zen, J. Chen, C. J. Pickard, A. Michaelides, The first-principles phase diagram of monolayer nanoconfined water, Nature, DOI 10.1038/s41586-022-05036-x.

Nature Materials

Impact Factor: 47.66

S. M. Moosavi, B. A. Novotny, D. Ongari, E. Moubarak, M. Asgari, O. Kadioglu, C. Charalambous, A. Ortega-Guerrero, A. H. Farmahini, L. Sarkisov, S. Garcia, F. Noé, B. Smit, A data-science approach to predict the heat capacity of nanoporous materials, Nature Materials, DOI 10.1038/s41563-022-01374-3.

L. Caretta, Y.-T. Shao, J. Yu, A. B. Mei, B. F. Grosso, C. Dai, P. Behera, D. Lee, M. McCarter, E. Parsonnet, H. K. P, F. Xue, X. Guo, E. S. Barnard, S. Ganschow, Z. Hong, A. Raja, L. W. Martin, L.-Q. Chen, M. Fiebig, K. Lai, N. A. Spaldin, D. A. Muller, D. G. Schlom, R. Ramesh, Non-volatile electric-field control of inversion symmetry, Nature Materials, DOI 10.1038/s41563-022-01412-0.

Advanced Materials

Impact Factor: 32.07

S. Q. Huang, L. F. Villalobos, S. X. Li, M. T. Vahdat, H. Y. Chi, K. J. Hsu, L. Bondaz, V. Bouraux, N. Marzari, K. V. Agrawal, In Situ nucleation-decoupled and site-specific incorporation of angstrom-scale pores in graphene via epoxidation, Advanced Materials, DOI 10.1002/adma.202206627.

L. A. Muscarella, A. Dučinskas, M. Dankl, M. Andrzejewski, N. P. M. Casati, U. Röthlisberger, J. Maier, M. Grätzel, B. Ehrler, J. V. Milić, Reversible pressure-dependent mechanochromism of Dion-Jacobson and Ruddlesden-Popper layered hybrid perovskites, Advanced Materials, DOI 10.1002/adma.202108720.

D. Kim, I. Efe, H. Torlakcik, A. Terzopoulou, A. Veciana, E. Siringil, F. Mushtaq, C. Franco, D. von Arx, S. Sevim, J. Puigmartí-Luis, B. Nelson, N. A. Spaldin, C. Gattinoni, X.-Z. Chen, S. Pané, Magnetoelectric effect in hydrogen harvesting: Magnetic field as a trigger of catalytic reactions, Advanced Materials, DOI 10.1002/adma.202110612.

Advanced Energy Materials

Impact Factor: 29.70

Y. R. Wang, A. Senocrate, M. Mladenović, A. Ducinškas, G. Y. Kim, U. Röthlisberger, J. V. Milić, D. Moia, M. Grätzel, J. Maier, Photo de-mixing in Dion-Jacobson 2D mixed halide perovskites, Advanced Energy Materials, DOI 10.1002/aenm.202200768.

Nature Machine Intelligence

Impact Factor: 25.90

P. R. Vlachas, G. Arampatzis, C. Uhler, P. Koumoutsakos, Multiscale simulations of complex systems by learning their effective dynamics, Nature Machine Intelligence, DOI 10.1038/s42256-022-00464-w.

Annual Review of Fluid Mechanics

Impact Factor: 25.29

A. D. Sandberg, V. Michelassi, Fluid dynamics of axial turbomachinery: Blade- and stage-level simulations and models, Annual Review of Fluid Mechanics, DOI 10.1146/annurev-fluid-031221-105530.

Wiley Interdisciplinary Reviews-Computational Molecular Science

Impact Factor: 25.11

S. C. Van Keulen, J. Martin, F. Colizzi, E. Frezza, D. Trpevski, N. C. Diaz, P. Vidossich, U. Röthlisberger, J. Hellgren Kotaleski, R. C. Wade, P. Carloni, Multiscale molecular simulations to investigate adenylyl cyclase-based signaling in the brain, Wiley Interdisciplinary Reviews-Computational Molecular Science, DOI 10.1002/wcms.1623.

Accounts of Chemical Research

Impact Factor: 24.47

F. Mouvet, J. Villard, V. Bolnykh, U. Röthlisberger, Recent advances in first-principles based molecular dynamics, Accounts of Chemical Research, DOI 10.1021/acs.accounts.1c00503.

[1)] Journal of Impact Factor 2022 - JCR, Web Of Science

Applied Catalysis B: Environmental

Impact Factor: 24.32

M. S. Ozer, Z. Eroglu, A. S. Yalin, M. Kılıç, U. Röthlisberger, O. Metin, Bismuthene as a versatile photocatalyst operating under variable conditions for the photoredox CH bond functionalization, Applied Catalysis B: Environmental, DOI 10.1016/j.apcatb.2021.120957.

Nature Chemistry

Impact Factor: 24.27

K. Koner, S. Karak, S. Kandambeth, S. Karak, N. Thomas, L. Leanza, C. Perego, L. Pesce, R. Capelli, M. Moun, M. Bhakar, T. G. Ajithkumar, G. M. Pavan, R. Banerjee, Porous covalent organic nanotubes and their assembly in loops and toroids, Nature Chemistry, DOI 10.1038/s41557-022-00908-1.

P. O. Heidarsson, D. Mercadante, A. Sottini, D. Nettels, M. B. Borgia, A. Borgia, A. Borgia, S. Kilic, B. Fierz, R. B. Best, B. Schuler, Release of linker histone from the nucleosome driven by polyelectrolyte competition with a disordered protein, Nature Chemistry, DOI 10.1038/s41557-021-00839-3.

ACS Energy Letters

Impact Factor: 23.99

A. Mishra, D. J. Kubicki, A. Boziki, R. D. Chavan, M. Dankl, M. Mladenović, D. Prochowicz, C. P. Grey, U. Röthlisberger, L. Emsley, Interplay of kinetic and thermodynamic reaction control explains incorporation of dimethylammonium iodide into CsPbI 3, ACS Energy Letters, DOI 10.1021/acsenergylett.2c00877.

ACS Nano

Impact Factor: 18.03

G. Di Muccio, B. M. della Rocca, M. Chinappi, Geometrically induced selectivity and unidirectional electroosmosis in uncharged nanopores, ACS Nano, DOI 10.1021/acsnano.1c03017.

C. Lionello, C. Perego, A. Gardin, R. Klajn, G. M. Pavan, Supramolecular semiconductivity through emerging ionic gates in ion-nanoparticle superlattices, ACS Nano, DOI 10.1021/acsnano.2c07558.

A. K. Adamczyk, T. A. P. M. Huijben, M. Sison, A. Di Luca, S. Vanni, S. Brasselet, K. I. Mortensen, F. D. Stefani, M. Pilo-Pais, G. P. Acuna, DNA self-assembly of single molecules with deterministic position and orientation, ACS Nano, DOI 10.1021/acsnano.2c06936.

Nature Communications

Impact Factor: 17.69

K. Eimre, J. I. Urgel, H. Hayashi, M. Di Giovannantonio, P. Ruffieux, S. Sato, S. Otomo, Y. S. Chan, N. Aratani, D. Passerone, O. Gröning, H. Yamada, R. Fasel, C. A. Pignedoli, On-surface synthesis and characterization of nitrogen-substituted undecacenes, Nature Communications, DOI 10.1038/s41467-022-27961-1.

H. Zhang, K. Darabi, N. Y. Nia, A. Krishna, P. Ahlawat, B. Guo, M. H. S. Almalki, T.-S. Su, D. Ren, V. Bolnykh, L. A. Castriotta, M. Zendehdel, L. Pan, S. Sanchez Alonso, R. Li, S. M. Zakeeruddin, A. Hagfeldt, U. Röthlisberger, A. Di Carlo, A. Amassian, M. Grätzel, A universal co-solvent dilution strategy enables facile and cost-effective fabrication of perovskite photovoltaics, Nature Communications, DOI 10.1038/s41467-021-27740-4.

A. J. Bae, P. Koumoutsakos, Scientific multi-agent reinforcement learning for wall-models of turbulent flows, Nature Communications, DOI 10.1038/s41467-022-28957-7.

G. Raino, N. Yazdani, S. C. Boehme, M. Kober-Czerny, C. L. Zhu, F. Krieg, M. D. Rossell, R. Erni, V. Wood, I. Infante, M. V. Kovalenko, Ultra-narrow room-temperature emission from single $CsPbBr_3$ perovskite quantum dots, Nature Communications, DOI 10.1038/s41467-022-30016-0.

G. Chi, Q. Liang, A. Sridhar, J. B. Cowgill, K. Sader, M. Radjainia, P. Qian, P. Castro-Hartmann, S. Venkaya, N. Kaur Singh, G. McKinley, A. Fernandez-Cid, S. M. M. Mukhopadhyay, N. A. Burgess-Brown, L. Delemotte, M. Covarrubias, K. L. Dürr, Cryo-EM structure of the human Kv3.1 channel reveals gating control by the cytoplasmic T1 domain, Nature Communications, DOI 10.1038/s41467-022-29594-w.

N. Uchida, A. Kohata, K. Okuro, A. Cardellini, C. Lionello, E. A. Zizzi, M. A. Deriu, G. M. Pavan, M. Tomishige, T. Hikima, T. Aida, Reconstitution of microtubule into GTP-responsive nanocapsules, Nature Communications, DOI 10.1038/s41467-022-33156-5.

M. Crippa, C. Perego, A. L. de Marco, G. M. Pavan, Molecular communications in complex systems of dynamic supramolecular polymers, Nature Communications, DOI 10.1038/s41467-022-29804-5.

E. Weyandt, L. Leanza, R. Capelli, G. M. Pavan, G. Vantomme, E. W. Meijer, Controlling the length of porphyrin supramolecular polymers via coupled equilibria and dilution-induced supramolecular polymerization, Nature Communications, DOI 10.1038/s41467-021-27831-2.

L. Reichen, A. M. Burgdorf, S. Brönnimann, J. Franke, R. Hand, V. Valler, E. Samakinwa, Y. Brugnara, T. Rutishauser, A decade of cold Eurasian winters reconstructed for the early 19th century, Nature Communications, DOI 10.1038/s41467-022-29677-8.

F. A. Burger, J. Terhaar, T. L. Frölicher, Compound marine heatwaves and ocean acidity extremes, Nature Communications, DOI 10.1038/s41467-022-32120-7.

Angewandte Chemie-International Edition

Impact Factor: 16.82

J. Bjork, C. Sanchez-Sanchez, Q. Chen, C. A. Pignedoli, J. Rosen, P. Ruffieux, X. Feng, A. Narita, K. Müllen, R. Fasel, The Role of metal adatoms in a surface-assisted cyclodehydrogenation reaction on a gold surface, Angewandte Chemie-International Edition, DOI 10.1002/anie.202212354.

J. Lan, V. V. Rybkin, A. Pasquarello, Temperature dependent properties of the aqueous electron, Angewandte Chemie-International Edition, DOI 10.1002/anie.202209398.

P. Knecht, D. Meier, J. Reichert, D. A. Duncan, M. Schwarz, J. T. Küchle, T.-L. Lee, P. S. Deimel, P. Feulner, F. Allegretti, W. Auwärter, G. Médard, A. P. Seitsonen, J. V. Barth, A. C. Papageorgiou, N-heterocyclic carbenes: Molecular porters of surface mounted Ru-porphyrins, Angewandte Chemie-International Edition, DOI 10.1002/anie.202211877.

Journal of the American Chemical Society

Impact Factor: 16.38

S. X. Li, M. T. Vahdat, S. Q. Huang, K. J. Hsu, M. Rezaei, M. Mensi, N. Marzari, K. V. Agrawal, Structure evolution of graphitic surface upon oxidation: Insights by scanning tunneling microscopy, Journal of American Chemical Society, DOI 10.1021/jacsau.1c00570.

O. S. Lecina, M. A. Hope, A. Venkatesh, S. Bjorgvinsdottir, K. Rossi, A. Loiudice, L. Emsley, R. Buonsanti, Colloidal-ALD-grown hybrid shells nucleate via a ligand-precursor complex, Journal of the American Chemical Society, DOI 10.1021/jacs.1c12538.

M. G. Goesten, Y. Xia, U. Aschauer, M. Amsler, Conformational gap control in CsTaS 3, Journal of the American Chemical Society, DOI 10.1021/jacs.1c10947.

Nature Astronomy

Impact Factor: 15.65

J. Moreno, S. Danieli, J. S. Bullock, R. Feldmann, P. F. Hopkins, O. Çatmabacak, A. Gurvich, A. Lazar, C. Klein, C. B. Hummels, Z. Hafen, F. J. Mercado, S. Yu, F. Jiang, C. Wheeler, A. Wetzel, D. Anglés-Alcázar, M. Boylan-Kolchin, E. Quataert, C.-A. Faucher-Giguère, D. Kereš, Galaxies lacking dark matter produced by close encounters in a cosmological simulation, Nature Astronomy, DOI 10.1038/s41550-021-01598-4.

Science Advances

Impact Factor: 14.96

P. Karnakov, S. Litvinov, P. Koumoutsakos, Computing foaming flows across scales: From breaking waves to microfluidics, Science Advances, DOI 10.1126/sciadv.abm0590.

J. A. Mundy, B. F. Grosso, C. A. Heikes, D. F. Segedin, Z. Wang, Y. T. Shao, C. Dai, B. H. Goodge, Q. N. Meier, C. T. Nelson, B. Prasad, F. Xue, S. Ganschow, D. A. Muller, L. F. Kourkoutis, L.-Q. Chen, W. D. Ratcliff, N. A. Spaldin, R. Ramesh, D. G. Schlom, Liberating a hidden antiferroelectric phase with interfacial electrostatic engineering, Science Advances, DOI 10.1126/sciadv.abg5860.

G. Di Lorenzo, F. Iavarone, M. Maddaluno, A. B. Plata-Gómez, S. Aureli, C. P. Quezada Meza, L. Cinque, A. Palma, A. Reggio, C. Cirillo, F. Sacco, A. Stolz, G. Napolitano, O. Marin, L. A. Pinna, M. Ruzzene, V. Limongelli, A. Efeyan, P. Grumati, C. Settembre, Phosphorylation of FAM134C by CK2 controls starvation-induced ER-phagy, Science Advances, DOI 10.1126/sciadv.abo1215.

ACS Catalysis

Impact Factor: 13.70

S. Lyu, J. Wiktor, A. Pasquarello, Oxygen evolution at the BiVO4-water interface: Mechanism of the water dehydrogenation reaction, ACS Catalysis, DOI 10.1021/acscatal.2c03331.

Proceedings of the National Academy of Sciences of the United States of America

Impact Factor: 12.78

E. Scalone, L. Broggini, C. Visentin, D. Erba, F. B. Toplek, K. Peqini, S. Pellegrino, S. Ricagno, C. Paissoni, C. Camilloni, Multi-eGO: An in silico lens to look into protein aggregation kinetics at atomic resolution, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2203181119.

V. Kapil, E. A. Engel, A complete description of thermodynamic stabilities of molecular crystals, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2111769119.

F. Shao, J. K. Wong, Q. H. Low, M. Iannuzzi, J. G. Li, J. G. Lan, In situ spectroelectrochemical probing of CO redox landscape on copper single-crystal surfaces, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2118166119.

Nano Letters

Impact Factor: 12.26

G. Pasquale, Z. Sun, K. Cernevics, R. Perea-Causin, F. Tagarelli, K. Watanabe, T. Taniguchi, E. Malic, O. V. Yazyev, A. Kis, Flat-band-induced many-body interactions and exciton complexes in a layered semiconductor, Nano Letters, DOI 10.1021/acs.nanolett.2c02965.

npj Computational Materials

Impact Factor: 12.26

L. Gigli, M. Veit, M. Kotiuga, G. Pizzi, N. Marzari, M. Ceriotti, Thermodynamics and dielectric response of BaTiO3 by data-driven modeling, npj Computational Materials, DOI 10.1038/s41524-022-00845-0.

S. Falletta, A. Pasquarello, Hubbard U through polaronic defect states, npj Computational Materials, DOI 10.1038/s41524-022-00958-6.

H. Wang, A. Tal, T. Bischoff, P. Gono, A. Pasquarello, Accurate and efficient band-gap predictions for metal halide perovskites at finite temperature, npj Computational Materials, DOI 10.1038/s41524-022-00869-6.

Environmental Science & Technology

Impact Factor: 11.37

G. A. Kelesidis, D. Neubauer, L. S. Fan, U. Lohmann, S. E. Pratsinis, Enhanced light absorption and radiative forcing by black carbon agglomerates, Environmental Science & Technology, DOI 10.1021/acs.est.2c00428.

npj 2D Materials and Applications

Impact Factor: 11.11

F. Ducry, D. Waldhoer, T. Knobloch, M. Csontos, N. Jimenez Olalla, J. Leuthold, T. Grasser, M. Luisier, An ab initio study on resistance switching in hexagonal boron nitride, npj 2D Materials and Applications, DOI 10.1038/s41699-022-00340-6.

ACS Applied Materials & Interfaces

Impact Factor: 10.38

Y. L. Müller, L. P. H. Jeurgens, A. Antušek, V. Turlo, Atomistic assessment of melting point depression and enhanced interfacial diffusion of Cu in confinement with AlN, ACS Applied Materials & Interfaces, DOI 10.1021/acsami.2c01347.

G. Cherkashinin, R. Eilhardt, S. Nappini, M. Cococcioni, I. Píš, S. dal Zilio, F. Bondino, N. Marzari, E. Magnano, L. Alff, Energy level alignment at the cobalt phosphate/electrolyte interface: Intrinsic stability vs interfacial chemical reactions in 5 V Lithium ion batteries, ACS Applied Materials & Interfaces, DOI 10.1021/acsami.1c16296.

Chemical Science

Impact Factor: 9.97

M. Delle Piane, L. Pesce, M. Cioni, G. M. Pavan, Reconstructing reactivity in dynamic host-guest systems at atomistic resolution: amide hydrolysis under confinement in the cavity of a coordination cage, Chemical Science, DOI 10.1039/d2sc02000a.

ACS Sustainable Chemistry & Engineering

Impact Factor: 9.22

A. P. Le Monnier, L. Savereide, M. Kilic, R. Schnyder, M. D. Mensi, C. E. Avalos, U. Röthlisberger, J. S. Luterbacher, Atom-by-atom synthesis of multiatom-supported catalytic clusters by liquid-phase atomic layer deposition, ACS Sustainable Chemistry & Engineering, DOI 10.1021/acssuschemeng.1c07056.

Cellular and Molecular Life Sciences

Impact Factor: 9.21

S. G. Royce, P. V. Licciardi, R. C. Beh, J. E. Bourke, C. Donovan, A. N. Hung, I. Khurana, J. J. Liang, S. Maxwell, N. Mazarakis, E. Pitsillou, Y. Y. Siow, K. J. Snibson, M. J. Tobin, K. Ververis, J. Vongsvivut, M. Ziemann, C. S. Samuel, M. L. K. Tang, A. El-Osta, T. C. Karagiannis, Sulforaphane prevents and reverses allergic airways disease in mice via anti-inflammatory, antioxidant, and epigenetic mechanisms, Cellular and Molecular Life Sciences, DOI 10.1007/s00018-022-04609-3.

Physical Review Letters

Impact Factor: 9.19

S. Falletta, A. Pasquarello, Many-body self-interaction and polarons, Physical Review Letters, DOI 10.1103/PhysRevLett.129.126401.

A. Petocchi, C. W. Nicholson, B. Salzmann, D. Pasquier, O. V. Yazyev, C. Monney, P. Werner, Mott versus hybridization gap in the low-temperature phase of 1T-TaS_2, Physical Review Letters, DOI 10.1103/PhysRevLett.129.016402.

S. Bhowal, N. A. Spaldin, Magnetoelectric classification of skyrmions, Physical Review Letters, DOI 10.1103/PhysRevLett.128.227204.

S. Bhowal, S. P. Collins, N. A. Spaldin, Hidden k-space magnetoelectric multipoles in nonmagnetic ferroelectrics, Physical Review Letters, DOI 10.1103/PhysRevLett.128.116402.

C. W. Myung, B. Hirshberg, M. Parrinello, Prediction of a supersolid phase in high-pressure deuterium, Physical Review Letters, DOI 10.1103/PhysRevLett.128.045301.

A. Chen, T. Gehrmann, N. Glover, A. Huss, T. Z. Yang, H. X. Zhu, Dilepton rapidity distribution in drell-yan production to third order in QCD, Physical Review Letters, DOI 10.1103/PhysRevLett.128.052001.

ChemSusChem

Impact Factor: 9.14

N. Weder, N. S. Grundmann, B. Probst, O. Blacque, R. Ketkaew, F. Creazzo, S. Luber, R. Alberto, Two novel dinuclear cobalt polypyridyl complexes in electro- and photocatalysis for hydrogen production: Cooperativity increases performance, ChemSusChem, DOI 10.1002/cssc.202201049.

Nano Research

Impact Factor: 8.90

B. D. Chen, F. F. Qin, M. Su, D. X. Xie, Z. Y. Zhang, Q. Pan, H. Wang, X. Yang, S. Chen, J. Huang, D. Derome, J. Carmeliet, Y. Song, One droplet reaction for synthesis of multi-sized nanoparticles, Nano Research, DOI 10.1007/s12274-022-5115-7.

Frontiers in Immunology

Impact Factor: 8.79

M. L. Fernández-Quintero, A. L. M. Fischer, J. Kokot, F. Waibl, C. A. Seidler, K. R. Liedl, The influence of antibody humanization on shark variable domain (VNAR) binding site ensembles, Frontiers in Immunology, DOI 10.3389/fimmu.2022.953917.

Journal of Molecular Graphics & Modelling

Impact Factor: 8.71

E. Pitsillou, J. L. Liang, A. D. Hung, T. C. Karagiannis, The SARS-CoV-2 helicase as a target for antiviral therapy: Identification of potential small molecule inhibitors by in silico modelling, Journal of Molecular Graphics & Modelling, DOI 10.1016/j.jmgm.2022.108193.

eLife

Impact Factor: 8.71

S. Sotillos, I. von der Decken, I. Domenech Mercadé, S. Srinivasan, D. Sirokha, L. Livshits, S. Vanni, S. Nef, A. Biason-Lauber, D. Rodríguez Gutiérrez, J. Castelli-Gair Hombría, A conserved function of Human DLC3 and *Drosophila* Cv-c in testis development, eLife, DOI 10.7554/eLife.82343.

A. Borsatto, O. Akkad, I. Galdadas, S. M. Ma, S. Damfo, S. Haider, F. Kozielski, C. Estarellas, Francesco Luigi Gervasio, Revealing druggable cryptic pockets in the Nsp1 of SARS-CoV-2 and other beta-coronaviruses by simulations and crystallography, eLife, DOI 10.7554/eLife.81167.

J. R. McArthur, J. R. Wen, A. D. Hung, R. K. Finol-Urdaneta, D. J. Adams, H. M. Colecraft, m-Theraphotoxin Pn3a inhibition of CaV3.3 channels reveals a novel isoform-selective drug binding site, eLife, DOI 10.7554/eLife.74040.

Advances in Physics-X

Impact Factor: 8.53

A. Gubbiotti, M. Baldelli, G. Di Muccio, P. Malgaretti, S. Marbach, M. Chinappi, Electroosmosis in nanopores: Computational methods and technological applications, Advances in Physics-X, DOI 10.1080/23746149.2022.2036638.

Nanoscale

Impact Factor: 8.31

E. Petretto, Q. K. Ong, F. Olgiati, T. Mao, P. Campomanes, F. Stellacci, S. Vanni, Monovalent ion-mediated charge-charge interactions drive aggregation of surface-functionalized gold nanoparticles, Nanoscale, DOI 10.1039/d2nr02824g.

Engineering with Computers

Impact Factor: 8.08

C. Ruiz-Herrera, T. Grandits, G. Plank, P. Perdikaris, F. S. Costabal, S. Pezzuto, Physics-informed neural networks to learn cardiac fiber orientation from multiple electroanatomical maps, Engineering with Computers, DOI 10.1007/s00366-022-01709-3.

Journal of Cell Biology

Impact Factor: 8.08

S. Rogers, L. Gui, A. Kovalenko, V. Zoni, M. Carpentier, K. Ramji, K. B. Mbarek, A. Bacle, P. Fuchs, P. Campomanes, E. Reetz, N. Ortiz Speer, E. Reynolds, A. R. Thiam, S. Vanni, D. Nicastro, W. M. Henne, Triglyceride lipolysis triggers liquid crystalline phases in lipid droplets and alters the LD proteome, Journal of Cell Biology, DOI 10.1083/jcb.202205053.

Papers Published in 2022 by Principal Investigator

Sebnem Aksoyoglu, Paul Scherrer Institute

J. H. Zohdirad, J. H. Jiang, S. Aksoyoglu, M. M. Namin, K. Ashrafi, A. S. H. Prévôt, Investigating sources of surface ozone in central Europe during the hot Summer in 2018: High temperatures, but not so high ozone, Atmospheric Environment, DOI 10.1016/j.atmosenv.2022.119099.

Kumar Varoon Agrawal, EPFL

S. Q. Huang, L. F. Villalobos, S. X. Li, M. T. Vahdat, H. Y. Chi, K. J. Hsu, L. Bondaz, V. Bouraux, N. Marzari, K. V. Agrawal, In Situ nucleation-decoupled and site-specific incorporation of angstrom-scale pores in graphene via epoxidation, Advanced Materials, DOI 10.1002/adma.202206627.

S. X. Li, M. T. Vahdat, S. Q. Huang, K. J. Hsu, M. Rezaei, M. Mensi, N. Marzari, K. V. Agrawal, Structure evolution of graphitic surface upon oxidation: Insights by scanning tunneling microscopy, Journal of American Chemical Society, DOI 10.1021/jacsau.1c00570.

Constantia Alexandrou, Cyprus Institute & University of Cyprus

C. Alexandrou, S. Bacchio, G. Bergner, M. Constantinou, M. Di Carlo, P. Dimopoulos, J. Finkenrath, E. Fiorenza, R. Frezzotti, M. Garofalo, K. Hadjiyiannakou, B. Kostrzewa, G. Koutsou, K. Jansen, V. Lubicz, M. Mangin-Brinet, F. Manigrasso, G. Martinelli, F. Pittler, G.C. Rossi, F. Sanfilippo, S. Simula, C. Tarantino, A. Todaro, C. Urbachj, U. Wenger, Determination of the light, strange and charm quark masses using twisted mass fermions, Proceedings of Science, DOI 10.22323/1.396.0171.

C. Alexandrou, S. Bacchio, M. Constantinou, J. Finkenrath, K. Hadjiyiannakou, K. Jansen, G. Koutsou, A. Vaquero, Nucleon form factors from N_f=2+1+1 twisted mass QCD at the physical point, Proceedings of Science, LATTICE2021, DOI 10.22323/1.396.0250.

K. Hadjiyiannakou, C. Alexandrou, S. Bacchio, M. Constantinou, J. Finkenrath, K. Jansen, G. Koutsou, H. Panagopoulos, G. Spanoudes, Decomposition of the proton spin from lattice QCD, Proceedings of Science, LATTICE2021, DOI 10.22323/1.396.0348.

C. Alexandrou, K. Hadjiannakou, G. Koutsou, S. Paul, F. Pittler, M. Petschliesd, A. Todaro, Elastic $\pi - N$ scattering in the I = 3/2 channel, Proceedings of Science, LATTICE2021, DOI 10.22323/1.396.0226.

C. Alexandrou, A. Athenodorou, K. Hadjiannakou, A. Todaro, A lattice QCD determination of the neutron electric dipole moment at the physical point, Proceedings of Science, LATTICE2021, DOI 10.22323/1.396.0120.

Ulrich Aschauer, University of Bern

M. Bouri, N. Niederhauser, B. Künzli, M. Amsler, U. Aschauer, Oxygen evolution reaction activity of $Sr_2Ta_2O_7$ and $Sr_2Nb_2O_7$ surfaces, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.2c00649.

M. G. Goesten, Y. Xia, U. Aschauer, M. Amsler, Conformational gap control in $CsTaS_3$, Journal of the American Chemical Society, DOI 10.1021/jacs.1c10947.

N. Vonrüti, R. Rao, L. Giordano, Y. Shao-Horn, U. Aschauer, Implications of nonelectrochemical reaction steps on the oxygen evolution reaction: Oxygen dimer formation on perovskite oxide and oxynitride surfaces, ACS Catalysis, DOI 10.1021/acscatal.1c03308.

M. Kaviani, U. Aschauer, Surface and interface effects in oxygen-deficient $SrMnO_3$ thin films grown on $SrTiO_3$, Physical Chemistry Chemical Physics, DOI 10.1039/d1cp04998d.

C. Ricca, U. Aschauer, Photochemical anisotropy and direction-dependent optical absorption in semiconductors, Journal of Chemical Physics, DOI 10.1063/5.0087293.

Marco Bacci, EAWAG

M. Bacci, M. Dal Molin, F. Fenicia, P. Reichert, J. Šukys, Application of stochastic time dependent parameters to improve the characterization of uncertainty in conceptual hydrological models, Journal of Hydrology, DOI 10.1016/j.jhydrol.2022.128057.

Dirk Bakowies, University of Basel

D. Bakowies, ATOMIC-2 protocol for thermochemistry, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.1c01272.

D. Bakowies, Ab initio thermochemistry with ATOMIC-2, Journal of Chemical Theory and Computation, DOI 10.5281/zenodo.5780172.

Justin Ball, EPFL

A. Volčokas, J. Ball, S. Brunner, Ultra long turbulent eddies, magnetic topology, and the triggering of internal transport barriers in tokamaks, Nuclear Fusion, DOI 10.1088/1741-4326/aca213.

J. Ball, S. Brunner, Local gyrokinetic simulations of tokamaks with non-uniform magnetic shear, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/aca715.

Nikolina Ban, University of Innsbruck

A. F. Prein, N. Ban, T. H. Ou, J. P. Tang, K. Sakaguchi, E. Collier, S. Jayanarayanan, L. Li, S. Sobolowski, X. Chen, X. Zhou, H.-W. Lai, S. Sugimoto, L. Zou, S. ul Hasson, M. Ekstrom, P. K. Pothapakula, B. Ahrens, R. Stuart, H. C. Steen-Larsen, R. Leung, D. Belusic, J. Kukulies, J. Curio, D. Chen, Towards ensemble-based kilometer-scale climate simulations over the third pole region, Climate Dynamics, DOI 10.1007/s00382-022-06543-3.

S. Berthou, M. J. Roberts, B. Vanniere, N. Ban, D. Belusic, C. Caillaud, T. Crocker, H. de Vries, A. Dobler, D. Harris, Convection in future winter storms over Northern Europe, Environmental Research Letters, DOI 10.1088/1748-9326/aca03a.

N. Peleg, N. K. L. A. Ban, M. J. Gibson, A. S. Chen, A. Paschalis, P. Burlando, J. P. Leitão, Mapping storm spatial profiles for flood impact assessments, Advances in Water Resources, DOI 10.1016/j.advwatres.2022.104258.

P. M. M. Soares, J. A. M. Careto, R. M. Cardoso, K. Goergen, E. Katragkou, S. Sobolowski, E. Coppola, N. Ban, D. Belušić, S. Berthou, C. Caillaud, A. Dobler, Ø. Hodnebrog, S. Kartsios, G. Lenderink, T. Lorenz, J. Milovac, H. Feldmann, E. Pichelli, H. Truhetz, M. E. Demory, H. de Vries, K. Warrach-Sagi, K. Keuler, M. Raffa, M. Tölle, K. Sieck, S. Bastin, The added value of km-scale simulations to describe temperature over complex orography: The CORDEX FPS-convection multi-model ensemble runs over the Alps, Climate Dynamics, DOI 10.1007/s00382-022-06593-7.

S. C. Chan, E. J. Kendon, H. J. Fowler, A. Kahraman, J. Crook, N. Ban, A. F. Prein, Large-scale dynamics moderate impact-relevant changes to organised convective storms, Communications Earth & Environment, DOI 10.1038/s43247-022-00669-2.

Quentin Barraud, EPFL

C. Kathe, M. A. Skinnider, T. H. Hutson, N. Regazzi, M. Gautier, R. Demesmaeker, S. Komi, S. Ceto, N. D. James, N. Cho, L. Baud, K. Galan, K. J. E. Matson, A. Rowald, K. Kim, R. Wang, K. Minassian, J. O. Prior, L. Asboth, Q. Barraud, S. P. Lacour, A. J. Levine, F. Wagner, J. Bloch, J. W. Squair, G. Courtine, The neurons that restore walking after paralysis, Nature, DOI 10.1038/s41586-022-05385-7.

Olivier Bignucolo, University of Lausanne

O. Bignucolo, C. Chipot, S. Kellenberger, B. Roux, Galvani offset potential and constant-ph simulations of membrane proteins, Journal of Physical Chemistry B, DOI 10.1021/acs.jpcb.2c04593.

Stefan Brönnimann, University of Bern

V. Valler, J. Franke, Y. Brugnara, S. Brönnimann, An updated global atmospheric paleo-reanalysis covering the last 400 years, Geoscience Data Journal, DOI 10.1002/gdj3.121.

L. Reichen, A. M. Burgdorf, S. Brönnimann, J. Franke, R. Hand, V. Valler, E. Samakinwa, Y. Brugnara, T. Rutishauser, A decade of cold Eurasian winters reconstructed for the early 19th century, Nature Communications, DOI 10.1038/s41467-022-29677-8.

S. Brönnimann, P. Stucki, J. Franke, V. Valler, Y. Brugnara, R. Hand, L. C. Slivinski, G. P. Compo, P. D. Sardeshmukh, M. Lang, B. Schaefli, Influence of warming and atmospheric circulation changes on multidecadal European flood variability, Climate of the Past, DOI 10.5194/cp-18-919-2022.

S. Brönnimann, From climate to weather reconstructions, PLOS Climate, DOI 10.1371/journal.pclm.0000034.

C. Camenisch, F. Jaume-Santero, S. White, Q. Pei, R. Hand, C. Rohr, S. Brönnimann, A Bayesian approach to historical climatology for the Burgundian low countries in the 15th century, Climate of the Past, DOI 10.5194/cp-18-2449-2022.

Dominik Brunner, Empa

I. Katharopoulos, D. Brunner, L. Emmenegger, M. Leuenberger, S. Henne, Lagrangian particle dispersion models in the grey zone of turbulence: Adaptations to FLEXPART-COSMO for simulations at 1 km grid resolution, Boundary-Layer Meteorology, DOI 10.1007/s10546-022-00728-3.

D. Rust, I. Katharopoulos, M. K. Vollmer, S. Henne, S. O'Doherty, D. Say, L. Emmenegger, R. Zenobi, S. Reimann, Swiss halocarbon emissions for 2019 to 2020 assessed from regional atmospheric observations, Atmospheric Chemistry and Physics, DOI 10.5194/acp-22-2447-2022.

S. M. Pieber, B. Tuzson, S. Henne, U. Karstens, C. Gerbig, F.-T. Koch, D. Brunner, M. Steinbacher, L. Emmenegger, Analysis of regional CO2 contributions at the high Alpine observatory Jungfraujoch by means of atmospheric transport simulations and $\delta^{13}C$, Atmospheric Chemistry and Physics, DOI 10.5194/acp-22-10721-2022.

Amedeo Caflisch, University of Zurich

I. M. Ilie, A. Caflisch, Antibody binding increases the flexibility of the prion protein, Biochimica Et Biophysica Acta-Proteins and Proteomics, DOI 10.1016/j.bbapap.2022.140827.

P. A. Vargas-Rosales, A. Caflisch, Domino effect in allosteric signaling of peptide binding, Journal of Molecular Biology, DOI 10.1016/j.jmb.2022.167661.

F. Nai, R. Nachawati, F. Zalesak, X. Wang, Y. Z. Li, A. Caflisch, Fragment ligands of the m^6A-RNA Reader YTHDF2, ACS Medicinal Chemistry Letters, DOI 10.1021/acsmedchemlett.2c00303.

I. M. Ilie, M. Bacci, A. Vitalis, A. Caflisch, Antibody binding modulates the dynamics of the membrane-bound prion protein, Biophysical Journal, DOI 10.1016/j.bpj.2022.06.007.

S. Garcia-Viñuales, I. M. Ilie, A. M. Santoro, V. Romanucci, A. Zarrelli, G. Di Fabio, A. Caflisch, D. Milardi, Silybins inhibit human IAPP amyloid growth and toxicity through stereospecific interactions, Biochimica Et Biophysica Acta-Proteins and Proteomics, DOI 10.1016/j.bbapap.2022.140772.

K. J. Nass, I. M. Ilie, M. J. Saller, A. J. M. Driessen, A. Caflisch, R. A. Kammerer, X. Li, The role of the N-terminal amphipathic helix in bacterial YidC: Insights from functional studies, the crystal structure and molecular dynamics simulations, Biochimica Et Biophysica Acta-Biomembranes, DOI 10.1016/j.bbamem.2021.183825.

J. Schilling, C. Jost, I. M. Ilie, J. Schnabl, O. Buechi, R. S. Eapen, R. Truffer, A. Caflisch, P. Forrer, Thermostable designed ankyrin repeat proteins (DARPins) as building blocks for innovative drugs, Journal of Biological Chemistry, DOI 10.1016/j.jbc.2021.101403.

C. Camilloni, University of Milan

E. Scalone, L. Broggini, C. Visentin, D. Erba, F. B. Toplek, K. Peqini, S. Pellegrino, S. Ricagno C. Paissoni, C. Camilloni, Multi-eGO: An in silico lens to look into protein aggregation kinetics at atomic resolution, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2203181119.

E. Karlsson, J. Schnatwinkel, C. Paissoni, E. Andersson, C. Herrmann, C. Camilloni, P. Jemth, Disordered regions flanking the binding interface modulate affinity between CBP and NCOA, Journal of Molecular Biology, DOI 10.1016/j.jmb.2022.167643.

Jan Carmeliet, ETH Zurich

J. L. Zhao, F. F. Qin, L. L. Fei, C. Z. Qin, Q. J. Kang, D. Derome, J. Carmeliet, Competition between main meniscus and corner film flow during imbibition in a strongly wetting square tube, Journal of Hydrology, DOI 10.1016/j.jhydrol.2022.128695.

B. D. Chen, F. F. Qin, M. Su, D. X. Xie, Z. Y. Zhang, Q. Pan, H. Wang, X. Yang, S. Chen, J. Huang, D. Derome, J. Carmeliet, Y. Song, One droplet reaction for synthesis of multi-sized nanoparticles, Nano Research, DOI 10.1007/s12274-022-5115-7.

J. L. Zhao, F. F. Qin, Q. J. Kang, C. Z. Qin, D. Derome, J. Carmeliet, A dynamic pore network model for imbibition simulation considering corner film flow, Water Resources Research, DOI 10.1029/2022WR032332.

J. M. Chi, Y. B. Wu, F. F. Qin, M. Su, N. Cheng, J. B. Zhang, C. Li, Z. Lian, X. Yang, L. Cheng, H. Xie, H. Wang, Z. Zhang, J. Carmeliet, Y. Song, All-printed point-of-care immunosensing biochip for one drop blood diagnostics, Lab on a Chip, DOI 10.1039/d2lc00385f.

L. L. Fei, F. F. Qin, J. L. Zhao, D. Derome, J. Carmeliet, Pore-scale study on convective drying of porous media, Langmuir, DOI 10.1021/acs.langmuir.2c00267.

L. L. Fei, F. F. Qin, G. Wang, K. H. Luo, D. Derome, J. Carmeliet, Droplet evaporation in finite-size systems: Theoretical analysis and mesoscopic modeling, Physical Review E, DOI 10.1103/PhysRevE.105.025101.

Michele Ceriotti, EPFL

J. Nigam, S. Pozdnyakov, G. Fraux, M. Ceriotti, Unified theory of atom-centered representations and message-passing machine-learning schemes, Journal of Chemical Physics, DOI 10.1063/5.0087042.

Mauro Chinappi, University of Rome Tor Vergata

G. Di Muccio, B. M. della Rocca, M. Chinappi, Geometrically induced selectivity and unidirectional electroosmosis in uncharged nanopores, ACS Nano, DOI 10.1021/acsnano.1c03017.

A. Gubbiotti, M. Baldelli, G. Di Muccio, P. Malgaretti, S. Marbach, M. Chinappi, Electroosmosis in nanopores: Computational methods and technological applications, Advances in Physics-X, DOI 10.1080/23746149.2022.2036638.

Bastien Chopard, University of Geneva

C. Kotsalos, F. Raynaud, J. Latt, R. Dutta, F. Dubois, K. Z. Boudjeltia, B. Chopard, Shear induced diffusion of platelets revisited, Frontiers in Physiology, DOI 10.3389/fphys.2022.985905.

R. Dutta, K. Z. Boudjeltia, C. Kotsalos, A. Rousseau, D. R. de Sousa, J. M. Desmet, A. Van Meerhaeghe, A. Mira, B. Chopard, Personalized pathology test for cardio-vascular disease: Approximate Bayesian computation with discriminative summary statistics learning, PLOS Computational Biology, DOI 10.1371/journal.pcbi.1009910.

Sergey V. Churakov, Paul Scherrer Institute & University of Bern

J. P. Owusu, K. Karalis, N. I. Prasianakis, S. V. Churakov, Mobility of dissolved gases in smectites under saturated conditions: Effects of pore size, gas types, temperature, and surface interaction, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.2c05678.

Florina M. Ciorba, University of Basel

A. Mohammed, J. H. M. Korndorfer, A. Eleliemy, F. M. Ciorba, Automated scheduling algorithm selection and chunk parameter calculation in OpenMP, IEEE Transactions on Parallel and Distributed Systems, DOI 10.1109/Tpds.2022.3189270.

J. H. M. Korndörfer, A. Eleliemy, A. Mohammed, F. M. Ciorba, LB4OMP: A dynamic load balancing library for multithreaded applications, IEEE Transactions on Parallel and Distributed Systems, DOI 10.1109/Tpds.2021.3107775.

H. Brunst, S. Chandrasekaran, F. M. Ciorba, N. Hagerty, R. Henschel, G. Juckeland, J. Li, V. G. Melesse Vergara, S. Wienke, M. Zavala, First experiences in performance benchmarking with the new SPEChpc 2021 suites, 22nd IEEE/ACM International Symposium on Cluster, Cloud and Internet Computing, DOI 10.1109/CCGrid54584.2022.00077.

Edouard L. Davin, Wyss Academy for Nature, University of Bern

A. S. Daloz, C. Schwingshackl, P. Mooney, S. Strada, D. Rechid, E. L. Davin, E. Katragkou, N. de Noblet-Ducoudré, M. Belda, T. Halenka, M. Breil, R. M. Cardoso, P. Hoffmann, D. C. A. Lima, R. Meier, P. M. M. Soares, G. Sofiadis, G. Strandberg, M. H. Toelle, M. T. Lund, Land-atmosphere interactions in sub-polar and alpine climates in the CORDEX flagship pilot study Land Use and Climate Across Scales (LUCAS) models - Part 1: Evaluation of the snow-albedo effect, Cryosphere, DOI 10.5194/tc-16-2403-2022.

P. A. Mooney, D. Rechid, E. L. Davin, E. Katragkou, N. de Noblet-Ducoudre, M. Breil, R. M. Cardoso, A. S. Daloz, P. Hoffmann, D. C. A. Lima, R. Meier, P. M. M. Soares, G. Sofiadis, S. Strada, G. Strandberg, M. H. Toelle, M. T. Lund, Land-atmosphere interactions in sub-polar and alpine climates in the CORDEX Flagship Pilot Study Land Use and Climate Across Scales (LUCAS) models - Part 2: The role of changing vegetation, Cryosphere, DOI 10.5194/tc-16-1383-2022.

G. Sofiadis, E. Katragkou, E. L. Davin, D. Rechid, N. de Noblet-Ducoudre, M. Breil, R. M. Cardoso, P. Hoffmann, L. Jach, R. Meier, P. A. Mooney, P. M. M. Soares, S. Strada, M. H. Tölle, K. Warrach Sagi, Afforestation impact on soil temperature in regional climate model simulations over Europe, Geoscientific Model Development, DOI 10.5194/gmd-15-595-2022.

Lucie Delemotte, KTH Royal Institute of Technology

K. Choudhury, R. J. Howard, L. Delemotte, An a-p transition in S6 shapes the conformational cycle of the bacterial sodium channel NavAb, Journal of General Physiology, DOI 10.1085/jgp.202213214.

G. Chi, Q. Liang, A. Sridhar, J. B. Cowgill, K. Sader, M. Radjainia, P. Qian, P. Castro-Hartmann, S. Venkaya, N. Kaur Singh, G. McKinley, A. Fernandez-Cid, S. M. M. Mukhopadhyay, N. A. Burgess-Brown, L. Delemotte, M. Covarrubias, K. L. Dürr, Cryo-EM structure of the human Kv3.1 channel reveals gating control by the cytoplasmic T1 domain, Nature Communications, DOI 10.1038/s41467-022-29594-w.

K. Choudhury, M. A. Kasimova, S. McComas, R. J. Howard, L. Delemotte, An open state of a voltage-gated sodium channel involving a π-helix and conserved pore-facing asparagine, Biophysical Journal, DOI 10.1016/j.bpj.2021.12.010.

Xavier Deupi, Paul Scherrer Institute

B. Plouffe, A. Karamitri, T. Flock, J. M. Gallion, S. Houston, C. A. Daly, A. Bonnefond, J.-L. Guillaume, C. Le Gouill, P. Froguel, O. Lichtarge, X. Deupi, R. Jockers, M. Bouvier, Structural elements directing G proteins and b-arrestin interactions with the human melatonin type 2 receptor revealed by natural variants, ACS Pharmacology & Translational Science, DOI 10.1021/acsptsci.1c00239.

Javier Diaz & Ignacio Pagonabarraga, EPFL

J. Diaz, M. Pinna, A. V. Zvelindovsky, I. Pagonabarraga, Hybrid time-dependent Ginzburg-Landau simulations of block copolymer nanocomposites: Nanoparticle anisotropy, Polymers, DOI 10.3390/polym14091910.

Carmen Domene, University of Bath

F. Pettini, C. Domene, S. Furini, Early steps in C-type inactivation of the hERG potassium channel, Journal of Chemical Information and Modeling, DOI 10.1021/acs.jcim.2c01028.

C. Domene, L. Darre, V. Oakes, S. Gonzalez-Resines, A potential route of capsaicin to its binding site in the TRPV1 ion channel, Journal of Chemical Information and Modeling, DOI 10.1021/acs.jcim.1c01441.

Robert Feldmann, University of Zurich

J. Moreno, S. Danieli, J. S. Bullock, R. Feldmann, P. F. Hopkins, O. Çatmabacak, A. Gurvich, A. Lazar, C. Klein, C. B. Hummels, Z. Hafen, F. J. Mercado, S. Yu, F. Jiang, C. Wheeler, A. Wetzel, D. Anglés-Alcázar, M. Boylan-Kolchin, E. Quataert, C.-A. Faucher-Giguère, D. Kereš, Galaxies lacking dark matter produced by close encounters in a cosmological simulation, Nature Astronomy, DOI 10.1038/s41550-021-01598-4.

O. Çatmabacak, R. Feldmann, D. Angles-Alcazar, C. A. Faucher-Giguère, P. F. Hopkins, D. Kereš, Black hole-galaxy scaling relations in FIRE: The importance of black hole location and mergers, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stac040.

M. Bernardini, R. Feldmann, D. Anglés-Alcázar, M. Boylan-Kolchin, J. Bullock, L. Mayer, J. Stadel, From EMBER to FIRE: Predicting high resolution baryon fields from dark matter simulations with deep learning, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab3088.

J. Gensior, R. Feldmann, L. Mayer, A. Wetzel, P. F Hopkins, C.-A. Faucher-Giguère, Realistic H i scale heights of Milky Way-mass galaxies in the FIREbox cosmological volume, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnrasl/slac138.

Andreas Fichtner, ETH Zurich

J.-F. Aubry, O. Bates, C. Boehm, K. Butts Pauly, D. Christensen, C. Cueto, P. Gélat, L. Guasch, J. Jaros, Y. Jing, R. Jones, N. Li, P. Marty, H. Montanaro, E. Neufeld, S. Pichardo, G. Pinton, A. Pulkkinen, A. Stanziola, A. Thielscher, B. Treeby, E. van 't Wout, Benchmark problems for transcranial ultrasound simulation: Intercomparison of compressional wave models, The Journal of the Acoustical Society of America, DOI 10.1121/10.0013426.

I. E. Ulrich, C. Boehm, A. Zunino, A. Fichtner, Analyzing resolution and model uncertainties for ultrasound computed tomography using Hessian information, Proceedings SPIE, Medical Imaging 2022: Ultrasonic Imaging and Tomography, DOI 10.1117/12.2608546.

C. Boehm, L. Krischer, I. Ulrich, P. Marty, M. Afanasiev, A. Fichtner, Using optimal transport to mitigate cycle-skipping in ultrasound computed tomography, Proceedings SPIE, Medical Imaging 2022: Ultrasonic Imaging and Tomography, DOI 10.1117/12.2605894.

J. C. Ma, H. P. Bunge, S. Thrastarson, A. Fichtner, D. P. van Herwaarden, Y. Tian, S.-J. Chang, T. Liu, Seismic full-waveform inversion of the crust-mantle structure beneath China and adjacent regions, Journal of Geophysical Research-Solid Earth DOI 10.1029/2022JB024957.

I. E. Ulrich, C. Boehm, A. Zunino, C. Bosch, A. Fichtner, Diffuse ultrasound computed tomography, Journal of the Acoustical Society of America, DOI 10.1121/10.0011540.

S. Thrastarson, D. P. Van Herwaarden, L. Krischer, C. Boehm, M. van Driel, M. Afanasiev, A. Fichtner, Data-adaptive global full-waveform inversion, Geophysical Journal International, DOI 10.1093/gji/ggac122.

P. Marty, C. Boehm, C. Paverd, M. Rominger, A. Fichtner, Full-waveform ultrasound modeling of soft tissue-bone interactions using conforming hexahedral meshes, Proceedings SPIE, Medical Imaging 2022: Physics of Medical Imaging, DOI 10.1117/12.2611548.

Thomas L. Frölicher, University of Bern

N. Le Grix, J. Zscheischler, K. B. Rodgers, R. Yamaguchi, T. L. Frölicher, Hotspots and drivers of compound marine heatwaves and low net primary production extremes, Biogeosciences, DOI 10.5194/bg-19-5807-2022.

F. A. Burger, J. Terhaar, T. L. Frölicher, Compound marine heatwaves and ocean acidity extremes, Nature Communications, DOI 10.1038/s41467-022-32120-7.

Thomas Gehrmann, University of Zurich

X. Chen, T. Gehrmann, N. Glover, A. Huss, T. Z. Yang, H. X. Zhu, Dilepton rapidity distribution in Drell-Yan production to third order in QCD, Physical Review Letters, DOI 10.1103/PhysRevLett.128.052001.

X. Chen, A. Huss, S. P. Jones, M. Kerner, J.-N. Lang, J. M. Lindert, H. Zhang, Top-quark mass effects in H+jet and H+2 jets production, Journal of High Energy Physics, DOI 0.1007/JHEP03(2022)096.

X. Chen, T. Gehrmann, E. W. N. Glover, A. Huss, Fiducial cross sections for the lepton-pair-plus-photon decay mode in Higgs production up to NNLO QCD, Journal of High Energy Physics, DOI 10.1007/Jhep01(2022)053.

Aude Gehrmann-De Ridder, University of Zurich

G. Coloretti, A. Gehrmann-De Ridder, C. T. Preuss, QCD predictions for event-shape distributions in hadronic Higgs decays, Journal of High Energy Physics, DOI 10.1007/JHEP06(2022)009.

R. Gauld, A. Gehrmann-De Ridder, T. Gehrmann, E. W. N. Glover, A. Huss, I. Majer, A. Rodriguez Garcia, Transverse momentum distributions in low-mass Drell-Yan lepton pair production at NNLO QCD, Physics Letters B, DOI 10.1016/j.physletb.2022.137111.

R. Gauld, A. Gehrmann-De Ridder, E. W. N. Glover, A. Huss, I. Majer, VH plus jet production in hadron-hadron collisions up to order alpha(3)(s) in perturbative QCD, Journal of High Energy Physics, DOI 10.1007/Jhep03(2022)008.

Francesco L. Gervasio, University of Geneva & University College London

A. Borsatto, O. Akkad, I. Galdadas, S. M. Ma, S. Damfo, S. Haider, F. Kozielski, C. Estarellas, F. L. Gervasio, Revealing druggable cryptic pockets in the Nsp1 of SARS-CoV-2 and other beta-coronaviruses by simulations and crystallography, eLife, DOI 10.7554/eLife.81167.

D. Lukauskis, M. L. Samways, S. Aureli, B. P. Cossins, R. D. Taylor, F. L. Gervasio, Open binding pose metadynamics: An effective approach for the ranking of protein-ligand binding poses, Journal of Chemical Information and Modeling, DOI 10.1021/acs.jcim.2c01142.

S. Di Gaetano, L. Pirone, I. Galdadas, S. Traboni, A. Iadonisi, E. Pedone, M. Saviano, F. L. Gervasio, D. Capasso, Design, synthesis, and anticancer activity of a selenium-containing galectin-3 and galectin-9N inhibitor, International Journal of Molecular Sciences, DOI 10.3390/ijms23052581.

Stefan Goedecker, University of Basel

B. Parsaeifard, S. Goedecker, Manifolds of quasi-constant SOAP and ACSF fingerprints and the resulting failure to machine learn four-body interactions, Journal of Chemical Physics, DOI 10.1063/5.0070488.

M. Gubler, J. A. Flores-Livas, A. Kozhevnikov, S. Goedecker, Missing theoretical evidence for conventional room-temperature superconductivity in low-enthalpy structures of carbonaceous sulfur hydrides, Physical Review Materials, DOI 10.1103/PhysRevMaterials.6.014801.

J. A. Finkler, S. Goedecker, Experimental absence of the non-perovskite ground state phases of MaPbI3 explained by a Funnel Hopping Monte Carlo study based on a neural network potential, Materials Advances, DOI 10.1039/d2ma00958g.

Gianvito Grasso, SUPSI

B. Barletti, G. Lucchesi, S. Muscat, S. Errico, D. Barbut, A. Danani, M. Zasloff, G. Grasso, F. Chiti, G. Caminati, Reorganization of the outer layer of a model of the plasma membrane induced by a neuroprotective aminosterol, Colloids and Surfaces B: Biointerfaces, DOI 10.1016/j.colsurfb.2022.113115.

Thomas Greber, University of Zurich & Ari P. Seitsonen, Ecole Normale Supérieure Paris

P. Knecht, D. Meier, J. Reichert, D. A. Duncan, M. Schwarz, J. T. Küchle, T.-L. Lee, P. S. Deimel, P. Feulner, F. AllegrettiW. Auwärter, G. Médard, A. P. Seitsonen, J. V. Barth, A. C. Papageorgiou, N-heterocyclic carbenes: Molecular porters of surface mounted Ru-porphyrins, Angewandte Chemie-International Edition, DOI 10.1002/anie.202211877.

Nicolas Gruber, ETH Zurich

E. E. Kohn, M. Munnich, M. Vogt, F. Desmet, N. Gruber, Strong habitat compression by extreme shoaling events of hypoxic waters in the Eastern Pacific, Journal of Geophysical Research-Oceans, DOI 10.1029/2022JC018429.

F. Desmet, N. Gruber, E. E. Kohn, M. Munnich, M. Vogt, Tracking the space-time evolution of ocean acidification extremes in the California current system and Northeast Pacific, Journal of Geophysical Research-Oceans, DOI 10.1029/2021JC018159.

Stefan Hackstein, University of Applied Sciences North Western Switzerland

S. Hackstein, V. Kinakh, C. Bailer, M. Melchior, Evaluation metrics for galaxy image generators, Astronomy and Computing, DOI 10.1016/j.ascom.2022.100685.

Torsten Hoefler, ETH Zurich

D. De Sensi, T. De Matteis, K. Taranov, S. Di Girolamo, T. Rahn, T. Hoefler, Noise in the clouds: Influence of network performance variability on application scalability, Proceedings of the ACM on Measurement and Analysis of Computing Systems, DOI 10.1145/3570609.

M. Copik, T. Grosser, T. Hoefler, P. Bientinesi, B. Berkels, Work-stealing prefix scan: Addressing load imbalance in large-scale image registration, IEEE Transactions on Parallel and Distributed Systems, DOI 10.1109/Tpds.2021.3095230.

S. G. Li, T. Hoefler, Near-optimal sparse allreduce for distributed Deep Learning, Proceedings of the 27th ACM Sigplan Symposium on Principles and Practice of Parallel Programming (PPoPP22), DOI 10.1145/3503221.3508399.

A. Strausz, F. Vella, S. Di Girolamo, M. Besta, T. Hoefler, Asynchronous distributed-memory triangle counting and LCC with RMA caching, IEEE 36th International Parallel and Distributed Processing Symposium (IPDPS22), DOI 10.1109/Ipdps53621.2022.00036.

J. D. Licht, C. A. Pattison, A. N. Ziogas, D. Simmons-Duffin, T. Hoefler, Fast arbitrary precision floating point on FPGA, IEEE 30th International Symposium on Field-Programmable Custom Computing Machines (FCCM22), DOI 10.1109/Fccm53951.2022.9786219.

S. Ashkboos, L. Huang, N. Dryden, T. Ben-Nun, P. Dueben, L. Gianinazzi, L. Kummer, T. Hoefler, ENS-10: A dataset for post-processing ensemble weather forecasts, Proceedings of the Neural Information Processing Systems Track on Datasets and Benchmarks, DOI 10.48550/arXiv.2206.14786.

M. Besta, C. Miglioli, P. S. Labini, J. Tětek, P. Iff, R. Kanakagiri, S. Ashkboos, K. Janda, M. Podstawski, G. Kwasniewski, N. Gleinig, F. Vella, O. Mutlu, T. Hoefler, ProbGraph: High-performance and high-accuracy graph mining with probabilistic set representations, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC22), DOI 10.5555/3571885.3571942.

T. Hoefler, T. Bonato, D. De Sensi, S. Di Girolamo, S. Li, M. Heddes, J. Belk, D. Goel, M. Castro, S. Scott, HammingMesh: A network topology for large-scale Deep Learning, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC22), DOI 10.5555/3571885.3571899.

S. Li, K. Osawa, T. Hoefler, Efficient quantized sparse matrix operations on tensor cores, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC22), DOI 10.5555/3571885.3571934.

A. N. Ziogas, G. Kwasniewski, T. Ben-Nun, T. Schneider, T. Hoefler, Deinsum: Practically I/O optimal multilinear algebra, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC22), DOI 10.5555/3571885.3571918.

P. Schaad, T. Ben-Nun, T. Hoefler, Boosting performance optimization with interactive data movement visualization, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC22), DOI 10.5555/3571885.3571970.

T. Ben-Nun, L. Groner, F. Deconinck, T. Wicky, E. Davis, J. Dahm, O. Elbert, R. George, J. McGibbon, L. Trümper, E. Wu, O. Fuhrer, T. Schulthess, T. Hoefler, Productive performance engineering for weather and climate modeling with python, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC22), DOI 10.5555/3571885.3571982.

M. Besta, R. Grob, C. Miglioli, N. Bernold, G. Kwasniewski, G. Gjini, R. Kanakagiri, S. Ashkboos, L. Gianinazzi, N. Dryden, T. Hoefler, Motif prediction with graph neural networks, Proceedings of the 28th SIGKDD Conference on Knowledge Discovery and Data Mining (KDD22), DOI 10.1145/3534678.3539343.

O. Rausch, T. Ben-Nun, N. Dryden, A. Ivanov, S. Li, T. Hoefler, A data-centric optimization framework for Machine Learning, Proceedings of the 2022 International Conference on Supercomputing (ICS22), DOI 10.1145/3524059.3532364.

A. Calotoiu, T. Ben-Nun, G. Kwasniewski, J. de Fine Licht, T. Schneider, P. Schaad, T. Hoefler, Lifting C semantics for dataflow optimization, Proceedings of the 2022 International Conference on Supercomputing (ICS22), DOI 10.1145/3524059.3532389.

Andrew Hung, RMIT University, Melbourne

S. G. Royce, P. V. Licciardi, R. C. Beh, J. E. Bourke, C. Donovan, A. N. Hung, I. Khurana, J. J. Liang, S. Maxwell, N. Mazarakis, E. Pitsillou, Y. Y. Siow, K. J. Snibson, M. J. Tobin, K. Ververis, J. Vongsvivut, M. Ziemann, C. S. Samuel, M. L. K. Tang, A. El-Osta, T. C. Karagiannis, Sulforaphane prevents and reverses allergic airways disease in mice via anti-inflammatory, antioxidant, and epigenetic mechanisms, Cellular and Molecular Life Sciences, DOI 10.1007/s00018-022-04609-3.

E. Pitsillou, J. J. Liang, R. C. Beh, A. D. Hung, T. C. Karagiannis, Molecular dynamics simulations highlight the altered binding landscape at the spike-ACE2 interface between the Delta and Omicron variants compared to the SARS-CoV-2 original strain, Computers in Biology and Medicine, DOI 10.1016/j.compbiomed.2022.106035.

J. R. McArthur, J. R. Wen, A. D. Hung, R. K. Finol-Urdaneta, D. J. Adams, H. M. Colecraft, m-Theraphotoxin Pn3a inhibition of $Ca_V3.3$ channels reveals a novel isoform-selective drug binding site, eLife, DOI 10.7554/eLife.74040.

E. Pitsillou, J. L. Liang, A. D. Hung, T. C. Karagiannis, The SARS-CoV-2 helicase as a target for antiviral therapy: Identification of potential small molecule inhibitors by in silico modelling, Journal of Molecular Graphics & Modelling, DOI 10.1016/j.jmgm.2022.108193.

E. Pitsillou, J. J. Liang, R. C. Beh, J. Prestedge, S. Catak, A. Hung, T. C. Karagiannis, Identification of novel bioactive compounds from *Olea europaea* by evaluation of chemical compounds in the OliveNet™ library: in silico bioactivity and molecular modelling, and in vitro validation of hERG activity, Computers in Biology and Medicine, DOI 10.1016/j.compbiomed.2022.105247.

J. J. Liang, E. Pitsillou, K. Ververis, V. Guallar, A. D. Hung, T. C. C. Karagiannis, Investigation of small molecule inhibitors of the SARS-CoV-2 papain-like protease by all-atom microsecond modelling, PELE Monte Carlo simulations, and in vitro activity inhibition, Chemical Physics Letters, DOI 10.1016/j.cplett.2021.139294.

Jürg Hutter, University of Zurich

A. S. Hehn, B. Sertcan, F. Belleflamme, S. K. Chulkov, M. B. Watkins, J. Hutter, Excited-state properties for extended systems: Efficient hybrid density functional methods, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.2c00144.

F. Stein, J. Hutter, Double-hybrid density functionals for the condensed phase: Gradients, stress tensor, and auxiliary-density matrix method acceleration, Journal of Chemical Physics, DOI 10.1063/5.0082327.

Marcella Iannuzzi, University of Zurich

F. Shao, J. K. Wong, Q. H. Low, M. Iannuzzi, J. G. Li, J. G. Lan, In situ spectroelectrochemical probing of CO redox landscape on copper single-crystal surfaces, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2118166119.

G. Melani, J. P. Guerrero-Felipe, A. M. Valencia, J. Krumland, C. Cocchi, M. Iannuzzi, Donors, acceptors, and a bit of aromatics: Electronic interactions of molecular adsorbates on hBN and MoS_2 monolayers, Physical Chemistry Chemical Physics, DOI 10.1039/d2cp01502a.

M. Pauletti, V. V. Rybkin, M. Iannuzzi, Surface tension of liquids and binary mixtures from molecular dynamics simulations, Journal of Physics-Condensed Matter, DOI 10.1088/1361-648X/ac2e8f.

Andrew Jackson, ETH Zurich

J. W. Luo, A. Jackson, Waves in the Earth's core. I. Mildly diffusive torsional oscillations, Proceedings of the Royal Society A – Mathematical, Physical and Engineering Sciences, DOI 10.1098/rspa.2021.0982.

J. W. Luo, P. Marti, A. Jackson, Waves in the Earth's core. II. Magneto-Coriolis modes, Proceedings of the Royal Society A – Mathematical, Physical and Engineering Sciences, DOI 10.1098/rspa.2022.0108.

Fortunat Joos, University of Bern

T. Frischknecht, A. Ekici, F. Joos, Radiocarbon in the land and ocean component of the Community Earth System Model, Global Biogeochemical Cycles, DOI 10.1029/2021GB007042.

Tomasz Kacprzak, ETH Zurich

J. Fluri, T. Kacprzak, A. Lucchi, A. Schneider, A. Refregier, T. Hofmann, Full wCDM analysis of KiDS-1000 weak lensing maps using deep learning, Physical Review D, DOI 10.1103/PhysRevD.105.083518.

Venkat Kapil, University of Cambridge

F. Musil, I. Zaporozhets, F. Noe, C. Clementi, V. Kapil, Quantum dynamics using path integral coarse-graining, Journal of Chemical Physics, DOI 10.1063/5.0120386.

V. Kapil, C. Schran, A. Zen, J. Chen, C. J. Pickard, A. Michaelides, The first-principles phase diagram of monolayer nanoconfined water, Nature, DOI 10.1038/s41586-022-05036-x.

V. Kapil, E. A. Engel, A complete description of thermodynamic stabilities of molecular crystals, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2111769119.

Ilya V. Karlin, ETH Zurich

S. A. Hosseini, B. Dorschner, I. V. Karlin, Towards a consistent lattice Boltzmann model for two-phase fluids, Journal of Fluid Mechanics, DOI 10.1017/jfm.2022.867.

N. G. Kallikounis, B. Dorschner, I. V. Karlin, Particles on demand for flows with strong discontinuities, Physical Review E, DOI 10.1103/PhysRevE.106.015301.

N. Sawant, B. Dorschner, I. V. Karlin, Consistent lattice Boltzmann model for reactive mixtures, Journal of Fluid Mechanics, DOI 10.1017/jfm.2022.345.

N. Sawant, B. Dorschner, I.V. Karlin, Detonation modeling with the Particles on Demand method, AIP Advances, DOI 10.1063/5.0095122.

Stephan Kellenberger, University of Lausanne

S. Roy, N. Johner, V. Trendafilov, I. Gautschi, O. Bignucolo, O. Molton, S. Bernèche, S. Kellenberger, Calcium regulates acid-sensing ion channel 3 activation by competing with protons in the channel pore and at an allosteric binding site, Open Biology, DOI 10.1098/rsob.220243.

Petros Koumoutsakos, ETH Zurich & Harvard University

M. Chatzimanolakis, P. Weber, P. Koumoutsakos, Vortex separation cascades in simulations of the planar flow past an impulsively started cylinder up to Re = 100 000, Journal of Fluid Mechanics, DOI 10.1017/jfm.2022.988.

P. R. Vlachas, G. Arampatzis, C. Uhler, P. Koumoutsakos, Multiscale simulations of complex systems by learning their effective dynamics, Nature Machine Intelligence, DOI 10.1038/s42256-022-00464-w.

H. J. Bae, P. Koumoutsakos, Scientific multi-agent reinforcement learning for wall-models of turbulent flows, Nature Communications, DOI 10.1038/s41467-022-28957-7.

S. M. Martin, D. Wälchli, G. Arampatzis, A. E. Economides, P. Karnakov, P. Koumoutsakos, Korali: Efficient and scalable software framework for Bayesian uncertainty quantification and stochastic optimization, Computer Methods in Applied Mechanics and Engineering, DOI 10.1016/j.cma.2021.114264.

P. Karnakov, S. Litvinov, P. Koumoutsakos, Computing foaming flows across scales: From breaking waves to microfluidics, Science Advances, DOI 10.1126/sciadv.abm0590.

E. Papadopoulou, C. M. Megaridis, J. H. Walther, P. Koumoutsakos, Nanopumps without pressure gradients: Ultrafast transport of water in patterned nanotubes, Journal of Physical Chemistry B, DOI 10.1021/acs.jpcb.1c07562.

Matthias Krack, Paul Scherrer Institute

D. Bocharov, A. Chesnokov, G. Chikvaidze, J. Gabrusenoks, R. Ignatans, R. Kalendarev, M. Krack, K. Kundzins, A. Kuzmin, N. Mironova-Ulmane, I. Pudza, L. Puust, I. Sildos, E. Vasil'chenko, M. Zubkins, J. Purans, A comprehensive study of structure and properties of nanocrystalline zinc peroxide, Journal of Physics and Chemistry of Solids, DOI 10.1016/j.jpcs.2021.110318.

A. Hartl, F. Juranyi, M. Krack, P. Lunkenheimer, A. Schulz, D. Sheptyakov, C. Paulmann, M. Appel, S.-H. Park, Dynamically disordered hydrogen bonds in the hureaulite-type phosphatic oxyhydroxide $Mn_5[(PO_4)_2(PO_3(OH))_2](HOH)_4$, Journal of Chemical Physics, DOI 10.1063/5.0083856.

Rolf Krause, Università della Svizzera italiana

H. Kothari, R. Krause, A generalized multigrid method for solving contact problems in Lagrange multiplier based unfitted Finite Element method, Computer Methods in Applied Mechanics and Engineering, DOI 10.1016/j.cma.2022.114630.

Martin Kunz, University of Geneva

F. Hassani, J. Adamek, R. Durrer, M. Kunz, Biased tracers as a probe of beyond-ΛCDM cosmologies, Astronomy & Astrophysics, DOI 10.1051/0004-6361/202244405.

Latévi Max Lawson Daku, University of Geneva

A. Missana, A. Hauser, L. M. Lawson Daku, Environmental control of the magnetic behavior of transition metal complexes: Density functional theory study of zeolite Y embedded complexes $[M(bpy)_3]^{2+}$@Y (M = Fe^{2+}, Co^{2+}), Journal of Physical Chemistry A, DOI 10.1021/acs.jpca.2c05070.

L. M. Lawson Daku, M. E. Casida, Modelling the physical properties of environmentally friendly optical magnetic switches: DFT and TD-DFT, Green Chemistry and Computational Chemistry, DOI 10.1016/B978-0-12-819879-7.00015-5.

Michael Lehning, WSL Institute for Snow and Avalanche Research SLF

F. Carletti, A. Michel, F. Casale, A. Burri, D. Bocchiola, M. Bavay, M. Lehning, A comparison of hydrological models with different level of complexity in Alpine regions in the context of climate change, Hydrology and Earth System Sciences, DOI 10.5194/hess-26-3447-2022.

Y. Zakari, A. Michel, M. Lehning, Future trends in wind resources and their consistency in the Indian sub-continent, Sustainable Energy Technologies and Assessments, DOI 10.1016/j.seta.2022.102460.

A. Michel, B. Schaefli, N. Wever, H. Zekollari, M. Lehning, H. Huwald, Future water temperature of rivers in Switzerland under climate change investigated with physics-based models, Hydrology and Earth System Sciences, DOI 10.5194/hess-26-1063-2022.

M. Jafari, V. Sharma, M. Lehning, Convection of water vapour in snowpacks, Journal of Fluid Mechanics, DOI 10.1017/jfm.2021.1146.

D. B. Melo, V. Sharma, F. Comola, A. Sigmund, M. Lehning, Modeling snow saltation: The effect of grain size and Interparticle cohesion, Journal of Geophysical Research-Atmospheres, DOI 10.1029/2021JD035260.

V. Sharma, F. Gerber, M. Lehning, Introducing CRYOWRF v1.0: Multiscale atmospheric flow simulations with advanced snow cover modelling, Geoscientific Model Development, DOI 10.5194/gmd-16-719-2023.

D. B. Melo, V. Sharma, F. Comola, A. Sigmund, M. Lehning, Modeling snow saltation: The effect of grain size and interparticle cohesion, Journal of Geophysical Research-Atmospheres, DOI 10.1029/2021JD035260.

Karl R. Liedl, University of Innsburck

M. L. Fernández-Quintero, K. B. Kroell, L. J. Grunewald, A. L. M. Fischer, J. R. Riccabona, K. R. Liedl, CDR loop interactions can determine heavy and light chain pairing preferences in bispecific antibodies, mAbs, DOI 10.1080/19420862.2021.2024118.

M. L. Fernández-Quintero, A. L. M. Fischer, J. Kokot, F. Waibl, C. A. Seidler, K. R. Liedl, The influence of antibody humanization on shark variable domain (VNAR) binding site ensembles, Frontiers in Immunology, DOI 10.3389/fimmu.2022.953917.

F. Waibl, M. L. Fernández-Quintero, F. S. Wedl, H. Kettenberger, G. Georges, K. R. Liedl, Comparison of hydrophobicity scales for predicting biophysical properties of antibodies, Frontiers in Molecular Biosciences, DOI 10.3389/fmolb.2022.960194.

M. L. Fernández-Quintero, E. F. DeRose, S. A. Gabel, G. A. Mueller, K. R. Liedl, Nanobody paratope ensembles in solution characterized by MD simulations and NMR, International Journal of Molecular Sciences, DOI 10.3390/ijms23105419.

M. L. Fernández-Quintero, A. Vangone, J. R. Loeffler, C. A. Seidler, G. Georges, K. R. Liedl, Paratope states in solution improve structure prediction and docking, Structure, DOI 10.1016/j.str.2021.11.001.

M. L. Fernández-Quintero, P. K. Quoika, F. S. Wedl, C. A. Seidler, K. B. Kroell, J. R. Loeffler, N. D. Pomarici, V. J. Hoerschinger, A. Bujotzek, G. Georges, H. Kettenberger, K. R. Liedl, Comparing antibody interfaces to inform rational design of new antibody formats, Frontiers in Molecular Biosciences, DOI 10.3389/fmolb.2022.864654.

N. D. Pomarici, M. L. Fernández-Quintero, P. K. Quoika, F. Waibl, A. Bujotzek, G. Georges, K. R. Liedl, Bispecific antibodies—effects of point mutations on CH_3-CH_3 interface stability, Protein Engineering, Design and Selection, DOI 10.1093/protein/gzac012.

F. Hofer, A.-L. Fischer, A. S. Kamenik, F. Waibl, M. L. Fernández-Quintero, K. R. Liedl, pH-dependent structural diversity of profilin allergens determines thermal stability, Frontiers in Allergy, DOI 10.3389/falgy.2022.1007000.

Vittorio Limongelli, Università della Svizzera italiana

S. Fiorucci, P. Rapacciuolo, B. Fiorillo, R. Roselli, S. Marchiano, C. Di Giorgio, M. Bordoni, R. Bellini, C. Cassiano, P. Conflitti, B. Catalanotti, V. Limongelli, V. Sepe, M. Biagioli, A. Zampella, Discovery of a potent and orally active dual GPBAR1/$CysLT_1R$ modulator for the treatment of metabolic fatty liver disease, Frontiers in Pharmacology, DOI 10.3389/fphar.2022.858137.

G. Di Lorenzo, F. Iavarone, M. Maddaluno, A. B. Plata-Gómez, S. Aureli, C. P. Quezada Meza, L. Cinque, A. Palma, A. Reggio, C. Cirillo, F. Sacco, A. Stolz, G. Napolitano, O. Marin, L. A. Pinna, M. Ruzzene, V. Limongelli, A. Efeyan, P. Grumati, C. Settembre, Phosphorylation of FAM134C by CK2 controls starvation-induced ER-phagy, Science Advances, DOI 10.1126/sciadv.abo1215.

B. Fiorillo, S. Marchianò, F. Moraca, V. Sepe, A. Carino, P. Rapacciulo, M. Biagioli, V. Limongelli, A. Zampella, B. Catalanotti, S. Fiorucci, Discovery of bile acid derivatives as potent ACE2 activators by virtual screening and essential dynamics, Journal of Chemical Information and Modeling, DOI 10.1021/acs.jcim.1c01126.

Ulrike Lohmann, ETH Zurich

C. Tully, D. Neubauer, N. Omanovic, U. Lohmann, Cirrus cloud thinning using a more physically based ice microphysics scheme in the ECHAM-HAM general circulation model, Atmospheric Chemistry and Physics, DOI 10.5194/acp-22-11455-2022.

G. A. Kelesidis, D. Neubauer, L. S. Fan, U. Lohmann, S. E. Pratsinis, Enhanced light absorption and radiative forcing by black carbon agglomerates, Environmental Science & Technology, DOI 10.1021/acs.est.2c00428.

G. K. Eirund, S. D. van Dusseldorp, B. T. Brem, Z. Dedekind, Y. Karrer, M. Stoll, U. Lohmann, Aerosol-cloud-precipitation interactions during a Saharan dust event - A summertime case-study from the Alps, Quarterly Journal of the Royal Meteorological Society, DOI 10.1002/qj.4240.

B. Jiménez-Esteve, D. I. V. Domeisen, The role of atmospheric dynamics and large-scale topography in driving heatwaves, Quarterly Journal of the Royal Meteorological Society, DOI 10.1002/qj.4306.

B. Jiménez-Esteve, K. Kornhuber, D. I. V. Domeisen, Heat extremes driven by amplification of phase-locked circumglobal waves forced by topography in an idealized atmospheric model, Geophysical Research Letters, DOI 10.1029/2021GL096337.

C. Tully, D. Neubauer, D. Villanueva, U. Lohmann, Does prognostic seeding along flight tracks produce the desired effects of cirrus cloud thinning?, EGUsphere, DOI 10.5194/egusphere-2022-1238.

Detlef Lohse, University of Twente

G. S. Yerragolam, R. J. A. M. Stevens, R. Verzicco, D. Lohse, O. Shishkina, Passive scalar transport in Couette flow, Journal of Fluid Mechanics, DOI 10.1017/jfm.2022.368.

Sandra Luber, University of Zurich

R. Ketkaew, S. Luber, DeepCV: A Deep Learning framework for blind search of collective variables in expanded configurational space, Journal of Chemical Information and Modeling, DOI 10.1021/acs.jcim.2c00883.

J. Mattiat, S. Luber, Comparison of length, velocity, and symmetric gauges for the calculation of absorption and electric circular dichroism spectra with real-time time-dependent density functional theory, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.2c00644.

N. Weder, N. S. Grundmann, B. Probst, O. Blacque, R. Ketkaew, F. Creazzo, S. Luber, R. Alberto, Two novel dinuclear cobalt polypyridyl complexes in electro- and photocatalysis for hydrogen production: Cooperativity increases performance, ChemSusChem, DOI 10.1002/cssc.202201049.

F. Creazzo, R. Ketkaew, K. Sivula and S. Luber, Effects of surface wettability on (001)-WO3 and (100)-WSe_2: A spin-polarized DFT-MD study, Applied Surface Science, DOI 10.1016/j.apsusc.2022.154203.

M. Malis, E. Vandaele, S. Luber, Spin-orbit couplings for nonadiabatic molecular dynamics at the DSCF level, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.1c01046.

C. Kumar, S. Luber, Robust DSCF calculations with direct energy functional minimization methods and STEP for molecules and materials, Journal of Chemical Physics, DOI 10.1063/5.0075927.

E. Ditler, T. Zimmermann, C. Kumar, S. Luber, Implementation of nuclear velocity perturbation and magnetic field perturbation theory in CP2K and their application to vibrational circular dichroism, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.2c00006.

R. Ketkaew, F. Creazzo, S. Luber, Machine learning-assisted discovery of hidden states in expanded free energy space, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.1c04004.

E. Vandaele, M. Malis, S. Luber, The photodissociation of solvated cyclopropanone and its hydrate explored via non-adiabatic molecular dynamics using DSCF, Physical Chemistry Chemical Physics, DOI 10.1039/d1cp05187c.

Mathieu Luisier, ETH Zurich

J. Cao, S. Fiore, C. Klinkert, M. Luisier, Bulk photovoltaic effect in partial overlap MoSe2-WSe2 van der Waals heterostructures: An ab initio quantum transport study, Solid-State Electronics, DOI 10.1016/j.sse.2022.108452.

F. Ducry, D. Waldhoer, T. Knobloch, M. Csontos, N. Jimenez Olalla, J. Leuthold, T. Grasser, M. Luisier, An ab initio study on resistance switching in hexagonal boron nitride, npj 2D Materials and Applications, DOI 10.1038/s41699-022-00340-6.

L. Deuschle, R. Rhyner, M. Frey, M. Luisier, Non-parabolic effective mass model for dissipative quantum transport simulations of III-V nano-devices, Journal of Applied Physics, DOI 10.1063/5.0102123.

J. Cao, S. Fiore, C. Klinkert, N. Vetsch, M. Luisier, Light-matter interactions in van der Waals photodiodes from first principles, Physical Review B, DOI 10.1103/PhysRevB.106.035306.

S. Papadopoulos, T. Agarwal, A. Jain, T. Taniguchi, K. Watanabe, M. Luisier, A. Emboras, L. Novotny, Ion migration in monolayer MoS_2 memristors, Physical Review Applied, DOI 10.1103/PhysRevApplied.18.014018.

S. Fiore, C. Klinkert, F. Ducry, J. Backman, M. Luisier, Influence of the hBN dielectric layers on the quantum transport properties of MoS_2 transistors, Materials, DOI 10.3390/ma15031062.

J. Cao, G. Gandus, T. Agarwal, M. Luisier, Y. Lee, Dynamics of van der Waals charge qubit in two-dimensional bilayer materials: Ab initio quantum transport and qubit measurement, Physical Review Research, DOI 10.1103/PhysRevResearch.4.043073.

J. Backman, Y. Lee, M. Luisier, Electron-phonon calculations using a Wannier-based supercell approach: applications to the monolayer MoS_2 mobility, Solid-State Electronics, DOI 10.1016/j.sse.2022.108461.

Ivan Lunati, Empa

L. Manickathan, C. Mucignat, I. Lunati, Kinematic training of convolutional neural networks for particle image velocimetry, Measurement Science and Technology, DOI 10.1088/1361-6501/ac8fae.

Nicola Marzari, EPFL

L. Gigli, M. Veit, M. Kotiuga, G. Pizzi, N. Marzari, M. Ceriotti, Thermodynamics and dielectric response of $BaTiO_3$ by data-driven modeling, npj Computational Materials, DOI 10.1038/s41524-022-00845-0.

I. Timrov, N. Marzari, M. Cococcioni, HP - A code for the calculation of Hubbard parameters using density-functional perturbation theory, Computer Physics Communications, DOI 10.1016/j.cpc.2022.108455.

M. Kotiuga, S. Halilov, B. Kozinsky, M. Fornari, N. Marzari, G. Pizzi, Microscopic picture of paraelectric perovskites from structural prototypes, Physical Review Research, DOI 10.1103/PhysRevResearch.4.L012042.

R. Mahajan, A. Kashyap, I. Timrov, Pivotal role of intersite Hubbard interactions in Fe-Doped α-MnO_2, Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.2c04767.

I. Timrov, F. Aquilante, M. Cococcioni, N. Marzari, Accurate electronic properties and intercalation voltages of olivine-type Li-ion cathode materials from extended Hubbard functionals, PRX Energy, DOI 10.1103/PRXEnergy.1.033003.

G. Cherkashinin, R. Eilhardt, S. Nappini, M. Cococcioni, I. Píš, S. dal Zilio, F. Bondino, N. Marzari, E. Magnano, L. Alff, Energy level alignment at the cobalt phosphate/electrolyte interface: Intrinsic stability vs interfacial chemical reactions in 5 V Lithium ion batteries, ACS Applied Materials & Interfaces, DOI 10.1021/acsami.1c16296.

John Mantzaras, Paul Scherrer Institute

M. Khatoonabadi, N. I. Prasianakis, J. Mantzaras, Lattice Boltzmann modeling and simulation of velocity and concentration slip effects on the catalytic reaction rate of strongly nonequimolar reactions in microflows, Physical Review E, DOI 10.1103/PhysRevE.106.065305.

Marina K. Marinkovic, ETH Zurich

R. Gruber, A. Kozhevnikov, M. K. Marinkovic, T. C. Schulthess, R. Solcà, Performance optimizations for porting the openQ*D package to GPUs, PoS: Proceedings of Science, DOI 10.22323/1.396.0491.

L. Bushnaq, I. Campos, M. Catillo, A. Cotellucci, M. Dale, J. Lücke, M. K. Marinković, A. Patella, M. Peardon, N. Tantalo, Implementing noise reduction techniques into the OpenQ*D package, PoS: Proceedings of Science, DOI 10.22323/1.396.0363.

M. E. B. Dale, L. Bushnaq, I. Campos, M. Catillo, A. Cotellucci, Baryon masses from full QCD+QED$_C$ simulations, PoS: Proceedings of Science, DOI 10.22323/1.396.0373.

J. Lücke, L. Bushnaq, I. Campos Plasencia, M. Catillo, A. Cotellucci, M. E. B. Dale, P. Fritzsch, M. K. Marinkovic, A. Patella, N. Tantalo, An update on QCD+QED simulations with C* boundary conditions, PoS: Proceedings of Science, DOI 10.22323/1.396.0293.

Lucio Mayer, University of Zurich

T. Tamfal, L. Mayer, T. R. Quinn, A. Babul, P. Madau, P. R. Capelo, S. Shen, M. Staub, The dawn of disk formation in a milky way-sized galaxy halo: Thin stellar disks at $z > 4$, Astrophysical Journal, DOI 10.3847/1538-4357/ac558e.

Davide Modesti, Delft University of Technology

H. Shahzad, S. Hickel, D. Modesti, Permeability and turbulence over perforated plates, Flow Turbulence and Combustion, DOI 10.1007/s10494-022-00354-6.

D. Modesti, S. Sathyanarayana, F. Salvadore, M. Bernardini, Direct numerical simulation of supersonic turbulent flows over rough surfaces, Journal of Fluid Mechanics, DOI 10.1017/jfm.2022.393.

S. Shahzad, J. M. Favre, S. Hickel, D. Modesti, Turbulent boundary layer over acoustic liners, APS Gallery of Fluid Motion, DOI 10.1103/APS.DFD.2022.GFM.V0019.

Rebecca Mott, WSL Institute for Snow- and Avalanche Research SLF

B. Kruyt, R. Mott, J. Fiddes, F. Gerber, V. Sharma, D. Reynolds, A downscaling intercomparison study: The representation of slope- and ridge-scale processes in models of different complexity, Frontiers in Earth Science, DOI 10.3389/feart.2022.789332.

Dominik Obrist, University of Bern

H. Zolfaghari, R. R. Kerswell, D. Obrist, P. J. Schmid, Sensitivity and downstream influence of the impinging leading-edge vortex instability in a bileaflet mechanical heart valve, Journal of Fluid Mechanics, DOI 10.1017/jfm.2022.49.

Michele Parrinello, Italian Institute of Technology Genoa

C. W. Myung, B. Hirshberg, M. Parrinello, Prediction of a supersolid phase in high-pressure deuterium, Physical Review Letters, DOI 10.1103/PhysRevLett.128.045301.

Alfredo Pasquarello, EPFL

J. Yang, S. Falletta, A. Pasquarello, One-shot approach for enforcing piecewise linearity on hybrid functionals: Application to band gap predictions, Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.2c00414.

S. Falletta, A. Pasquarello, Many-body self-interaction and polarons, Physical Review Letters DOI 10.1103/PhysRevLett.129.126401.

S. Falletta, A. Pasquarello, Polarons free from many-body self-interaction in density functional theory, Physical Review B, DOI 10.1103/PhysRevB.106.125119.

S. Falletta, A. Pasquarello, Hubbard U through polaronic defect states, npj Computational Materials, DOI 10.1038/s41524-022-00958-6.

J. Lan, V. V. Rybkin, A. Pasquarello, Temperature dependent properties of the aqueous electron, Angewandte Chemie-International Edition, DOI 10.1002/anie.202209398.

S. Lyu, J. Wiktor, A. Pasquarello, Oxygen evolution at the $BiVO_4$-water interface: Mechanism of the water dehydrogenation reaction, ACS Catalysis, DOI 10.1021/acscatal.2c03331.

H. Wang, A. Tal, T. Bischoff, P. Gono, A. Pasquarello, Accurate and efficient band-gap predictions for metal halide perovskites at finite temperature, npj Computational Materials, DOI 10.1038/s41524-022-00869-6.

Giovanni M. Pavan, SUPSI

C. Lionello, C. Perego, A. Gardin, R. Klajn, G. M. Pavan, Supramolecular semiconductivity through emerging ionic gates in ion-nanoparticle superlattices, ACS Nano, DOI 10.1021/acsnano.2c07558.

M. Becchi, R. Capelli, C. Perego, G. M. Pavan, C. Micheletti, Density-tunable pathway complexity in a minimalistic self-assembly model, Soft Matter, DOI 10.1039/d2sm00968d.

N. Uchida, A. Kohata, K. Okuro, A. Cardellini, C. Lionello, E. A. Zizzi, M. A. Deriu, G. M. Pavan, M. Tomishige, T. Hikima, T. Aida, Reconstitution of microtubule into GTP-responsive nanocapsules, Nature Communications, DOI 10.1038/s41467-022-33156-5.

M. Delle Piane, L. Pesce, M. Cioni, G. M. Pavan, Reconstructing reactivity in dynamic host-guest systems at atomistic resolution: Amide hydrolysis under confinement in the cavity of a coordination cage, Chemical Science, DOI 10.1039/d2sc02000a.

A. Gardin, C. Perego, G. Doni, G. M. Pavan, Classifying soft self-assembled materials via unsupervised machine learning of defects, Communications Chemistry, DOI 10.1038/s42004-022-00699-z.

K. Koner, S. Karak, S. Kandambeth, S. Karak, N. Thomas, L. Leanza, C. Perego, L. Pesce, R. Capelli, M. Moun, M. Bhakar, T. G. Ajithkumar, G. M. Pavan, R. Banerjee, Porous covalent organic nanotubes and their assembly in loops and toroids, Nature Chemistry, DOI 10.1038/s41557-022-00908-1.

M. Crippa, C. Perego, A. L. de Marco, G. M. Pavan, Molecular communications in complex systems of dynamic supramolecular polymers, Nature Communications, DOI 10.1038/s41467-022-29804-5.

C. Empereur-mot, R. Capelli, M. Perrone, C. Caruso, G. Doni, G. M. Pavan, Automatic multi-objective optimization of coarse-grained lipid force fields using SwarmCG, Journal of Chemical Physics, DOI 10.1063/5.0079044.

E. Weyandt, L. Leanza, R. Capelli, G. M. Pavan, G. Vantomme, E. W. Meijer, Controlling the length of porphyrin supramolecular polymers via coupled equilibria and dilution-induced supramolecular polymerization, Nature Communications, DOI 10.1038/s41467-021-27831-2.

Simone Pezzuto, Università della Svizzera italiana

C. Ruiz-Herrera, T. Grandits, G. Plank, P. Perdikaris, F. S. Costabal, S. Pezzuto, Physics-informed neural networks to learn cardiac fiber orientation from multiple electroanatomical maps, Engineering with Computers, DOI 10.1007/s00366-022-01709-3.

N. J. Verzaal, C. J. M. van Deursen, S. Pezzuto, L. Wecke, W. M. van Everdingen, K. Vernooy, T. Delhaas, A. Auricchio, F. W. Prinzen, Synchronization of repolarization after cardiac resynchronization therapy: A combined clinical and modeling study, Journal of Cardiovascular Electrophysiology, DOI 10.1111/jce.15581.

L. Gander, S. Pezzuto, A. Gharaviri, R. Krause, P. Perdikaris, F. S. Costabal, Fast characterization of inducible regions of atrial fibrillation models with multi-fidelity Gaussian process classification, Frontiers in Physiology, DOI 10.3389/fphys.2022.757159.

S. Pezzuto, P. Perdikaris, F. Sahli Costabal, Learning cardiac activation maps from 12-lead ECG with multi-fidelity Bayesian optimization on manifolds, IFAC-PapersOnLine, DOI 10.1016/j.ifacol.2022.09.091.

T. Grandits, S. Pezzuto, G. Plank, Smoothness and continuity of cost functionals for ECG mismatch computation, IFAC-PapersOnLine, DOI 10.1016/j.ifacol.2022.09.092.

V. G. Marques, A. Gharaviri, S. Pezzuto, P. Bonizzi, S. Zeemering, U. Schotten, Spatial relationship between atrial fibrillation drivers and the presence of repetitive conduction patterns using recurrence analysis on in-silico models, Computing in Cardiology Conference (CinC), DOI 10.23919/CinC53138.2021.9662692.

Carlo A. Pignedoli, Empa

K. Eimre, J. I. Urgel, H. Hayashi, M. Di Giovannantonio, P. Ruffieux, S. Sato, S. Otomo, Y. S. Chan, N. Aratani, D. Passerone, O. Gröning, H. Yamada, R. Fasel, C. A. Pignedoli, On-surface synthesis and characterization of nitrogen-substituted undecacenes, Nature Communications, DOI 10.1038/s41467-022-27961-1.

C. Li, X. Z. Meng, A. Weismann, J. S. von Glasenapp, S. Hamer, F. F. Xiang, C. A. Pignedoli, R. Herges, R. Berndt, Effect of an axial ligand on the self-assembly of molecular platforms, Physical Chemistry Chemical Physics, DOI 10.1039/d2cp04760h.

J. Bjork, C. Sanchez-Sanchez, Q. Chen, C. A. Pignedoli, J. Rosen, P. Ruffieux, X. Feng, A. Narita, K. Müllen, R. Fasel, The Role of metal adatoms in a surface-assisted cyclodehydrogenation reaction on a gold surface, Angewandte Chemie-International Edition, DOI 10.1002/anie.202212354.

M. R. Ajayakumar, M. Di Giovannantonio, C. A. Pignedoli, L. Yang, P. Ruffieux, J. Ma, R. Fasel, X. Feng, On-surface synthesis of porous graphene nanoribbons containing nonplanar [14]annulene pores, Journal of Polymer Science, DOI 10.1002/pol.20220003.

Fernando Porté-Agel, EPFL

D. Vahidi, F. Porté-Agel, A physics-based model for wind turbine wake expansion in the atmospheric boundary layer, Journal of Fluid Mechanics, DOI 10.1017/jfm.2022.443.

Nikolaos I. Prasianakis, Paul Scherrer Institute

M. Mahrous, E. Curti, S. V. Churakov, N. I. Prasianakis, Petrophysical initialization of core-scale reactive transport simulations on Indiana limestones: Pore-scale characterization, spatial autocorrelations, and representative elementary volume analysis, Journal of Petroleum Science and Engineering, DOI 10.1016/j.petrol.2022.110389.

T. Jäger, A. Mokos, N. I. Prasianakis, S. Leyer, Pore-level multiphase simulations of realistic distillation membranes for water desalination, Membranes, DOI 10.3390/membranes12111112.

Christoph C. Raible, University of Bern

P. Velasquez, M. Messmer, C. C. Raible, The role of ice-sheet topography in the Alpine hydro-climate at glacial times, Climate of the Past, DOI 10.5194/cp-18-1579-2022.

H. Mackay, G. Plunkett, B. J. L. Jensen, T. J. Aubry, C. Corona, W. M. Kim, M. Toohey, M. Sigl, M. Stoffel, K. J. Anchukaitis, C. Raible, M. S. M. Bolton, J. G. Manning, T. P. Newfield, N. Di Cosmo, F. Ludlow, C. Kostick, Z. Yang, L. Coyle McClung, M. Amesbury, A. Monteath, P. D. M. Hughes, P. G. Langdon, D. Charman, R. Booth, K. L. Davies, A. Blundell, G. T. Swindles, The 852/3CE Mount Churchill eruption: Examining the potential climatic and societal impacts and the timing of the Medieval Climate Anomaly in the North Atlantic region, Climate of the Past, DOI 10.5194/cp-18-1475-2022.

J. J. Gomez-Navarro, C. C. Raible, J. A. Garcia-Valero, M. Messmer, J. P. Montavez, O. Martius, Event selection for dynamical downscaling: A neural network approach for physically-constrained precipitation events, Climate Dynamics, DOI 10.1007/s00382-019-04818-w.

Paolo Ricci, EPFL

B. J. Frei, A. C. D. Hoffmann, P. Ricci, Local gyrokinetic collisional theory of the ion-temperature gradient mode, Journal of Plasma Physics, DOI 10.1017/S0022377822000344.

A. Coroado, P. Ricci, Numerical simulations of gas puff imaging using a multi-component model of the neutral-plasma interaction in the tokamak boundary, Physics of Plasmas, DOI 10.1063/5.0077336.

B. J. Frei, S. Ernst, P. Ricci, Numerical implementation of the improved Sugama collision operator using a moment approach, Physics of Plasmas, DOI 10.1063/5.0091244.

A. Coroado, P. Ricci, A self-consistent multi-component model of plasma turbulence and kinetic neutral dynamics for the simulation of the tokamak boundary, Nuclear Fusion, DOI 10.1088/1741-4326/ac47b8.

M. Giacomin, P. Ricci, Turbulent transport regimes in the tokamak boundary and operational limits, Physics of Plasmas, DOI 10.1063/5.0090541.

A. J. Coelho, J. Loizu, P. Ricci, M. Giacomin, Global fluid simulation of plasma turbulence in a stellarator with an island divertor, Nuclear Fusion, DOI 10.1088/1741-4326/ac6ad2.

Marcello Righi, Zurich University of Applied Sciences

M. Righi, D. Anderegg, S. Düzel, ROM-based uncertainties quantification of flutter speed prediction of the BSCW wing, AIAA SciTech Forum, DOI 10.2514/6.2022-0179.

M. Righi, D. Anderegg, L. Manfriani, M. Ammann, Optimisation of symmetrical aerofoils for a vertical axis wind turbine, AIAA AVIATION Forum, DOI 10.2514/6.2022-3384.

Fabio Riva, Istituto Ricerche Solari IRSOL, Università della Svizzera italiana

F. Riva, O. Steiner, Methodology for estimating the magnetic Prandtl number and application to solar surface small-scale dynamo simulations, Astronomy & Astrophysics, DOI 10.1051/0004-6361/202142644.

Kevin Rossi, EPFL

O. S. Lecina, M. A. Hope, A. Venkatesh, S. Bjorgvinsdottir, K. Rossi, A. Loiudice, L. Emsley, R. Buonsanti, Colloidal-ALD-grown hybrid shells nucleate via a ligand-precursor complex, Journal of the American Chemical Society, DOI 10.1021/jacs.1c12538.

Ursula Röthlisberger, EPFL

A. Mishra, D. J. Kubicki, A. Boziki, R. D. Chavan, M. Dankl, M. Mladenović, D. Prochowicz, C. P. Grey, U. Röthlisberger, L. Emsley, Interplay of kinetic and thermodynamic reaction control explains incorporation of dimethylammonium iodide into $CsPbI_3$, ACS Energy Letters, DOI 10.1021/acsenergylett.2c00877.

S. C. Van Keulen, J. Martin, F. Colizzi, E. Frezza, D. Trpevski, N. C. Diaz, P. Vidossich, U. Röthlisberger, J. Hellgren Kotaleski, R. C. Wade, P. Carloni, Multiscale molecular simulations to investigate adenylyl cyclase-based signaling in the brain, Wiley Interdisciplinary Reviews-Computational Molecular Science, DOI 10.1002/wcms.1623.

Y. R. Wang, A. Senocrate, M. Mladenović, A. Ducinškas, G. Y. Kim, U. Röthlisberger, J. V. Milić, D. Moia, M. Grätzel, J. Maier, Photo de-mixing in Dion-Jacobson 2D mixed halide perovskites, Advanced Energy Materials, DOI 10.1002/aenm.202200768.

N. Arora, A. Greco, S. Meloni, A. Hinderhofer, A. Mattoni, U. Röthlisberger, J. Hagenlocher, C. Caddeo, S. M. Zakeeruddin, F. Schreiber, M. Grätzel, R. H. Friend, M. I. Dar, Kinetics and energetics of metal halide perovskite conversion reactions at the nanoscale, Communications Materials, DOI 10.1038/s43246-022-00239-1.

B. P. Le Monnier, L. Savereide, M. Kilic, R. Schnyder, M. D. Mensi, C. E. Avalos, U. Röthlisberger, J. S. Luterbacher, Atom-by-atom synthesis of multiatom-supported catalytic clusters by liquid-phase atomic layer deposition, ACS Sustainable Chemistry & Engineering, DOI 10.1021/acssuschemeng.1c07056.

L. A. Muscarella, A. Dučinskas, M. Dankl, M. Andrzejewski, N. P. M. Casati, U. Röthlisberger, J. Maier, M. Grätzel, B. Ehrler, J. V. Milić, Reversible pressure-dependent mechanochromism of Dion-Jacobson and Ruddlesden-Popper layered hybrid perovskites, Advanced Materials, DOI 10.1002/adma.202108720.

A. Boziki, P. Baudin, E. Liberatore, N. A. Astani, U. Röthlisberger, A theoretical perspective of the ultrafast transient absorption dynamics of CsPbBr3, Journal of Computational Chemistry, DOI 10.1002/jcc.26815.

F. Mouvet, J. Villard, V. Bolnykh, U. Röthlisberger, Recent advances in first-principles based molecular dynamics, Accounts of Chemical Research, DOI 10.1021/acs.accounts.1c00503.

M. S. Ozer, Z. Eroglu, A. S. Yalin, M. Kılıç, U. Röthlisberger, O. Metin, Bismuthene as a versatile photocatalyst operating under variable conditions for the photoredox CH bond functionalization, Applied Catalysis B: Environmental, DOI 10.1016/j.apcatb.2021.120957.

H. Zhang, K. Darabi, N. Y. Nia, A. Krishna, P. Ahlawat, B. Guo, M. H. S. Almalki, T.-S. Su, D. Ren, V. Bolnykh, L. A. Castriotta, M. Zendehdel, L. Pan, S. Sanchez Alonso, R. Li, S. M. Zakeeruddin, A. Hagfeldt, U. Röthlisberger, A. Di Carlo, A. Amassian, M. Grätzel, A universal co-solvent dilution strategy enables facile and cost-effective fabrication of perovskite photovoltaics, Nature Communications, DOI 10.1038/s41467-021-27740-4.

Eugene Rozanov, PMO-DWRC, Davos

A. Karagodin-Doyennel, E. Rozanov, T. Sukhodolov, T. Egorova, J. Sedlacek, W. Ball, T. Peter, The historical ozone trends simulated with the SOCOLv4 and their comparison with observations and reanalyses, Atmospheric Chemistry and Physics, DOI 10.5194/acp-22-15333-2022.

O. Morgenstern, D. E. Kinnison, M. Mills, M. Michou, L. W. Horowitz, P. Lin, M. Deushi, K. Yoshida, F. M. O'Connor, Y. Tang, N. L. Abraham, J. Keeble, F. Dennison, E. Rozanov, T. Egorova, T. Sukhodolov, G. Zeng, Comparison of Arctic and Antarctic stratospheric climates in chemistry versus no-chemistry climate models, Journal of Geophysical Research-Atmospheres, DOI 10.1029/2022JD037123.

Andrei V. Ruban, KTH Royal Institute of Technology

S. He, D. Scheiber, T. Jechtl, F. Moitzi, O. Peil, L. Romaner, S. Zamberger, E. Povoden-Karadeniz, V. Razumovskiy, A. V. Ruban, Solubility and segregation of B in paramagnetic fcc Fe, Physical Review Materials, DOI 10.1103/PhysRevMaterials.6.023604.

Richard Sandberg, University of Melbourne

R. D. Sandberg, V. Michelassi, Fluid dynamics of axial turbomachinery: Blade- and stage-level simulations and models, Annual Review of Fluid Mechanics, DOI 10.1146/annurev-fluid-031221-105530.

Yohei Sato, Paul Scherrer Institute

M. Corrado, Y. Sato, Magnetohydrodynamics simulation of the nonlinear behavior of single rising bubbles in liquid metals in the presence of a horizontal magnetic field, Fluids, DOI 10.3390/fluids7110349.

Christoph Schär, ETH Zurich

A. M. Fischer, K. M. Strassmann, M. Croci-Maspoli, A. M. Hama, R. Knutti, S. Kotlarski, C. Schär, C. Schnadt Poberaj, N. Ban, M. Bavay, U. Beyerle, D.N. Bresch, S. Brönnimann, P. Burlando, A. Casanueva, S. Fatichi, I. Feigenwinter, E.M. Fischer, M. Hirschi, M.A. Liniger, C. Marty, I. Medhaug, N. Peleg, M. Pickl, C.C. Raible, J. Rajczak, O. Rössler, S.C. Scherrer, C. Schwierz, S. I. Seneviratne, M. Skelton, S.L. Sørland, C. Spirig, F. Tschurr, J. Zeder, E.M. Zubler, Climate Scenarios for Switzerland CH2018-Approach and Implications, Climate Services, DOI 10.1016/j.cliser.2022.100288.

C. Zeman, C. Schär, An ensemble-based statistical methodology to detect differences in weather and climate model executables, Geoscientific Model Development, DOI 10.5194/gmd-15-3183-2022.

Simon Scheidegger, University of Lausanne

M. Azinovic, L. Gaegauf, S. Scheidegger, Deep equilibrium nets, International Economic Review, DOI 10.1111/iere.12575.

A. Eftekhari, S. Scheidegger, High-Dimensional dynamic stochastic model representation, SIAM Journal on Scientific Computing, DOI 10.1137/21m1392231.

Benjamin Schuler, University of Zurich

K. J. Buholzer, J. McIvor, F. Zosel, C. Teppich, D. Nettels, D. Mercadante, B. Schuler, Multilayered allosteric modulation of coupled folding and binding by phosphorylation, peptidyl-prolyl cis/trans isomerization, and diversity of interaction partners, Journal of Chemical Physics, DOI 10.1063/5.0128273.

P. O. Heidarsson, D. Mercadante, A. Sottini, D. Nettels, M. B. Borgia, A. Borgia, S. Kilic, B. Fierz, R. B. Best, B. Schuler, Release of linker histone from the nucleosome driven by polyelectrolyte competition with a disordered protein, Nature Chemistry, DOI 10.1038/s41557-021-00839-3.

Sonia I Seneviratne, ETH Zurich

G. Mussetti, E. L. Davin, J. Schwaab, J. A. Acero, J. Ivanchev, V. K. Singh, L. Jin, S. I. Seneviratne, Do electric vehicles mitigate urban heat? The case of a tropical city, Frontiers in Environmental Science, DOI 10.3389/fenvs.2022.810342.

Berend Smit, EPFL

S. M. Moosavi, B. A. Novotny, D. Ongari, E. Moubarak, M. Asgari, O. Kadioglu, C. Charalambous, A. Ortega-Guerrero, A. H. Farmahini, L. Sarkisov, S. Garcia, F. Noé, B. Smit, A data-science approach to predict the heat capacity of nanoporous materials, Nature Materials, DOI 10.1038/s41563-022-01374-3.

H. L. Xu, R. Cabriolu, B. Smit, Effects of degrees of freedom on calculating diffusion properties in nanoporous materials, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.2c00094.

Nicola A. Spaldin, ETH Zurich

L. Caretta, Y.-T. Shao, J. Yu, A. B. Mei, B. F. Grosso, C. Dai, P. Behera, D. Lee, M. McCarter, E. Parsonnet, H. K. P, F. Xue, X. Guo, E. S. Barnard, S. Ganschow, Z. Hong, A. Raja, L. W. Martin, L.-Q. Chen, M. Fiebig, K. Lai, N. A. Spaldin, D. A. Muller, D. G. Schlom, R. Ramesh, Non-volatile electric-field control of inversion symmetry, Nature Materials, DOI 10.1038/s41563-022-01412-0.

R. Zhang, M. E. Merkel, S. Beck, C. Ederer, Training biases in machine learning for the analytic continuation of quantum many-body Green's functions, Physical Review Research, DOI 10.1103/PhysRevResearch.4.043082.

T. N. Tosic, Q. N. Meier, N. A. Spaldin, Influence of the triangular Mn-O breathing mode on magnetic ordering in multiferroic hexagonal manganites, Physical Review Research, DOI 10.1103/PhysRevResearch.4.033204.

M. Si, A. Izardar, C. Ederer, Effect of chemical disorder on the magnetic anisotropy in L10 FeNi from first-principles calculations, Physical Review Research, DOI 10.1103/PhysRevResearch.4.033161.

T. Esswein, N. A. Spaldin, Ferroelectric, quantum paraelectric, or paraelectric? Calculating the evolution from $BaTiO_3$ to $SrTiO_3$ to $KTaO_3$ using a single-particle quantum mechanical description of the ions, Physical Review Research, DOI 10.1103/PhysRevResearch.4.033020.

S. Beck, A. Hampel, O. Parcollet, C. Ederer, A. Georges, Charge self-consistent electronic structure calculations with dynamical mean-field theory using Quantum ESPRESSO, Wannier 90 and TRIQS, Journal of Physics-Condensed Matter, DOI 10.1088/1361-648X/ac5d1c.

S. Bhowal, N. A. Spaldin, Magnetoelectric classification of skyrmions, Physical Review Letters, DOI 10.1103/PhysRevLett.128.227204.

D. Kim, I. Efe, H. Torlakcik, A. Terzopoulou, A. Veciana, E. Siringil, F. Mushtaq, C. Franco, D. von Arx, S. Sevim, J. Puigmartí-Luis, B. Nelson, N. A. Spaldin, C. Gattinoni, X.-Z. Chen, S. Pané, Magnetoelectric effect in hydrogen harvesting: Magnetic field as a trigger of catalytic reactions, Advanced Materials, DOI 10.1002/adma.202110612.

A. Izardar, C. Ederer, Impact of chemical disorder on magnetic exchange interactions in $L1_0$-FeNi, Physical Review B, DOI 10.1103/PhysRevB.105.134428.

S. Bhowal, S. P. Collins, N. A. Spaldin, Hidden *k*-space magnetoelectric multipoles in nonmagnetic ferroelectrics, Physical Review Letters, DOI 10.1103/PhysRevLett.128.116402.

J. A. Mundy, B. F. Grosso, C. A. Heikes, D. F. Segedin, Z. Wang, Y. T. Shao, C. Dai, B. H. Goodge, Q. N. Meier, C. T. Nelson, B. Prasad, F. Xue, S. Ganschow, D. A. Muller, L. F. Kourkoutis, L.-Q. Chen, W. D. Ratcliff, N. A. Spaldin, R. Ramesh, D. G. Schlom, Liberating a hidden antiferroelectric phase with interfacial electrostatic engineering, Science Advances, DOI 10.1126/sciadv.abg5860.

Joachim Stadel, University of Zurich

J. M. Y. Woo, C. Reinhardt, M. Cilibrasi, A. Chau, R. Helled, J. Stadel, Did Uranus' regular moons form via a rocky giant impactor, Icarus, DOI 10.1016/j.icarus.2021.114842.

Thomas Stocker, University of Bern

S. J. Gonzalez-Roji, M. Messmer, C. C. Raible, T. F. Stocker, Sensitivity of precipitation in the highlands and lowlands of Peru to physics parameterization options in WRFV3.8.1, Geoscientific Model Development, DOI 10.5194/gmd-15-2859-2022.

Judit Szulágyi, ETH Zurich

J. Szulágyi, F. Binkert, C. Surville, Meridional circulation of dust and gas in the circumstellar disk: Delivery of solids onto the circumplanetary region, The Astrophysical Journal, DOI 10.3847/1538-4357/ac32d1.

X. Chen, J. Szulágyi, Observability of forming planets and their circumplanetary discs – IV. With JWST and ELT, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stac1976.

Paul J. Tackley, ETH Zurich

X. Borgeat, P. J. Tackley, Hadean/Eoarchean tectonics and mantle mixing induced by impacts: a three-dimensional study, Progress in Earth and Planetary Science, DOI 10.1186/s40645-022-00497-0.

Romain Teyssier, University of Zurich & Princeton University

J. R. C. Cuissa, R. Teyssier, Toward fully compressible numerical simulations of stellar magneto-convection with the RAMSES code, Astronomy & Astrophysics, DOI 10.1051/0004-6361/202142754.

Y. K. Liu, M. Kretschmer, R. Teyssier, A subgrid turbulent mean-field dynamo model for cosmological galaxy formation simulations, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stac1266.

M. Kretschmer, A. Dekel, R. Teyssier, On the origin of surprisingly cold gas discs in galaxies at high redshift, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab3648.

D. A. V. Romero, F. S. Masset, R. Teyssier, Eccentricity driving of pebble accreting low-mass planets, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab3334.

Christian Theiler, EPFL

D. S. Oliveira, T. Body, D. Galassi, C. Theiler, E. Laribi, P. Tamain, A. Stegmeir, M. Giacomin, W. Zholobenko, P. Ricci, H. Bufferand, J. A. Boedo, G. Ciraolo, C. Colandrea, D. Coster, H. de Oliveira, G. Fourestey, S. Gorno, F. Imbeaux, F. Jenko, V. Naulin, N. Offeddu, H. Reimerdes, E. Serre, C. K. Tsui, N. Varini, N. Vianello, M. Wiesenberger, C. Wüthrich, TCV team, Validation of edge turbulence codes against the TCV-X21 diverted L-mode reference cases, Nuclear Fusion, DOI 10.1088/1741-4326/ac4cde.

D. Galassi, C. Theiler, T. Body, F. Manke, P. Micheletti, J. Omotani, M. Wiesenberger, M. Baquero-Ruiz, I. Furno, M. Giacomin, E. Laribi, F. Militello, P. Ricci, A. Stegmeir, P. Tamain, H. Bufferand, G. Ciraolo, H. De Oliveira, A. Fasoli, V. Naulin, S. Newton, N. Offeddu, D. S. Oliveira, E. Serre, N. Vianello, Validation of edge turbulence codes in a magnetic X-point scenario in TORPEX, Physics of Plasmas, DOI 10.1063/5.0064522.

Javier Trujillo Bueno, Instituto de Astrofisica de Canarias

S. H. Dayananda, J. Trujillo Bueno, Á. de Vicente, T. del Pino Alemán, Polarization of the Lyα lines of H I and He II as a tool for exploring the solar corona, Astrophysical Journal, DOI 10.3847/1538-4357/ac1068.

Vladyslav Turlo, Empa

Y. L. Müller, L. P. H. Jeurgens, A. Antušek, V. Turlo, Atomistic assessment of melting point depression and enhanced interfacial diffusion of Cu in confinement with AlN, ACS Applied Materials & Interfaces, DOI 10.1021/acsami.2c01347.

J. F. Troncoso, V. Turlo, Evaluating the applicability of classical and neural network interatomic potentials for modeling body centered cubic polymorph of magnesium, Modelling and Simulation in Materials Science and Engineering, DOI 10.1088/1361-651X/ac5ebc.

Andrii Tykhonov, University of Geneva

M. Stolpovskiy, X. Wu, A. Tykhonov, M. Deliyergiyev, C. Perrina, M. M. Salinas, D. Droz, A. Ruina, E. Catanzani on behalf of the DAMPE collaboration, Machine learning-based method of calorimeter saturation correction for helium flux analysis with DAMPE experiment, Journal of Instrumentation, DOI 10.1088/1748-0221/17/06/P06031.

Martin van Driel, ETH Zurich

J. Kemper, M. van Driel, F. Munch, A. Khan, D. Giardini, A spectral element approach to computing normal modes, Geophysical Journal International, DOI 10.1093/gji/ggab476.

Harry van Lenthe, ETH Zurich

C. J. Collins, P. R. Atkins, N. Ohs, M. Blauth, K. Lippuner, R. Müller, Clinical observation of diminished bone quality and quantity through HR-pQCT-derived remodeling and mechanoregulation, Scientific Reports, DOI 10.1038/s41598-022-22678-z.

A. Sas, A. Sermon, G. H. van Lenthe, Experimental validation of a voxel-based finite element model simulating femoroplasty of lytic lesions in the proximal femur, Scientific Reports, DOI 10.1038/s41598-022-11667-x.

Stefano Vanni, University of Fribourg

E. Petretto, Q. K. Ong, F. Olgiati, T. Mao, P. Campomanes, F. Stellacci, S. Vanni, Monovalent ion-mediated charge-charge interactions drive aggregation of surface-functionalized gold nanoparticles, Nanoscale, DOI 10.1039/d2nr02824g.

A. K. Adamczyk, T. A. P. M. Huijben, M. Sison, A. Di Luca, S. Vanni, S. Brasselet, K.I. Mortensen, F.D. Stefani, M. Pilo-Pais, G.P. Acuna, DNA self-assembly of single molecules with deterministic position and orientation, ACS Nano, DOI 10.1021/acsnano.2c06936.

S. Rogers, L. Gui, A. Kovalenko, V. Zoni, M. Carpentier, K. Ramji, K. B. Mbarek, A. Bacle, P. Fuchs, P. Campomanes, E. Reetz, N. Ortiz Speer, E. Reynolds, A. R. Thiam, S. Vanni, D. Nicastro, W. M. Henne, Triglyceride lipolysis triggers liquid crystalline phases in lipid droplets and alters the LD proteome, Journal of Cell Biology, DOI 10.1083/jcb.202205053.

S. Sotillos, I. von der Decken, I. Domenech Mercadé, S. Srinivasan, D. Sirokha, L. Livshits, S. Vanni, S. Nef, A. Biason-Lauber, D. Rodríguez Gutiérrez, J. Castelli-Gair Hombría, A conserved function of Human DLC3 and *Drosophila* Cv-c in testis development, eLife, DOI 10.7554/eLife.82343.

Franco Vazza, University of Bologna

E. Carretti, S. P. O'Sullivan, V. Vacca, F. Vazza, C. Gheller, T. Vernstrom, A. Bonafede, Magnetic field evolution in cosmic filaments with LOFAR data, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stac2966.

M. S. S. L. Oei, R. J. van Weeren, M. J. Hardcastle, F. Vazza, T. W. Shimwell, F. Leclercq, M. Brüggen, H. J A Röttgering, An intergalactic medium temperature from a giant radio galaxy, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stac2948.

T. Hodgson, F. Vazza, M. Johnston-Hollitt, B. McKinley, Stacking the synchrotron cosmic web with FIGARO, Publications of the Astronomical Society of Australia, DOI 10.1017/pasa.2022.26.

V. P. Pomakov, S. P. O'Sullivan, M. Bruggen, F. Vazza, E. Carretti, G. H. Heald, C. Horellou, T. Shimwell, A. Shulevski, T. Vernstrom, The redshift evolution of extragalactic magnetic fields, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stac1805.

M. S. S. L. Oei, R. J. van Weeren, F. Vazza, F. Leclercq, A. Gopinath, H. J. A. Rottgering, Filamentary baryons and where to find them: A forecast of synchrotron radiation from merger and accretion shocks in the local Cosmic Web, Astronomy & Astrophysics, DOI 10.1051/0004-6361/202140364.

Laurent Villard, EPFL

M. Murugappan, L. Villard, S. Brunner, B. F. McMillan, A. Bottino, Gyrokinetic simulations of turbulence and zonal flows driven by steep profile gradients using a delta-f approach with an evolving background Maxwellian, Physics of Plasmas, DOI 10.1063/5.0106661.

P. Donnel, J. B. Fontana, J. Cazabonne, L. Villard, S. Brunner, S. Coda, J. Decker, Y. Peysson, Electron-cyclotron resonance heating and current drive source for flux-driven gyrokinetic simulations of tokamaks, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/ac7974.

M. Sadr, A. Mishchenko, T. Hayward-Schneider, A. Koenies, A. Bottino, A. Biancalani, P. Donnel, E. Lanti, L. Villard, Linear and nonlinear excitation of TAE modes by external electromagnetic perturbations using ORB5, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/ac73eb.

Peter E. Vincent, Imperial College London

L. Caros, O. Buxton, T. Shigeta, T. Nagata, T. Nonomura, K. Asai, P. Vincent, Direct numerical simulation of flow over a triangular airfoil under martian conditions, AIAA Journal, DOI 10.2514/1.J061454.

G. Giangaspero, L. Amerio, S. Downie, A. Zasso, P. Vincent, High-order scale-resolving simulations of extreme wind loads on a model high-rise building, Journal of Wind Engineering and Industrial Aerodynamics, DOI 10.1016/j.jweia.2022.105169.

Nuri Yazdani & Vanessa Wood, ETH Zurich

G. Raino, N. Yazdani, S. C. Boehme, M. Kober-Czerny, C. L. Zhu, F. Krieg, M. D. Rossell, R. Erni, V. Wood, I. Infante, M. V. Kovalenko, Ultra-narrow room-temperature emission from single $CsPbBr_3$ perovskite quantum dots, Nature Communications, DOI 10.1038/s41467-022-30016-0.

Y. H. Xing, N. Yazdani, W. M. M. Lin, M. Yarema, R. Zahn, V. Wood, Effect of positional disorders on charge transport in nanocrystal quantum dot thin films, ACS Applied Electronic Materials, DOI 10.1021/acsaelm.1c01011.

Oleg V. Yazyev, EPFL

I. Zivkovic, R. Yadav, J. R. Soh, C. J. Yi, Y. G. Shi, O. V. Yazyev, H. M. Rønnow, Unraveling the origin of the peculiar transition in the magnetically ordered phase of theWeyl semimetal $Co_3Sn_2S_2$, Physical Review B, DOI 10.1103/PhysRevB.106.L180403.

G. Pasquale, Z. Sun, K. Cernevics, R. Perea-Causin, F. Tagarelli, K. Watanabe, T. Taniguchi, E. Malic, O. V. Yazyev, A. Kis, Flat-band-induced many-body interactions and exciton complexes in a layered semiconductor, Nano Letters, DOI 10.1021/acs.nanolett.2c02965.

A. Crepaldi, M. Puppin, D. Gosalbez-Martinez, L. Moreschini, F. Cilento, H. Berger, O. V. Yazyev, M. Chergui, M. Grioni, Optically induced changes in the band structure of the Weyl charge-density-wave compound (TaSe4)2I, Journal of Physics-Materials, DOI 10.1088/2515-7639/ac9647.

Y. F. Guan, O. V. Yazyev, A. Kruchkov, Reentrant magic-angle phenomena in twisted bilayer graphene in integer magnetic fluxes, Physical Review B, DOI 10.1103/PhysRevB.106.L121115.

F. Alsallom, L. Herviou, O. V. Yazyev, M. Brzezinska, Fate of the non-Hermitian skin effect in many-body fermionic systems, Physical Review Research, DOI 10.1103/PhysRevResearch.4.033122.

F. Petocchi, C. W. Nicholson, B. Salzmann, D. Pasquier, O. V. Yazyev, C. Monney, P. Werner, Mott versus hybridization gap in the low-temperature phase of 1T-TaS_2, Physical Review Letters, DOI

10.1103/PhysRevLett.129.016402.
X. J. Weng, Q. S. Wu, X. Shao, O. V. Yazyev, X. L. He, X. Dong, H.-T. Wang, X.-F. Zhou, Y. Y. Tian, Phase transition of layer-stacked borophene under pressure, Physical Review B, DOI 10.1103/PhysRevB.105.235410.

Y. F. Guan, A. Bouhon, O. V. Yazyev, Landau levels of the Euler class topology, Physical Review Research, DOI 10.1103/PhysRevResearch.4.023188.

D. Pasquier, O. V. Yazyev, Ab initio theory of magnetism in two-dimensional 1T-TaS2, Physical Review B, DOI 10.1103/PhysRevB.105.L081106.

Heini Wernli, ETH Zurich

A. J. de Vries, F. Aemisegger, S. Pfahl, H. Wernli, Stable water isotope signals in tropical ice clouds in the West African monsoon simulated with a regional convection-permitting model, Atmospheric Chemistry and Physics, DOI 10.5194/acp-22-8863-2022.

I. Thurnherr, F. Aemisegger, Disentangling the impact of air–sea interaction and boundary layer cloud formation on stable water isotope signals in the warm sector of a Southern Ocean cyclone, Atmospheric Chemistry and Physics, DOI 10.5194/acp-22-10353-2022.

Gabriel Wlazłowski, Warsaw University of Technology

P. Magierski, G. Wlazłowski, A. Makowski, K. Kobuszewski, Spin-polarized vortices with reversed circulation, Physical Review A, DOI 10.1103/PhysRevA.106.033322.

P. Magierski, A. Makowski, M. C. Barton, K. Sekizawa, G. Wlazłowski, Pairing dynamics and solitonic excitations in collisions of medium-mass, identical nuclei, Physical Review C, DOI 10.1103/PhysRevC.105.064602.

K. Hossain, K. Kobuszewski, M. M. Forbes, P. Magierski, K. Sekizawa, G. Wlazłowski, Rotating quantum turbulence in the unitary Fermi gas, Physical Review A, DOI 10.1103/PhysRevA.105.013304.

Savvas Zafeiropoulos, Aix Marseille University

C. Egerer, C. Kallidonis, J. Karpie, N. Karthik, C. J. Monahan, W. Morris, K. Orginos, A. Radyushkin, E. Romero, R. S. Sufian, S. Zafeiropoulos (On behalf of the HadStruc Collaboration), Transversity parton distribution function of the nucleon using the pseudodistribution approach, Physical Review D, DOI 10.1103/PhysRevD.105.034507.

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Background

1997-2001	PhD in computational chemistry, LUC, Belgium
2001-2006	Postdoc, ETH Zurich
2006-2010	User and application specialist, CSCS
2010-2013	User Support Group Leader, CSCS
2013-2021	Associate Director and Head of User Engagement & Support, CSCS
2021-Present	Associate Director, Head of User Program & Roadmaps, CSCS

Specialisation

I oversee all national calls for proposals, I coordinate the peer review process to assess the scientific merit of project proposals, and I implement the distribution of computational and data resources. I am also responsible for the training program and for the communication with the entire user community, and I contribute to outreach activities of the Centre. In essence, I am responsible for the set-up and process of strategic roadmaps that shape the Center's future and innovation.

What working at CSCS means to me

I am part of a multi-ethnic workforce full of talented individuals who share their knowledge and know-how to solve difficult and challenging problems. It means we are at the forefront of science and technology and helping scientists to advance their impact on society.

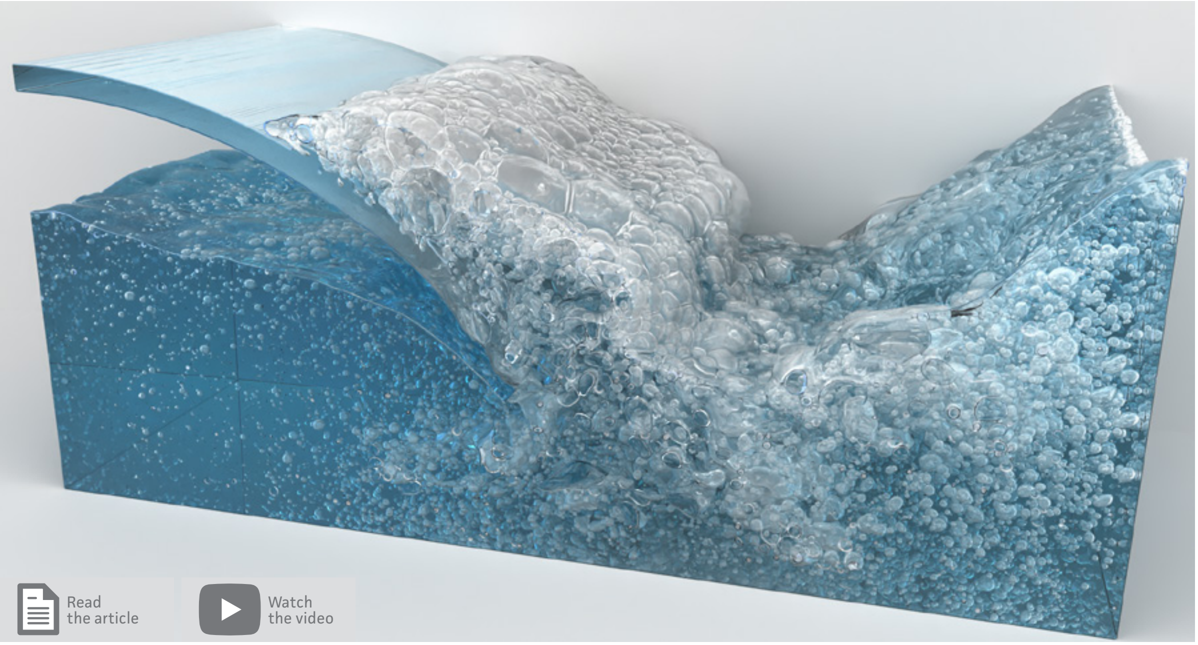
What I like most about my work

I like being able to help scientists achieve their goals, being part of an exciting world where something new is learned every day. Knowing that my contributions help to advance science and assist researchers in their endeavors to understand climate change, to improve health care, or to resolve the mysteries of deep space, is rewarding.

What challenges me at my work

New technology evolves rapidly, and our challenge is to keep scientists onboard, reach out to them, and help them to adapt their software and research workflows to new architectures and new programming paradigms. It is important to help them take full advantage of the infrastructure, and also to remain highly competitive worldwide by delivering outstanding science.

A new method cracks the simulation of foam formation



Scientists use CSCS's "Piz Daint" to simulate this foaming waterfall with many thousands of individual bubbles. (Image: CSElab, ETH Zurich)

Whether in the wake of a waterfall, on a cappuccino, or as an agent used in industry — foam is omnipresent. Simulating foam is a complex problem that has troubled researchers for years. Until now, only simulations of a few dozen flowing bubbles were feasible because of the high computational cost of larger, realistic representations. However, realistic simulations could greatly facilitate the production of emulsions and foams with desired properties — for example for foods and cosmetics.

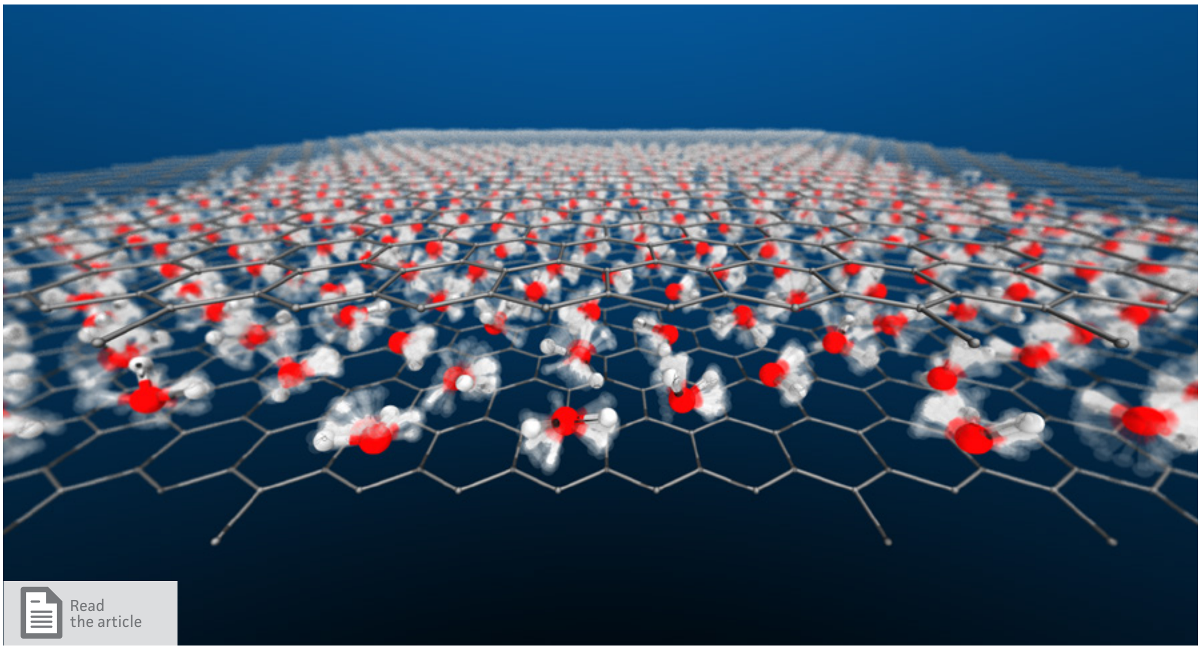
Now, a team led by Petros Koumoutsakos, a former professor at ETH Zurich and now at Harvard University, has developed a new, more efficient method to simulate foams. The researchers based their procedure on the volume-of-fluid (VOF) method, in which individual foam bubbles are represented on a grid. To prevent two bubbles in the same grid cell from being regarded as connected, individual volume fraction fields are used to calculate individual bubbles. The computational demand involved in this calculation is, however, proportional to the number of bubbles in the simulation — too high to represent realistic systems.

Koumoutsakos and his team found a solution to overcome this limitation: they succeeded in combining several volume fraction fields, and thus keeping the number of fields constant. Thus, the cost of a simulation no longer depends on the number of bubbles. In particular, the new method called Multi-VOF considers multiple layers of volume fraction fields and labels the bubbles with colours to distinguish them. Based on this idea of colour labels, the scientists developed an algorithm to identify sections of the same bubbles distributed across different grid cells. This way, the researchers reduced the complexity of the calculations.

Using this method on "Piz Daint", the researchers succeeded in simulating an unprecedented 20,000 interacting bubbles. They performed several simulations such as bubble formation in microfluidic devices, or a miniature waterfall, and validated them using experimental data. According to the researchers, the new Multi-VOF algorithm also captures complex processes such as the breakup of bubbles and can be used to realistically simulate a large variety of flows.

Reference
Karnakov et al. (2022): DOI: doi.org/10.1126/sciadv.abm0590

Researchers explore materials with new machine learning approach



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The "hexatic" (intermediate between a solid and a liquid) phase of water is simulated with almost fixed but rotating water molecules. (Image: Christoph Schran, University of Cambridge)

Be it for more efficient solar cells, tiny electronic components, or clean fuels: material scientists are constantly searching for promising chemical compounds. However, until now, accurate ab initio calculations of a materials' structures were only feasible for a small number of 100, rarely 1 000 atoms over experimental timescales. Now, Venkat Kapil, an Oppenheimer Research Fellow at University of Cambridge, UK, and his team have developed an approach that uses so-called machine learning potentials (MLPs) in combination with quantum-mechanical simulations to speed up computations. This way, they hope to realistically simulate tens of thousands of molecules.

One of the challenges in the process lies in simulating the stability of a material by calculating its 'free energy'. With their new approach, the researchers can rigorously including all physical effects in the simulations at a moderate computational cost. By doing so, they were able to reproduce the relative free energies for a variety of molecular crystals in agreement with experimental results. The development of such MLPs can be generalized across other crystal structures and will facilitate the search for thermodynamically stable materials of importance to industry, say the researchers.

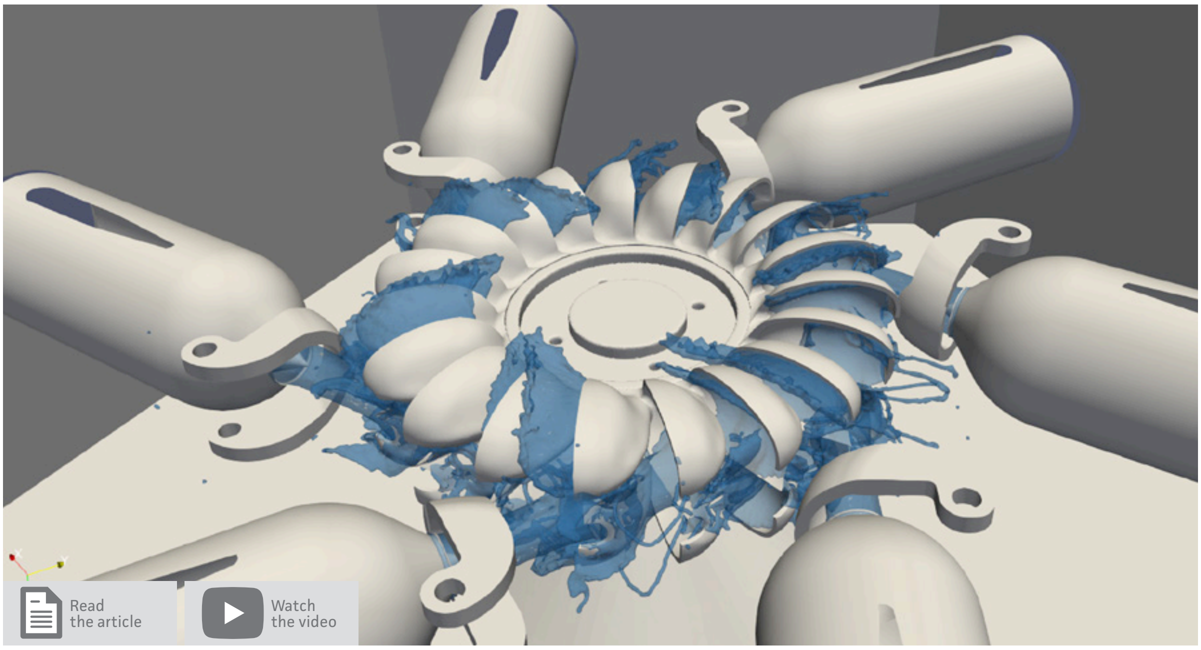
More recently, the team has even used this approach to predict the full phase diagram and properties of monolayer water confined in nanometre-sized graphene-like channels. Water, after all, is what makes life possible. Nonetheless, it is still not fully understood. The team applied MLPs to obtain a phase diagram of this monolayer water structure in a wide pressure and temperature range. According to the researchers, the phase diagram shows that monolayer water exhibits a surprisingly rich and diverse phase behaviour that depends on the temperature and van der Waals pressure in the nanochannel. Among other things, they found evidence of a hexatic phase that lies between a solid and a liquid, and a superionic phase with a high electrical conductivity. This conductivity should exceed that of batteries by up to a factor of 1,000. "The stability of superionic water at easily accessible conditions in confinement means that we can perhaps think of it as a technologically useful material in future," Kapil says.

Reference

Kapil et al. (2022): DOI: doi.org/10.1073/pnas.2111769119

Kapil et al. (2022): DOI: doi.org/10.1038/s41586-022-05036-x

Swiss Hydropower: from slow and steady to flexible and ready



A snapshot from the simulation of one of the six-jet Pelton turbines of the Gletsch-Oberwald power plant: Each of the six injectors feeds the buckets of the turbine runner with a high-velocity water jet. Since the forces are violent, there is a risk of mechanical stress if the turbine is operated under pressures and velocities for which it is not specifically designed. (Image: HES-SO Valais-Wallis Hydroelectricity Group)

Hydropower has long been Switzerland's traditional and priceless bonus in clean energy. But especially small and medium hydropower plants must now change: They need to better adapt to seasonal changes and, due to a new tariff system, meet the fluctuating needs of the market. "Such a flexible operation is not trivial, since it will impact the lifetime of the Pelton turbines used in most alpine hydropower plants," explains Cécile Münch-Alligné, a professor at the School of Engineering at HES-SO in Valais, Switzerland. With simulations run on "Piz Daint", her team recently investigated if and how run-of-the-river plants can indeed be operated flexibly.

The team based their simulations on the Gletsch-Oberwald facility in the Swiss canton Valais. It is powered by water from the Rhone river, which is guided through a pressure tunnel 300 metres down to two Pelton turbine units. The turbines' runner geometry is specifically designed for this given height difference and potential energy it holds, called "head" in technical terms. "If it changes, this can result in hydrodynamic instabilities that cause vibrations and fatigue on the components," says Münch-Alligné. Her goal was therefore to predict the influence of head variations on the torque of the runner.

The team's simulations combined two methodologies to represent the complex water flow in a Pelton turbine: on the one hand a single-phase flow inside the turbine's injectors, where no air is present and pressure is high, and on the other hand, the flow at the outlet of the injectors where the water contacts open air and undergoes a velocity boost. The results of the simulations investigating 12 different turbine operating conditions showed that the head can be lowered substantially — to a head value as low as 210 metres. A little lower, and the turbine's efficiency decreases in a sharp drop, while vibrations on the runner increase.

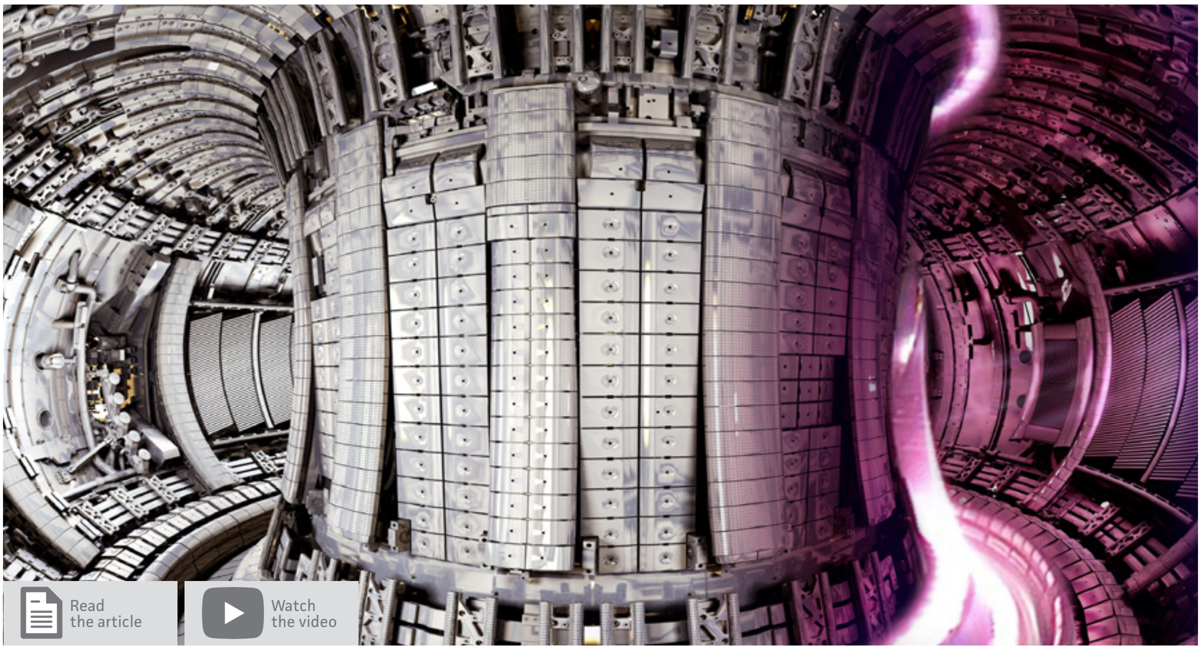
The results were confirmed by measurements in the Gletsch-Oberwald plant. According to the plant owners' estimates, the newly established flexible use when water levels are low will more than double the plant's energy production in winter.

Reference

Alimirzazadeh et al. (2021): DOI: doi.org/10.1088/1755-1315/774/1/012033

Münch-Alligné et al. (2021): DOI: doi.org/10.1088/1755-1315/774/1/012037

Explained: advances in nuclear fusion energy production



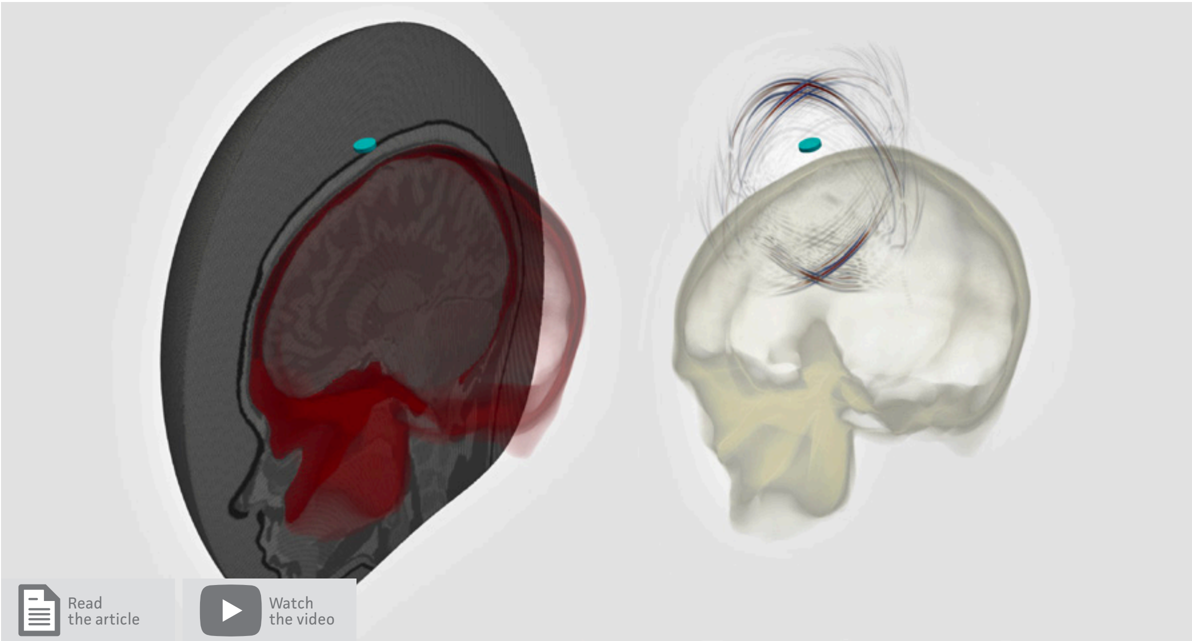
Jet in Oxfordshire, UK, is the largest existing nuclear fusion reactor of the tokamak type. The image shows the interior of the reactor with an illustration of the burning plasma blended in on the right. (Image: Wikimedia commons, EUROfusion)

In February 2022, fusion technology reached a new milestone: Researchers of the joint European undertaking EUROfusion generated 59 megajoules of energy from a 5-second-long plasma pulse using the Joint European Torus (JET) fusion experiment facility located in Oxfordshire, UK. This corresponds to the energy generated by burning 1.6 litres of oil, "which is impressive if you consider that the energy was created from a mere 0.1 milligrams of hydrogen and only released 0.1 milligrams of helium," says Laurent Villard, an adjoint professor at EPFL. He is investigating fusion plasma through simulations using the CSCS supercomputer "Piz Daint".

Among other things, his team studies the physics of future experiments in ITER, the large research fusion reactor being built in southern France, where the plasma will have a 10-fold larger volume than in JET. In particular, the scientists study the effect of the high-energy helium created by the fusion reaction. "Their energy is, in fact, what makes the fusion reaction self-sustaining, but such fast-traveling helium ions can also trigger unwanted instabilities in the plasma," says Villard. His team has recently developed a new functionality in their ORB5 code that allows them work towards understanding this balance, such as, how these fast helium ions are driven, and how they are damped. Also, the team newly implemented the modelling of microwave heating in their code. "We need to understand how plasma particles react to such an energy feed and how best to use microwaves to regulate the plasma."

In addition, the research projects conducted by Paolo Ricci, an associate professor at EPFL are focused on the outer rim of the plasma and the interaction with the reactor wall. Recently, his team performed a large set of simulations on "Piz Daint" to test the effect of factors like input power, size of the device, plasma volume or plasma density on plasma-wall interactions, and plasma turbulence. From the results, the scientists were able to derive the equation to calculate the maximum achievable plasma density for a certain reactor configuration, meaning the maximum density before plasma turbulence becomes too potent to allow for a confined plasma. "Going towards ITER, we have to prepare and learn about such properties and limits," says Ricci.

Seismologist images the brain with ultrasound waves



This simulation shows (left) a hexahedral finite-element mesh of the skull and brain and (right) a snapshot of the resulting ultrasound simulation. (Image: ETH Zurich/research group Andreas Fichtner)

Seismologists are wave specialists: They map the Earth's interior by recording the propagation of waves through matter. From these data, they can draw conclusions about the materials' composition and properties. Incidentally, the same applies to ultrasound waves used in medical imaging. That's what has led Andreas Fichtner, head of the Seismology and Wave Physics Group at ETH Zurich, to also study medical ultrasound.

In a first project, Fichtner's group developed ultrasound methods for the early detection of breast cancer. More recently, the team is investigating the brain. Their aim: to create a method to one day enable doctors to monitor stroke patients or identify brain tumours. So far, however, ultrasound imaging through hard structures like the skull has been difficult because bone reflects and dampens most of the incoming waves.

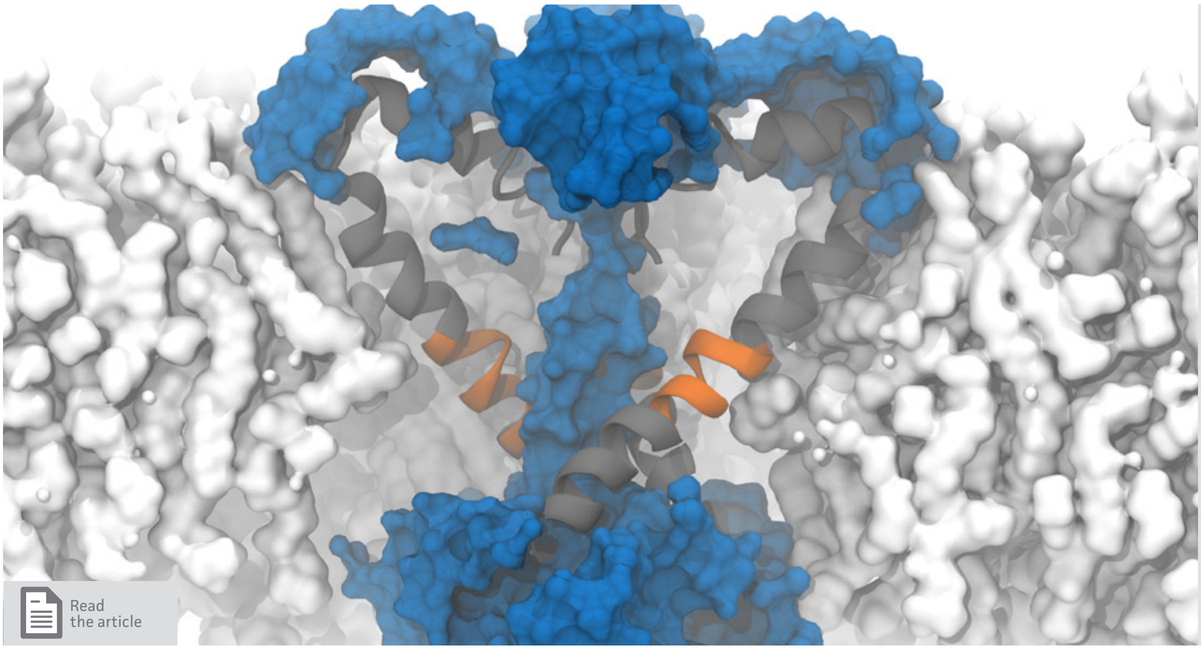
To overcome these challenges, the team is currently simulating the propagation of ultrasound waves through the brain on the "Piz Daint" supercomputer by developing algorithms that perform these calculations over complex grids known as meshes. They employ a software package named Salvus that was originally developed for seismic simulations and uses a method particularly well suited for high-contrast materials—like brain tissue and bone. Also, while conventional ultrasound only uses the arrival time of the waves, this new method exploits the shape, frequency, velocity, and amplitude of waves, and can therefore produce medical images that offer doctors more detailed information for patient diagnoses.

To create their model, the researchers use an MRI scan as a reference and then adjust the parameters used in the ultrasound calculations until the simulated image matches the MRI. The result is a quantitative reconstruction instead of the less informative greyscale image from conventional ultrasound. This makes it possible to distinguish between different tissue types—like healthy brain from tumour tissue.

One of the remaining challenges is the complex geometry of the skull with eye, nose, and jaw cavities. To address this, the team is working to create individual numerical meshes that are made up of deformed cubes (hexahedra) for arbitrary skull shapes, thereby accelerating the calculations by 100 to 1000-fold. And: The same methods may be transferable to other body parts like knees or elbows—a promising basis for developing a corresponding ultrasound device.

Reference
Marty et al. (2022): DOI: doi.org/10.1117/12.2611548

HPC simulations predict a mysterious biological process of the cell



This simulation shows the open-state model of a sodium channel (grey ribbon) in its membrane environment (white surface). A π-helical defect in the helices lining the pore (orange) promotes pore hydration (water depicted as cyan surface) and ion conduction across the membrane.
(Image: Lucie Delemotte)

Our dreaming, or the movement of our muscles are dependent on signals being transmitted to muscle or nerve cells via ion transfer through channels in the cells' membrane. "If the function of these ion channels is impaired by genetic mutations, this can lead to diseases such as epilepsy or muscular paralyses," says Lucie Delemotte, an associate professor at the KTH Royal Institute of Technology in Stockholm, Sweden. Her research is focused on understanding the function of these ion channels to help treat such diseases better in the future.

One of the questions her group addressed is the mechanism of how these ion channels open their pores, which was not fully understood. Clear was, however, that ions can only pass through the channels' pores if these are hydrated. To investigate the opening mechanism and the role of water molecules in more detail, the team performed molecular dynamics simulations on "Piz Daint".

Their subject was a bacterial ion channel with a supposedly open structure as described in experiments. To the surprise of the researchers, however, the simulation revealed the pores to be closed for ion passage. Fortunately, a special circumstance helped the researchers to understand the appearance of the channel being permeable: to speed up the simulation, the team increased the membrane potential five to ten times higher than what is found in reality or possible in experiments. Due to this unusually high voltage field, they caught a conformational change in the ion channel pore. In the simulation, the researchers were able to observe a kink spontaneously forming in a certain protein α-helix of the pore's structure, which led to the formation of another structure known as a π-helix.

Following this observation, Delemotte's team designed a dedicated "π-model", with which they showed that a specific rotation of this π-helix leads to a spontaneous hydration of the pore, and ultimately enables its opening as well as stable ion exchange. The researchers also hypothesised that such an opening model could apply to eukaryotic channels as well. Indeed, just recently, experimental researchers reported a transformation from a α-helix to a π-helix in a human channel.

Reference
Choudhury et al. (2021): DOI: doi.org/10.1016/j.bpj.2021.12.010

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Background

2001-2008	Diplom-Ingenieur, Luft- und Raumfahrttechnik con Universität Stuttgart, Germany
2008-2011	PhD, Dynamique de fluides, at Institut National Polytechnique de Toulouse, France
2011-2012	Post-Doctoral fellow at CERFACS, France

2017-2022 Computational Scientist, CSCS
2022-Present HPC Application Engineer & Service Manager, CSCS

Specialisation

I am currently responsible for the HPC platform service offered to the users of CSCS. This role involves ensuring that the underlying internal services comprising the current platform "Piz Daint" are working as intended and are being properly supported. This means I facilitate communication in my everyday work. In the case of an intervention becoming necessary on the system, for instance, I assist in organizing the work internally so that it causes as little impact to the users as possible. I also centralize the monitoring of the platform, ensuring the desired level of quality. The data is collected through tools observing the system's state directly, but also through more indirect means, e.g., the service requests submitted by users. Finally, a service offered to users like this HPC platform, naturally, is subject to continuous development in order to adapt to changing requirements, be it the users' workflows or from a system perspective. The latter is particularly true today with the next generation production system "Alps" arriving at CSCS.

What working at CSCS means to me

Working at CSCS is exciting due to it being a national supercomputing centre, which gives me the opportunity to work on technology not available in many other places. Moreover, contributing to the centre's efforts of providing reliable systems is important to me, because this is what enables our users in Switzerland and abroad to advance with their work.

What I like most about my work

As a service manager, I have to keep a more system-wide view of the solutions that are delivered to our users. I find it interesting to plan and implement a system at a level that others rely on for their daily work. In addition, I like the working environment. Being part of teams with members from different disciplines and different cultural backgrounds is always interesting; and, when it comes to tackling a problem, I have the impression that a wider solution space is considered in such groups.

What challenges me at my work

For the use cases that are run on our systems, there is usually no one-size-fits-all solution. Accommodating the different user needs within a single platform can be difficult at times and makes for an interesting challenge. Also, being inside a research environment, it is not always easy to find the balance between a stable, established system and moving to the next new technology.

At CSCS, energy efficiency is a key priority, even at high performance

The term "high-performance computer" already implies a high energy demand. Energy efficiency is therefore a central consideration in the procurement and use of supercomputers at the Swiss National Supercomputing Centre (CSCS) — just as it was during the planning of the new building in Lugano more than a decade ago.

The five-storey office block has been built to meet the Minergie Eco standard and offers a total surface area of 2600 square metres (Image: CSCS)

CSCS develops and operates a high-performance computing (HPC) and data research infrastructure that supports world-class science in Switzerland, including research at CERN and the Paul Scherrer Institute (PSI). High-performance computers and the simulations performed on them are indispensable for research where theory reaches its limits or experiments are impossible. Neither the universe nor the climate, for example, can be reproduced and observed in the laboratory. Simulations also support experimental researchers in the search for new, stable material compounds that are used, for example, in efficient solar cells, electronic components, or medicines; simulations now even make it possible to predict biological processes that were only seen afterwards in experiments.

High energy efficiency in computer design

In 2012, CSCS procured the high-performance computer "Piz Daint", one of the world's most energy-efficient computers in the petaflop performance class (a computer that can perform a quadrillion computing operations per second) at the time. A collaborative initiative in which CSCS worked closely with hardware manufacturers, software developers, mathematicians, and scientists made this achievement possible. CSCS has since launched the Platform for Advanced Scientific Computing (PASC) as part of the High Performance Computing and Networking (HPCN) strategy adopted by the ETH Board. On one hand, this involves working with hardware manufacturers to select energy-efficient hardware, such as graphics processing units (GPU), and thus build modern, energy-efficient computer architectures. On the other hand, PASC supports the optimisation of codes and algorithms in the software used by the researchers within these modern computer architectures, so research is carried out more efficiently and goals are reached faster than on conventional supercomputers — saving not only time, but also energy.

The latest computer technologies continue to improve in this regard. Take "Piz Daint" for example, which has been upgraded several times with more efficient processor generations: Since the Green500 list of the world's most energy-efficient computers was introduced in 2013, the supercomputer has been in the top 10 a total of five times. In November 2016, it was even listed in second place among the world's most energy-efficient computers. With "Alps", which is scheduled to go into operation in 2023, CSCS will again increase the energy efficiency relative to the computing power many times over, thanks to new technologies. Already today, there are systems similar to "Alps" that are able to perform up to five times more computing operations per watt than previous technologies. "Alps" is thus expected to put CSCS once again in a top position worldwide in energy efficiency in supercomputing.

Carbon-neutral electricity

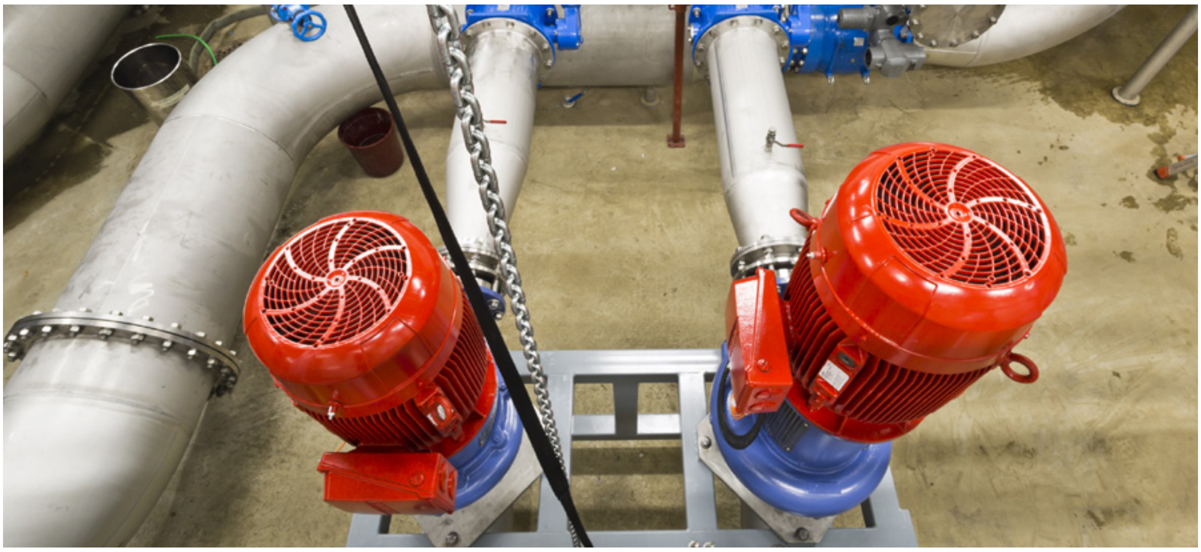
CSCS sources 100 percent of its electricity from hydropower and is carbon neutral. Furthermore, the energy consumption of the entire Centre in 2021 was around 37 gigawatt hours with an average output of around 4 megawatts. By way of comparison, the CERN and PSI research facilities have electricity requirements of 1300 gigawatt hours and 126 gigawatt hours respectively, according to recent media reports.

In addition to "Piz Daint", CSCS also operates the MeteoSwiss computer and other systems on behalf of partners and houses the ETH Euler computer and the Blue Brain computer. These partner systems account for approximately 35 percent of the total energy demand of the Centre. In addition, CSCS also provides computing capacity on "Piz Daint" — and eventually on "Alps" — to the MARVEL materials research network, the University of Zurich, and the PSI.

High efficiency starts with infrastructure

Careful planning made CSCS one of the world's most energy-efficient data centres in the world when in it opened in August 2012, and it remains so today with a PUE (Power Usage Effectivness) rating below 1.2. The PUE value indicates how effectively the supplied energy is consumed in a data centre. The closer the value approaches to 1.0, the more energy-efficient the data centre.

The new supercomputing infrastructure "Alps" is expected to be in a top position worldwide with respect to energy efficiency. (Image: CSCS)



Powered by the water circuit as it flows back toward Lake Lugano, these two micro-turbines in the pumping station produce an extra 200 megawatt hours of energy per year. (Image: CSCS)

Even ten years after the new building was completed in Lugano, additional new data centre buildings still aim for "only" a PUE below 1.2. This is also the case for ETH Zurich's plans for a data centre on the Hönggerberg campus (more on this soon).

The CSCS data centre especially owes its energy efficiency to its sophisticated and innovative cooling system that uses lake water from Lake Lugano. The cooling infrastructure is designed to cool high-performance computers with an output of up to 14 megawatts — research infrastructures such as "Piz Daint" or its successor "Alps" — in a so-called first cooling circuit. This cooling circuit is also used to cool the Minergie-certified CSCS office building in summer.

After the first cooling cycle, the relatively heated water in the second circuit is still able to cool computers with a total output of up to 7 megawatts. The second circuit cools, among other things, the air of housings — known as cooling islands — in which these smaller systems and data storage devices are housed.

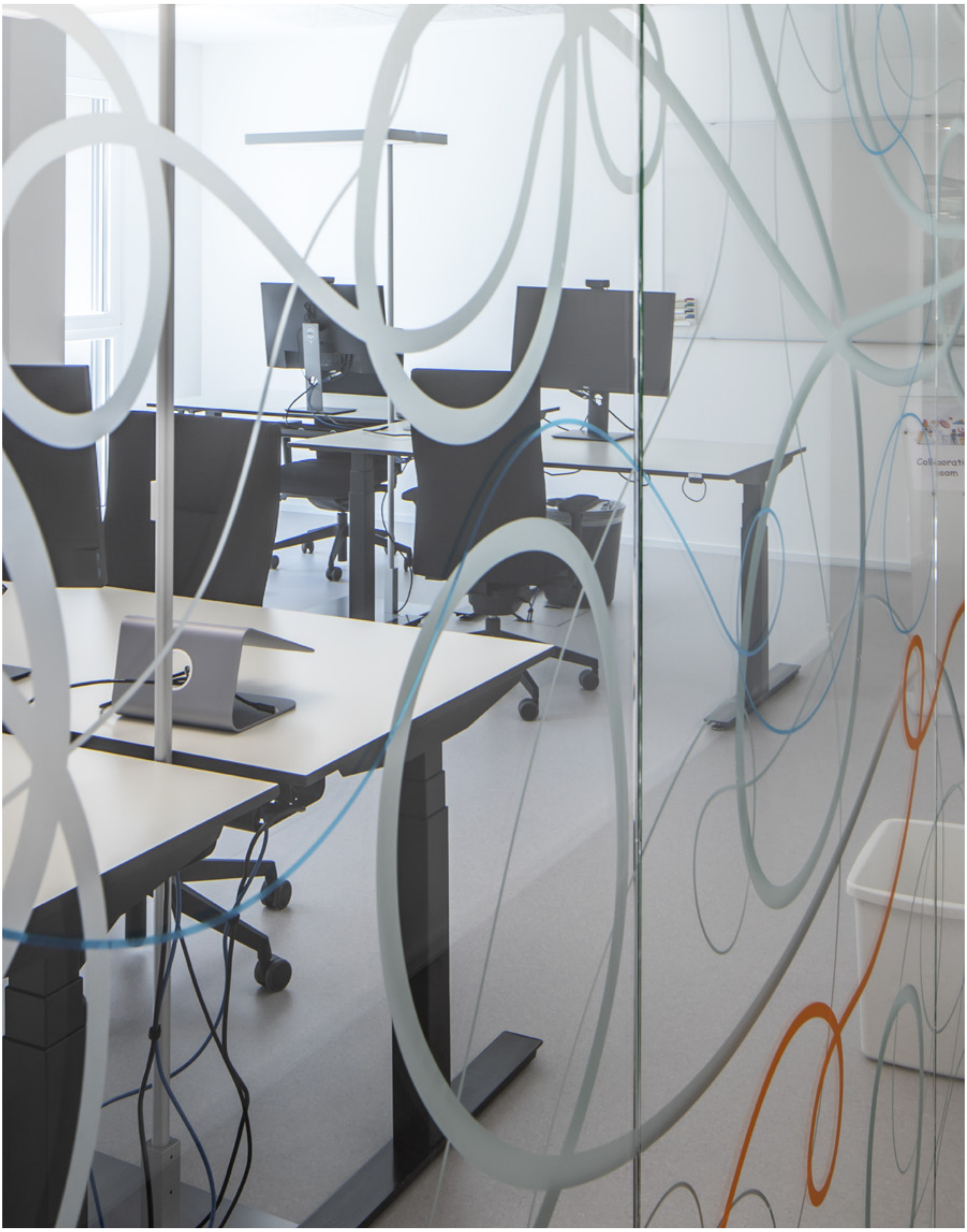
The CSCS building is also heated with the waste heat from the return of the second cooling circuit together with a heat pump. The heating flow is thus low at 30 degrees Celsius. Thanks to this carefully designed system, one and the same infrastructure is used in the office building for heating in winter and cooling in summer.

Energy synergy

In order to reduce the energy demand as much as possible and to reuse energy where possible, CSCS has taken even further innovative measures in recent years: Before the water circuit enters the lake again, it drives two micro-turbines to produce even more electricity. At 200 megawatt hours per year, the electricity generated by the turbine covers more than 30 percent of the energy needs of the pumping station itself, which pumps the water over a distance of 2.8 kilometres and 30 metres uphill to the data centre.

Additionally, the waste heat from the computers is not only used to heat the CSCS office building. Together with the Ticino electricity supplier AIL (Aziende Industriali Lugano), CSCS built an infrastructure that supplies heat to the city of Lugano as well as the new campus of the Università della Svizzera italiana with the SUPSI University of Applied Sciences — the campus requires around 742 megawatt hours of thermal energy per year to heat the buildings. AIL is also currently building a thermal power plant that will make it possible to produce a further six megawatts of heat with the waste heat from CSCS. The heat output can eventually be increased to up to 30 megawatts when combined with heat pumps.

All in all, the operation of CSCS's high-performance computers is embedded within a well thought-out and sustainable energy strategy.



Name
Angela Schneebeli

Nationality
Swiss

Position
Communications Officer

Working at CSCS since
September 2012

Background

2004-2008	Bachelor's in Public Relations and Advertising, Università IULM, Italy
2008-2011	Master's of Science in Communication and Economics, Corporate Communication and Corporate Social Responsibility, Università della Svizzera italiana, Lugano
2011-2012	Brand management trainee, The North Face, VF Corporation, Lugano
2012-Present	Communications Officer, CSCS

Specialisation

I develop and implement communications for internal and external audiences, including staff, partners, stakeholders, and media. I am responsible for all the content to promote CSCS's brand image, activities, and products. I mainly act as a liaison between CSCS, the employees, the public, and the media to ensure that the brand remains top-of-mind. My activities range from managing the website and social media channels to the internal newsletter, publications, and working on employer branding activities to ameliorate the perception of CSCS as an employer.

What working at CSCS means to me

Working at CSCS means working in an academic, international, and constantly developing environment. It means being able to be in contact with different realities and continually updating myself to keep up with the multiple changes. It also means being proud to work for a national organization that stands at the front of science and technology and helps to make great strides in scientific research and our society.

What I like most about my work

What I like most is that I deal with communication at 360 degrees. I'm not specialized in anything specific, and I do not have to work only on one side of the communication; but I can work on all internal and external communication activities. This has broadened my knowledge and skill set. I like that I learn something new daily and that CSCS allows me to take courses and training that expand my knowledge.

What challenges me at my work

The communications industry changes year after year, especially as communications technology and platforms continue to evolve. Work, for example, is now predominantly remote and digital, and we are losing the in-person part. This means that, now more than ever, we have to put a greater emphasis on effective communication. However, establishing optimized communication procedures tailored to everyone's needs is not easy. It requires a great deal of effort and some creativity. In addition, CSCS has grown a lot in recent years, and along with it the number of activities and events related to communication. It is often challenging to do everything consistently and sustainably, which raises the importance of standards and clear processes.

Finances

Expenditures in CHF

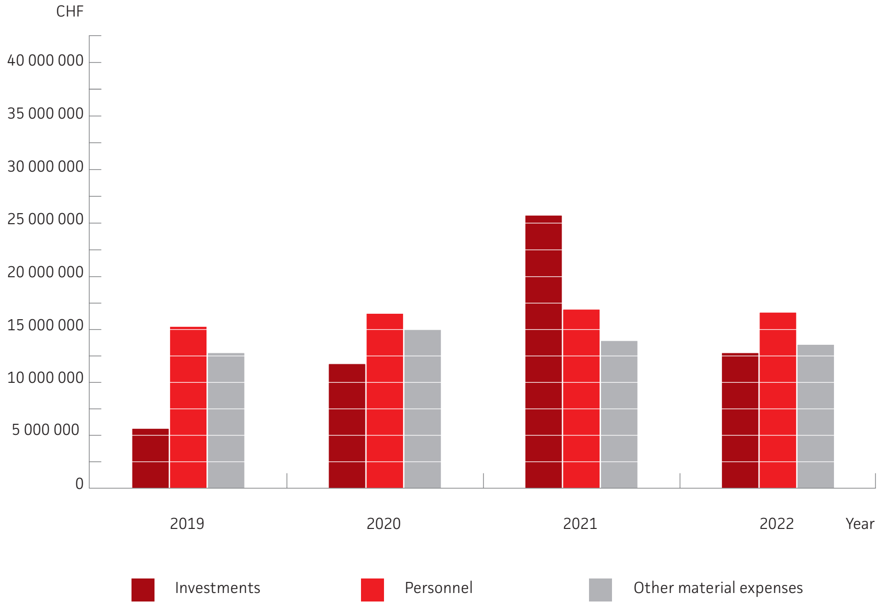
	User Lab	Third Party	Total
HPCN-24 Investments	**11 188 996.23**	**0.00**	**11 188 996.23**
New System	10 095 375.82		10 095 375.82
Data Center	381 544.51		381 544.51
Secondary Installation	712 075.90		712 075.90
IT Investments	**99 361.05**	**1 354 756.40**	**1 454 117.45**
Personnel	**11 423 385.29**	**5 039 556.40**	**16 462 941.69**
Payroll	11 246 522.65	5 039 556.40	16 286 079.05
Further education, Recruitment	176 862.64		176 862.64
Material expenses	**10 339 270.87**	**3 119 365.62**	**13 458 636.49**
Maintenance building & technical infrastructure	538 910.79	59 000.00	597 910.79
Energy	3 162 323.35	955 987.95	4 118 311.30
Maintenance hardware, Licenses, IT services & Telecommunication	4 293 079.46	369 182.16	4 662 261.62
Remunerations, Marketing, Workshops, Services, Travel, Membership fees	1 410 490.92	544 651.51	1 955 142.43
Granting of funds for PASC projects	934 466.35		934 466.35
Granting of funds for EuroHPC LUMI		1 190 544.00	1 190 544.00
Total expenditures	**33 051 013.44**	**9 513 678.42**	**42 564691.86**

Income in CHF

	User Lab	Third Party	Total
Contribution ETH Zurich	21 770 014.00		21 770 014.00
Contribution ETH Rat - HPCN investments	20 100 000.00		20 100 000.00
Contribution ETH Rat - PASC initiative	3 270 985.00		3 270 985.00
Contribution SERI - EuroHPC LUMI		1 190 544.00	1 190 544.00
Research collaboration projects		3 029 993.09	3 029 993.09
Services for paying customers		8 258 409.23	8 258 409.23
Other income		328 951.19	328 951.19
Total income	**45 140 999.00**	**12 807 897.51**	**57 948 896.51**

User Lab Expenses Development in CHF

	2019	2020	2021	2023
Investments	5 507 317	11 647 611	25 642 089	12 643 114
Personnel	15 158 424	16 398 117	16 735 133	16 462 942
Other material expenses	12 660 330	14 927 812	13 779 635	13 458 636



Name
Stefano Schuppli

Nationality
Swiss

Position
Unit Head Engineer & Senior Architect

Working at CSCS since
June 2017

Background

2003-2007	Diploma as software developer, Swisscom AG
2003-2008	Founder and software engineer, WebTi.ch
2008-2010	BSc in computer science (incomplete due to overseas work assignment), SUPSI

2008-2017	IT support engineer, system administrator, automation engineer, manager of IT service delivery, and head of desktop services, B-Source SA, then Avaloq ASSL AG, Switzerland, Singapore, and Hong Kong
2015-2019	BSc in computing and information systems, Goldsmiths University, UK
2017-2022	IT support and software development, CSCS
2020	MSc in data science, Goldsmiths University, UK
2022-Present	Unit Head Engineer & Senior Architect, CSCS

Specialisation

Unit heads at CSCS cover multiple roles in their respective field of competence: As line managers, we support, coach, and develop a group of engineers; as senior architects, we contribute to the evolution of the Centre's HPC architecture; and as part of the leadership team, we share the responsibility for the success of the Centre. My field covers a broad spectrum within the area of microservices development and infrastructural services, including those meant to support machine learning workloads on our systems.

What working at CSCS means to me

It means being part of a future-oriented organization that supports innovation and scientific discovery at national and international levels, thus contributing to the public interest. This makes it easy to find purpose and motivation in what we do.

What I like most about my work

CSCS provides amazing opportunities to work on meaningful projects, often with fresh technological advancements alongside brilliant people in exciting collaborations. We get to deepen our skills in the process and I find pleasure in the constant learning and updates required for the job, as well as the exposure we have to the latest innovations. More importantly, I feel fortunate to work with and support incredibly smart colleagues to which I look up to everyday.

What challenges me at my work

It is an exciting challenge to explore fields that might not yet be mature, where it might still be difficult to identify established practices and products.

Name
Mikael Simberg

Nationality
Finnish

Position
Software Engineer

Working at CSCS since
September 2017

Background

2010-2015	Master's degree in Operations Research, Aalto University, Finland
2015-2017	Software Engineer at SwissLitho AG, Zurich
2017-Present	Software Engineer, CSCS

Specialisation

I'm focused on various aspects of concurrency and parallelism in C++. I'm responsible for maintaining and developing a task-based runtime for use in projects at CSCS. A large part of my work involves helping and educating users to allow them to get the best performance out of their applications.

What working at CSCS means to me

I get to help science and scientists move their work forward in understanding the world. Despite my own work only occasionally being in direct contact with scientists, it motivates me to know that it is contributing to something useful for all of society.

What I like most about my work

The most valuable thing about working at CSCS is the people, who are kind, patient, and from whom I always find something new to learn. At the same time, it motivates me every day to know that I'm working on technologies that are at the leading edge of progress, and occasionally we get to push that edge a bit forward as well.

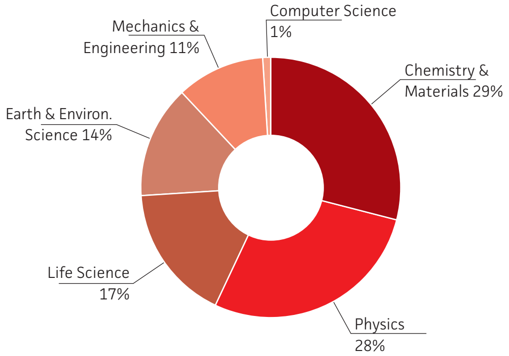
What challenges me at my work

Every day brings new technical challenges, whether it's a high-level API design that needs to fit a user's wishes or a concurrency bug deep in a runtime. This forces me to think and rethink about how I approach problems, to learn new techniques, and constantly push myself forward.

Usage Statistics

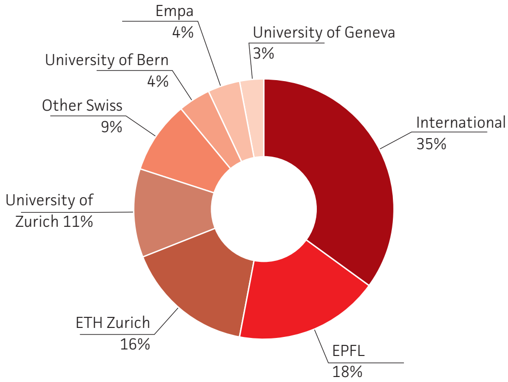
User Lab Usage by Research Field

Research Field	Node h	%
Chemistry & Materials	12 746 893	29
Physics	12 458 975	28
Life Science	7 358 629	17
Earth & Environmental Science	6 273 935	14
Mechanics & Engineering	4 886 911	11
Computer Science	683 728	2
Total Usage	**44 409 071**	**100**



User Lab Usage by Institution

Institution	Node h	%
International	15 462 301	35
EPFL	7 966 851	18
ETH Zurich	7 083 010	16
University of Zurich	5 030 735	11
Other Swiss	3 946 368	9
University of Bern	1 962 797	4
Empa	1 636 941	4
University of Geneva	1 320 068	3
Total Usage	**44 409 071**	**100**



Compute Infrastructure

Computing Systems Overview

Name	Model	Installation / Upgrades	User	TFlops
Piz Daint	Cray XC50 / Cray XC40	2012 / 13 / 16 / 17	User Lab, CHIPP	27 154 + 2 193
Tsa / Arolla	Cray CS-Storm 500	2020	MeteoSwiss	1 169
Alps	HPE Cray EX	2020	User Lab, Research & Development, UZH, CHIPP	4 719

Computing Systems Specifications

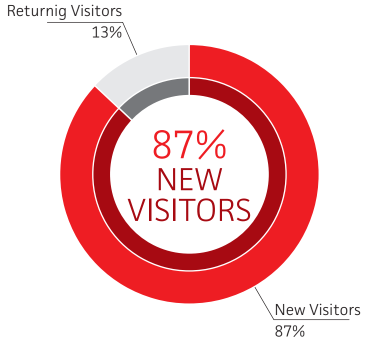
Name	Interconnect Type	CPU Type	Cores	Sockets	GPUs	Nodes
Piz Daint	Cray Aries	Intel Xeon E5-2690 v3/Nvidia Tesla P100	12	1	1	5 704
		Intel Xeon E5-2695 v4	18	2		1 813
Tsa / Arolla	100 Gb Ethernet	Intel Xeon Skylake 6143 Nvidia Tesla V100	8	2	8	18
		Intel Xeon Skylake 6148	20	2	0	20
Alps	HPE Cray Slingshot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

Communications Statistics

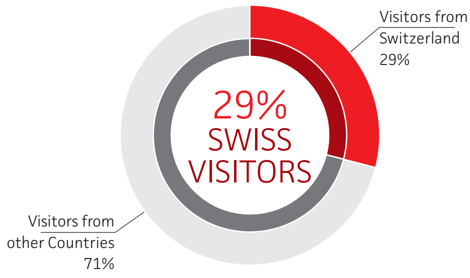
Website cscs.ch

	2021	2022
Total Website Visitors	79 907	73 215
Average Website Visits (Minutes)	2:52	1:92

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

Instagram

2021 creation of the CSCS page

	2021	2022
Followers	158	209

Twitter

	2021	2022
Followers	2 025	2 166

LinkedIn

	2021	2022
Followers	9 496	10 125

YouTube

	2021	2022
Watch Time (Minutes)	469 866	354 180
Average View Duration (Minutes)	4:46	3:32
Number of Views	98 400	89 800

Facebook

	2021	2022
Followers	259	265

CSCS in the News

	2021	2022
News Websites	232	133
Print	75	77
Radio & TV	9	8

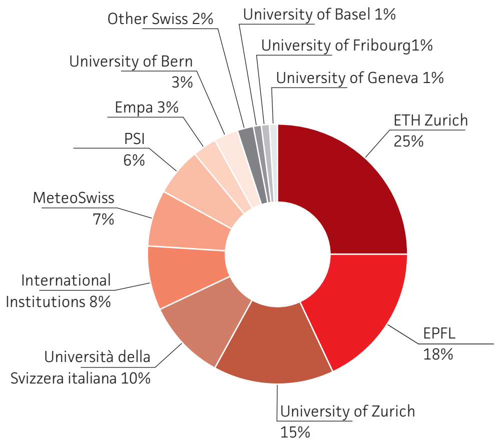
Word Cloud of News Related to CSCS

User Satisfaction

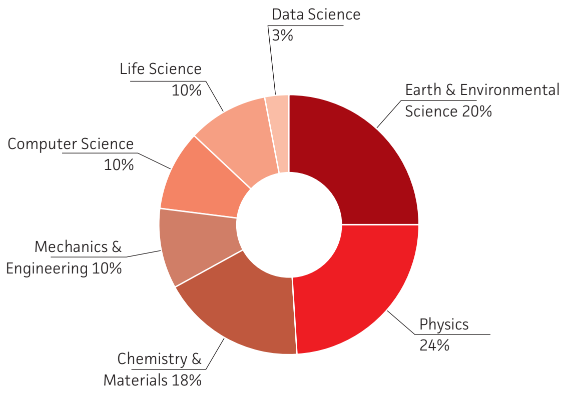
A user satisfaction survey was submitted to 2 441 users in January 2023. The response rate was 14.7% (360 answers).

User Profile

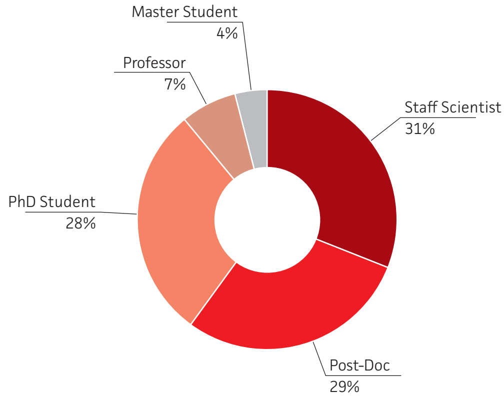
Your institution



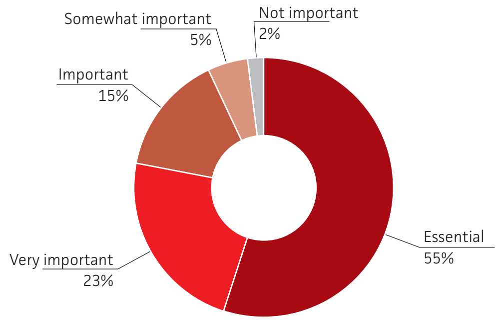
Your scientific field



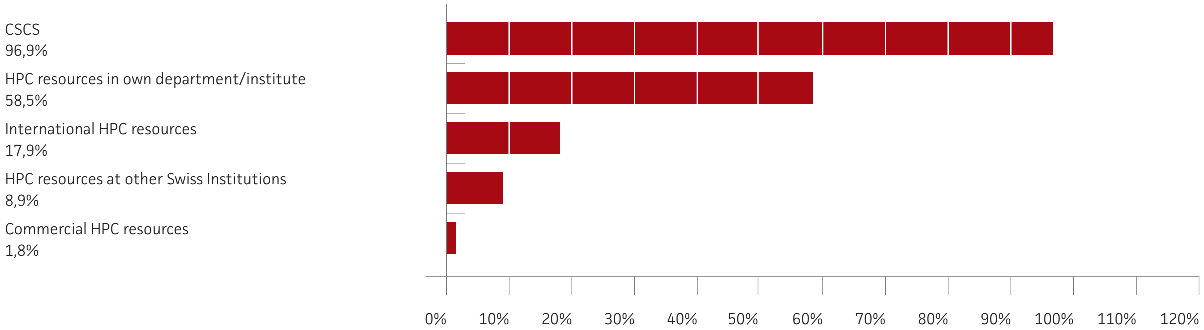
Your position



For my reserach, CSCS resources are



Which HPC resources are you using?



User Support

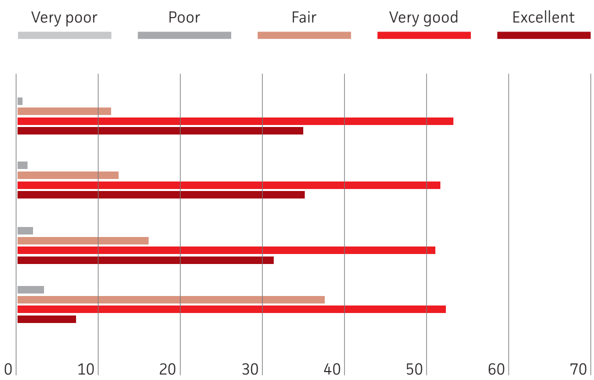
How do you rate the quality of...

Helpdesk support

System support

Application support

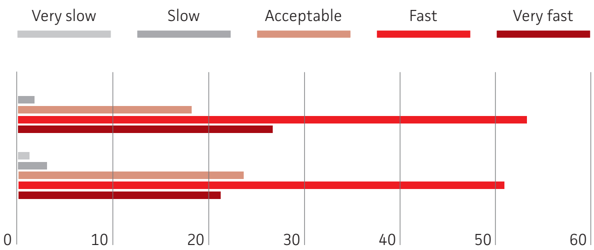
The offer of training courses and user events



How fast does support handle your request?

The reaction time of the helpdesk is

The time to solution for the support requests is



Service Availability, Stability and Usability

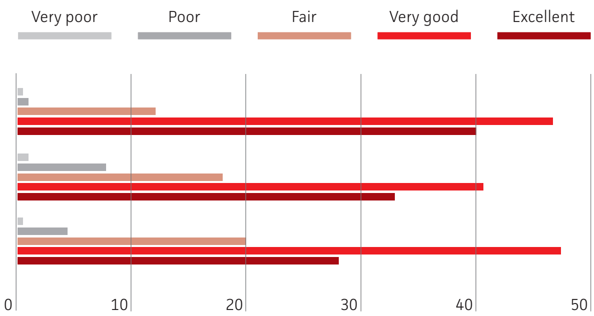
60

How you perceive...

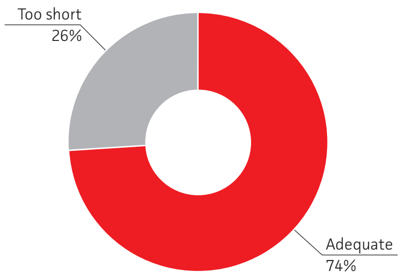
The availability of CSCS services?

The stability of CSCS services?

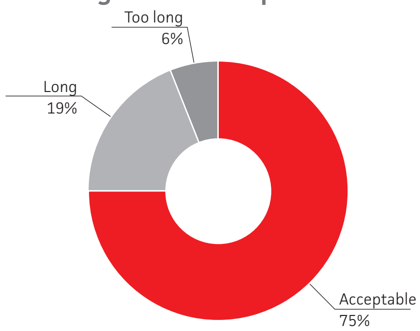
The ease of use of CSCS services?



The run time limits for batch jobs are

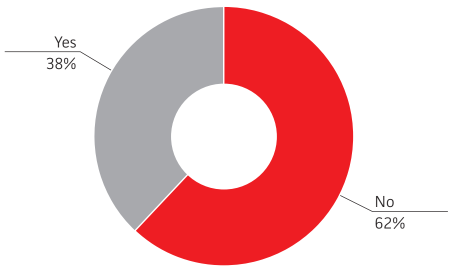


The job waiting time in the queue is

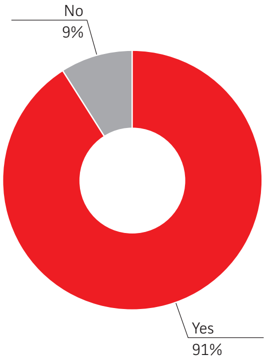


Project Proposal Process

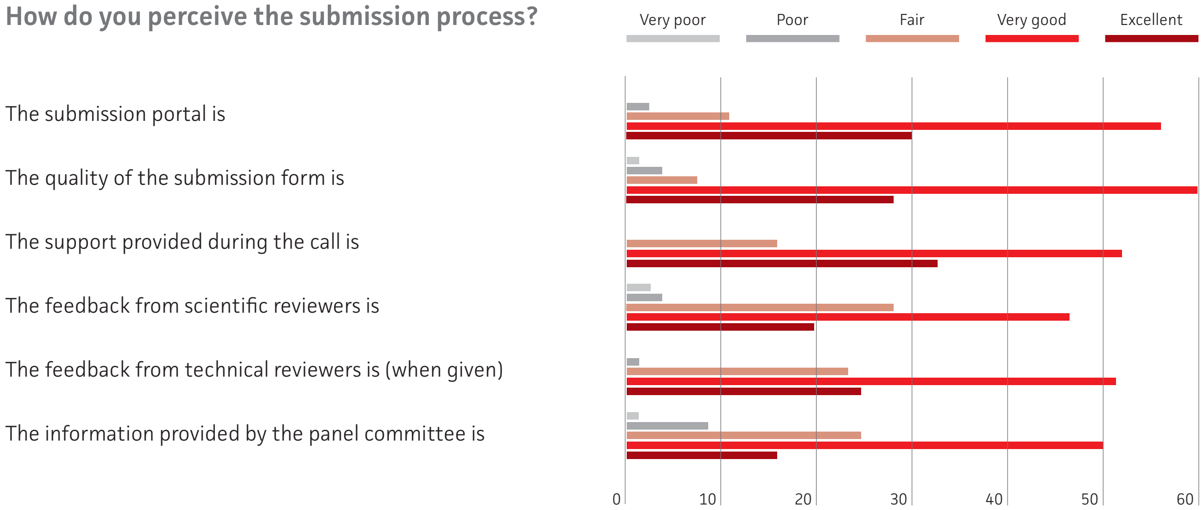
Have you been submitting project proposals to CSCS (as PI or supporting the PI?)



Is the reviewing process transparent?

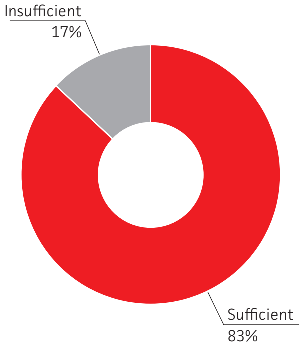


How do you perceive the submission process?

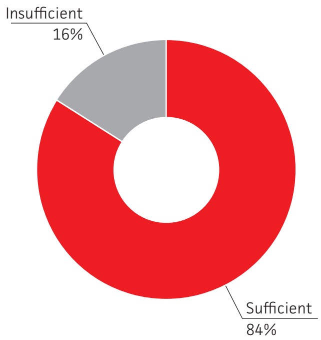


Adequacy of Allocated Resources

The resources assigned to my project are

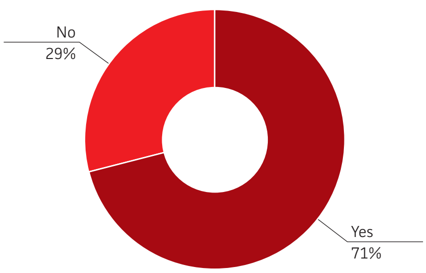


My storage allocation on “project” is

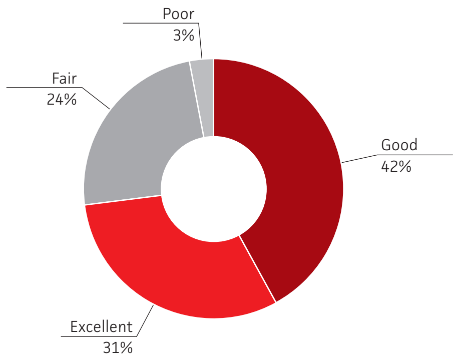


Application Development

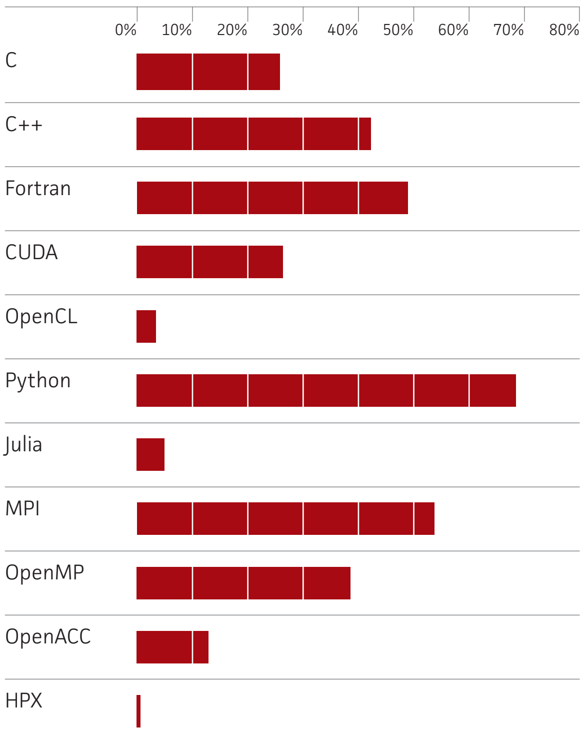
Do you develop and maintain application codes?



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

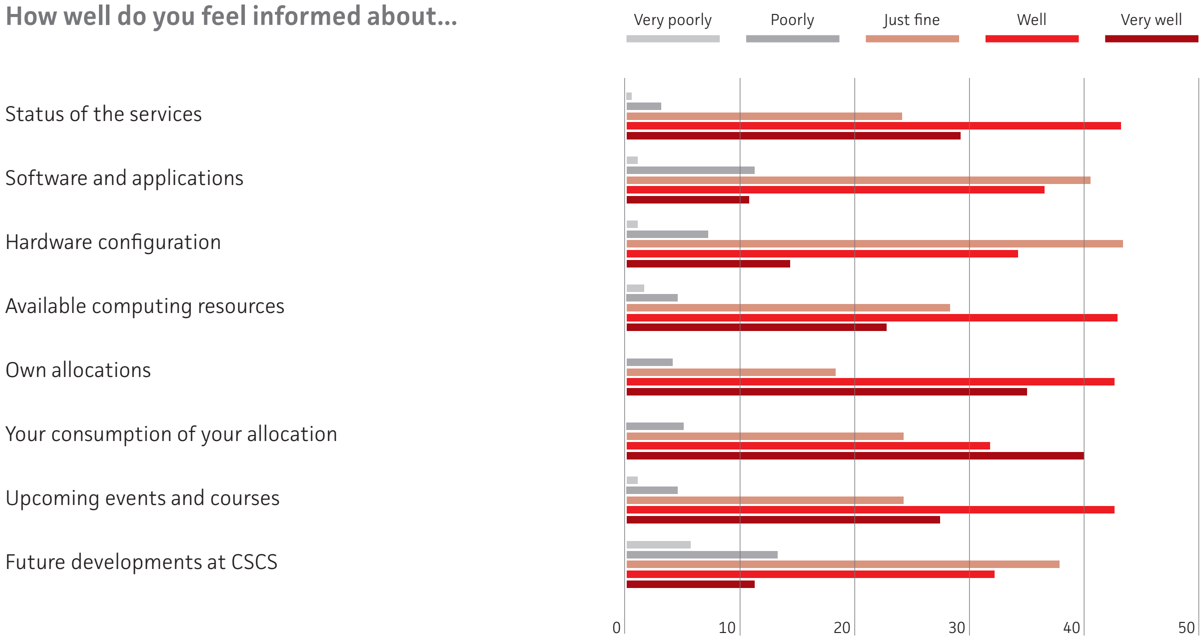


Which programming languages and parallelization paradigms are you using primarily?



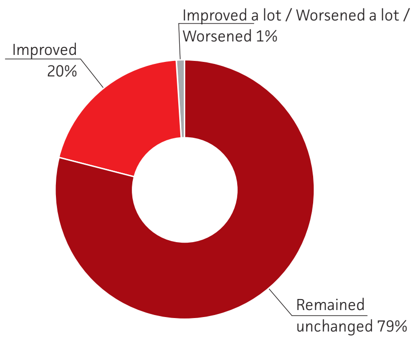
Information & Communication

How well do you feel informed about...

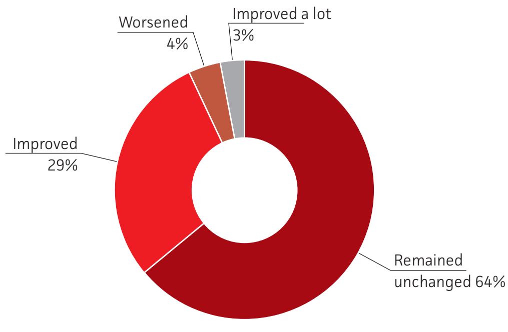


Perception of CSCS

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




PHONE
BOOTH

Impressum

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Design & Layout
Humus Brand Culture

Photos
CSCS, Marco Abram, Matteo Aroldi, Alessandro Della Bella
Staff portraits: Alessandro Della Bella

Printing
Lepori & Storni

Print-run
300