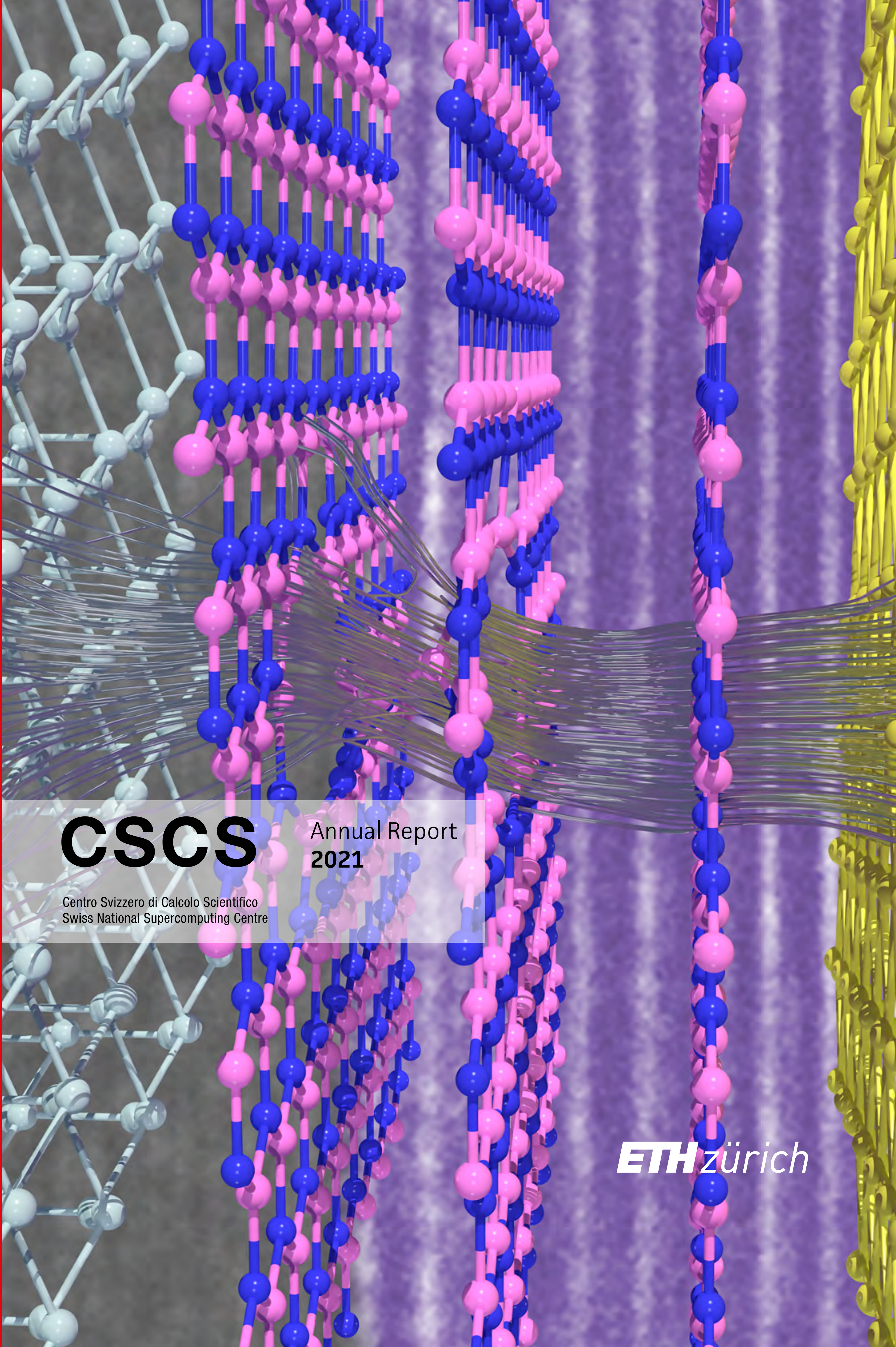


CSCS

Annual Report
2021

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

Annual Report 2021

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

The cover page depicts the rendering of the electron trajectories through a defective, three-layer hexagonal boron nitride (h-BN) insulator embedded between a gold (left) and silicon (right) electrode. The background shows the actual device structure.
Image: Jean M. Favre (CSCS), Mathieu Luisier (ETH Zurich)

The photographers Alessandro Della Bella and Rebecca J. Howard have portrayed six scientists of different scientific fields who use CSCS supercomputers for their research work: Carlo Antonio Pignedoli (Empa), Lucie Delemotte (Royal Institute of Technology KTH), Paolo Ricci (EPF Lausanne), Sergey V. Churakov (Paul Scherrer Institute), Siddhartha Mishra (ETH Zurich), Sonia I. Seneviratne (ETH Zurich).

Welcome from the Director

Thomas Schulthess, Director of CSCS.

Last year in our annual report, we introduced you to our innovative, software-defined research infrastructure "Alps", which will feature the future flagship supercomputer of CSCS. In 2021, "Eiger", a first partition of the infrastructure under construction, went into operation. The University of Zurich and researchers from the SNF-funded national centre of competence in research NCCR MARVEL on computational design and discovery of novel materials, were the first to use it successfully. An interview with our Chief Technology Officer Sadaf Alam on page 70 describes the initial experiences with the state-of-the-art infrastructure. With funding from the HPCN initiative, we are continuing to build and develop "Alps" together with researchers.

In the context of these developments, we were working on several projects with which we want to get the maximum out of our research infrastructure on the one hand, and on the other hand want to support our users and respond more effectively to their individual needs. One such project was SELVEDAS (Services for Large Volume Experiment-Data Analysis utilising Supercomputing and Cloud technologies) funded by swissuniversities.

Together with the Paul Scherrer Institute, which operates large-scale research facilities that produce petabytes of data every year, we have been looking for solutions to exchange and analyse data between the facilities more quickly and efficiently.

Now, technologies that resulted from SELVEDAS offer a solution to this complex problem. It leverages other software products developed at CSCS, Sarus and FirecREST. The new container engine Sarus allows scientific workflows to run in portable containers while ensuring the native performance of the HPC system. FirecREST provides a novel application programming interface to the supercomputing infrastructure designed for developers to support the complex scientific workflows.

In order to answer urgent questions in the area of weather and climate, researchers at ETH Zurich launched the EXCLAIM research initiative in 2021 together with the CSCS, as well as MeteoSwiss, the Swiss Data Science Center, Empa and international project partners. Among other things, CSCS provides a platform with "Alps" for their ambitious simulations, which will achieve significantly higher resolution models and increase the precision of forecasts on a global level.

Parallel to the commissioning of the first "Alps" computing partitions and the launched projects, substantial conversion work and extensions to the technical infrastructure of the CSCS facility took place. These had become necessary to enable the complete installation of "Alps" in 2023 and to be able to operate the powerful supercomputing infrastructure.

But not only the architecture of the technical infrastructure is being transformed. The organisation of the centre is currently being transformed to better align with the new architecture of the research infrastructure. "Alps" makes us all rethink the way we work together and run the centre. I am grateful to my staff and to ETH Zurich for many fruitful discussions, how we will turn the visionary concept of "Alps" into a new, future-oriented organisation of the Swiss National Supercomputing Centre.

Finally, allow me to point out another successful year in the User Lab. As always, you will find details and figures on this in this annual report, as well as examples of the scientific output of research projects by CSCS' users. I am also particularly pleased that we can again present 15 new PASC projects.

I wish you pleasant reading,

Thomas Schulthess

Content

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

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

Granted Resources for User Lab
2021: 56 321 000 node h
2020: 54 955 535 node h

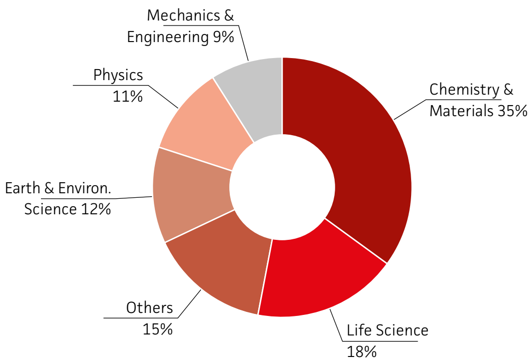
User Community
2021: 153 projects, 2 318 users
2020: 134 projects, 2 270 users

Employees
2021: 118
2020: 116

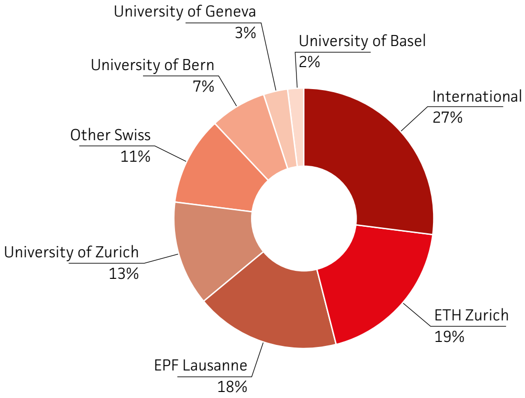
Investments
2021: 21.45 Mio. CHF
2020: 9.8 Mio. CHF

Operational Costs
2021: 26.2 Mio. CHF
2020: 23.6 Mio. CHF

User Lab Usage by Research Field



User Lab Usage by Institution



Computing Systems Overview

Name	Model	Installation / Upgrades	User	TFlops
Piz Daint	Cray XC50 / Cray XC40	2012 / 13 / 16 / 17	User Lab, UZH, NCCR Marvel, CHIPP	27 154 + 2 193
Grand Tavé	Cray X40	2017	Research & Development	437
Tsa / Arolla	Cray CS-Storm 500	2020	MeteoSwiss	1 169
Alps	HPE Cray EX	2020	User Lab, Research & Development	4 719

Carlo Antonio Pignedoli – Empa

“High performance computing is key to the success of computational materials science. CSCS is constantly working to offer scientists access to top-level architectures. The reliability of the services offered by CSCS is a shining example of HPC excellence in Europe”.

Name
Carlo Antonio Pignedoli

Position
Senior Scientist

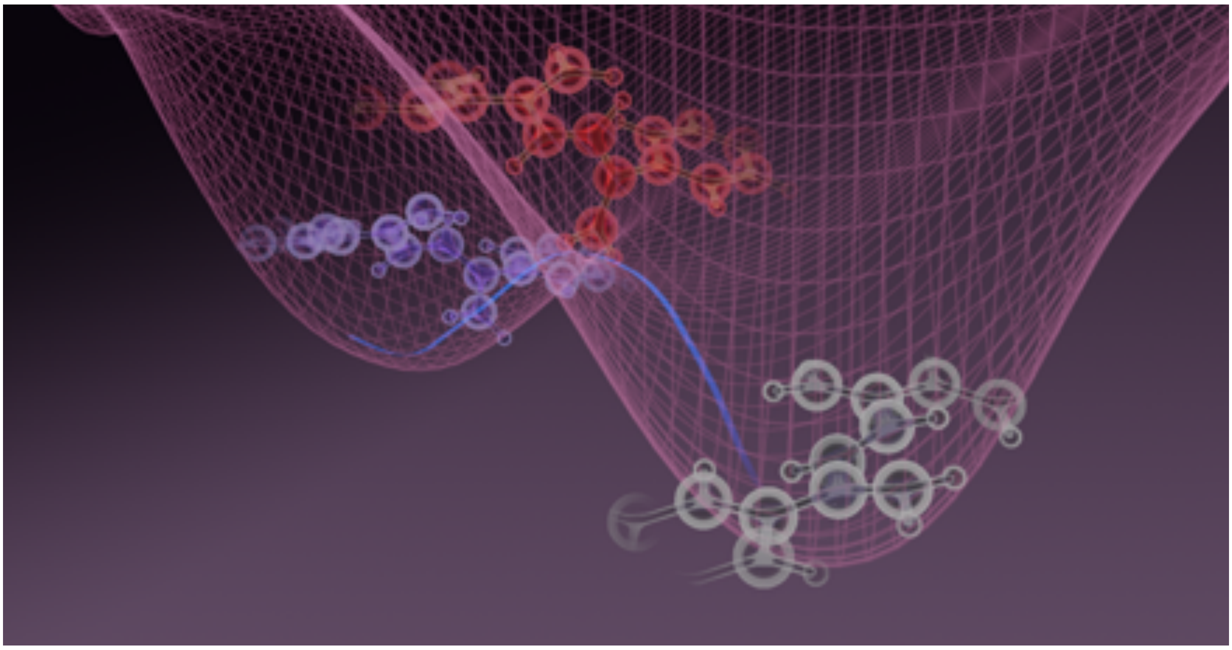
Institution
Empa

Background
2001–2003 PhD in physics, University of Modena & Reggio Emilia, Italy
2003–2007 Postdoc, IBM Research, Zürich Research Laboratory
2007–Present Senior scientist, Empa

Area of research
Computational materials science.

Specialised in
Surface supported chemical reactions.

HPC means for me
To me, HPC represents the possibility to understand experiments, to anticipate them, or to conduct them *in-silico*, which might otherwise be impossible in practice.



Characterization of on-surface reactions in the fabrication of atomically precise nanographenes with non-hexagonal rings

On-surface synthesis is an important technique in organic molecule and polymer preparation. Experimentalists in the nanotech@surfaces Laboratory of Empa use this approach to fabricate novel carbon-based nanomaterials with outstanding electronic and magnetic properties. Carlo Pignedoli and coworkers use HPC to understand the key mechanism in the experimental fabrication process at the atomic level.

The combined theoretical and experimental efforts allowed for unraveling a novel and intriguing surface-catalyzed reaction: the selective formation of phenylene rings by cycloaromatization of two isopropyl-substituted arylenes on gold surfaces. The image shows an artistic representation of a key reaction step that precedes the cyclization, where the coupled substituents rotate along a newly formed C-C bond. (Image: Amogh Kinikar)

January

04

A new beginning

The year begins as the previous one ended — heavily impacted by the pandemic. Most of the staff is working from home, and only the staff members essential for the operations go to the office. In spite of this, the center continues to provide full services to all users.

February

26 Read the article

New service desk to better support user community

A new web interface with a user-friendly dashboard is introduced, which allows users to report new issues, upload relevant files, and consult the status of open and past issues. Users no longer need to keep track of the e-mail exchange and history, as everything is available in the portal.

March

24

Webinar: "What is new in ParaView 5.9?"

The webinar focuses on the new features available in ParaView 5.9: the rendering enhancements, plugin updates, filters and I/O modules changes, and Python scripting improvements. It also includes interactive live demonstrations and gives users the chance to ask questions not just about ParaView, but also about 3D scientific visualization in general.

April

01

23.1 Mio node hours distributed in the User Lab and PRACE

A total of 23.1 million node hours are distributed in the first national call for proposals and in the PRACE Tier-0 Call 22 for the allocation period between April 1, 2021 and March 31, 2022.

12 Read the article

"Alps": the world's most powerful AI-capable supercomputer

CSCS, Hewlett Packard Enterprises, and NVIDIA announce "Alps", the new system that, among others, is expected to be one of the world's most powerful AI-capable supercomputers. Planned to come online in 2023, the "Alps" infrastructure will replace "Piz Daint" and serve as a general-purpose system open to the broad community of researchers in Switzerland and the rest of the world. "Alps" will use the HPE Cray EX supercomputing infrastructure, which is based on a cloud-native software architecture, to implement a software-defined research infrastructure. It will also use NVIDIA's novel Grace CPU to converge AI technologies and classic supercomputing in one single, powerful data centre infrastructure. This innovative system will enable breakthrough research on a wide range of fields, including climate and weather, materials sciences, astrophysics, computational fluid dynamics, life sciences, molecular dynamics, quantum chemistry and particle physics, as well as domains like economics and social sciences.

24

Online tutorial: "Interactive computing with Jupyter on 'Piz Daint', using Python, ParaView and Julia"

The online tutorial is held to discuss how to use JupyterHub service on "Piz Daint" for data analysis, visualization and rapid prototyping of code.

May

05/06

2021 Swiss Conference and HPCXXL User Group

Encouraging shared knowledge for over a decade, the Swiss Conference and HPCXXL User Group conference continues online this year due to the pandemic. 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.

14

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.

17/18

Online course on scientific visualization

The online course is targhetting "Piz Daint" users and is focusing on scientific visualization. The event includes and interactive live demonstrations and gives users the chance to ask questions about scientific visualization in general.

20

HPC-CH forum

The 22nd Community Forum Virtualization is hosted by the University of Lausanne. Representatives of the Swiss HPC Service Provider Community meet to discuss computational resources abstraction and efficient management of data.

June

06

Participation in the project EXCLAIM

The project EXCLAIM aims to develop extreme-scale computing and data platforms for cloud-resolving weather and climate modeling — an ICON-model based infrastructure that is capable of running kilometer-scale climate simulations at both regional and global level. The platform will become a foundation for weather and climate modeling for decades to come, involves the collaboration the ETH Center for Climate Systems Modeling (C2SM), ETH computer scientists, the Swiss Data Science Center (CSCS), Empa and MeteoSwiss, and international project partners. Among other things, CSCS provides a platform with "Alps" for their ambitious simulations, which will achieve significantly higher resolution models and increase the precision of forecasts on a global level.

17

SELVEDAS reaches its end

PSI and CSCS successfully terminated the project Services for Large Volume Experiment-Data Analysis utilizing Supercomputing and Cloud technologies (SELVEDAS) financed by swissuniversities. CSCS and PSI co-investigated how best to enable quick and efficient data workflows between the institutions. The project aimed at developing scalable and extensible services for data management, data processing, and data analysis to the Swiss academic user community by leveraging HPC, storage, networking and cloud technologies.

23

Webinar: "Long-term storage service at CSCS"

Scientists need a reliable, accessible, long-term storage service and a way to find or cite a particular dataset independent from future infrastructural changes. The webinar aims at describing the new service of long-term storage from a user perspective, covering who can access, what can be done, and how.

23/26

High-performance computing with Python

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

30

Webinar: "Deploying high-performance containers with Sarus on 'Piz Daint'"

Sarus is a container engine developed at CSCS that aims at bridging the gap between container portability and native HPC performance. This webinar provides an introduction to Sarus on "Piz Daint" from the user's perspective, covering fundamental workflows and the command line interface, as well as best practices for running containers with MPI and GPUs. Examples ranging from simple benchmark runs to a real-world HPC application are used to illustrate the presented information.

SARUS

30

Read the article

Fifteen PASC projects funded for the period 2021 to 2024

Since 2009, innovative software development projects are funded through the Platform for Advanced Scientific Computing (PASC) every three years. For the new period starting on July 1, 2021, 15 projects from the fields of astrophysics, chemistry and materials, computer science and high-performance computing, earth and climate sciences, life sciences and physics have been selected.

July

01

Webinar: "FirecREST for RESTful HPC"

FirecREST, another software product developed at CSCS, is bringing the world of programmable web applications to HPC infrastructure. It uses web-enabled REST API to expose — in a programable way — the access of HPC resources, including the capability to interact with the workload manager or to move data from/to storage. The webinar provides an introduction to the core concepts and the architecture of FirecREST.

FIRECREST

05/07

PASC21 Conference

The PASC21 Conference — with the theme "New Challenges, New Computing Paradigms"— takes place online due to the pandemic and is virtually hosted by the University of Geneva. With 500 participants from 28 countries, the conference has grown in attendee numbers every year since its inception. The technical program included keynote talks, minisymposium sessions, a peer-reviewed paper track, poster sessions, and panel-style discussions.

13 / 24

Online CSCS-USI Summer School 2021

CSCS and Università della Svizzera italiana (USI) host their annual Summer School online this year due to COVID-19 restrictions. A total of 100 students and working professionals log 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.

23

Read the article

AIL-CSCS: a collaboration in the name of sustainability

CSCS and the Aziende Industriali di Lugano (AIL) sign an agreement in the name of sustainability and the promotion of local renewable energy production. The contract concerns the purchase of electricity coming 100% from Ticino hydroelectric sources, for an annual quantity of up to 30 GWh.

August

01

"Eiger" on "Alps"

The first virtual cluster named "Eiger" has been opened and is now available on the "Alps" research infrastructure. "Eiger" is used by the researchers of University of Zurich and NCCR MARVEL currently.

26

ETH Foundation visiting CSCS

The director of the centre Thomas Schulthess welcomes the ETH Foundation and a group of patrons 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.

September

03

Read the article

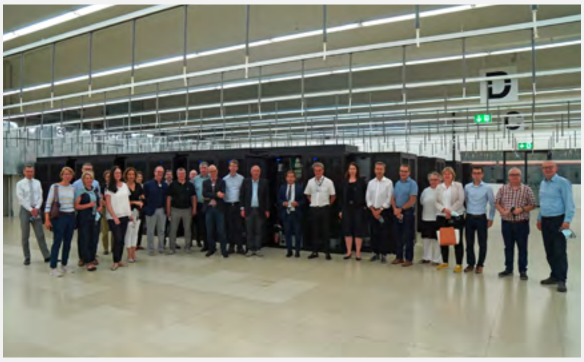
User Lab Day

CSCS welcomes current and possible future users to a one-day hybrid event. The event takes place both online and in person at the KKL in Lucerne. Attended by about 90 researchers, half in person and half virtually, the event provides ample time for presentation of CSCS roadmaps and plans and for conversation with CSCS staff about the current infrastructure, as well as the new services already on the horizon.

10

Visit of the Federal Chancellery

The Federal Chancellery, led by the Federal Chancellor Walter Thurnherr, visits the centre. Thomas Schulthess welcomes the delegation and presents the centre and its activities to show their relevance for Switzerland.



20 / 29

Online EuroHack21: GPU programming hackathon

The seventh GPU-programming hackathon takes place online. EuroHack21 engages a total of nine teams from Switzerland and around the world for a total of 28 participants. With the support of expert mentors, the hackathon is designed to help researchers port their codes to a GPU-hybrid supercomputing environment.

24

Read the article

Launch of software product website in support of EuroCC Project

A brand-new web portal is launched to provide detailed information about the new products, Sarus and FirecREST, developed at CSCS. The website provides information about the products including use cases, downloads, documentation, and contact information.

October

01

24.3 Mio node hours distributed in the User Lab and PRACE

A total of 24.3 million node hours are distributed in the second national call for proposals and in the PRACE Tier-0 Call 23 for the allocation period between October 1, 2021 and September 30, 2022.

11 / 13

Advanced C++

A three-day course is organized to provide the fundamental tools for effective C++ programming in the context of HPC. The tools include generic programming techniques, API development, and specific C++-11/14/17 constructs. Starting from a basic knowledge of C++, the attendees are able to start using C++ language to engineer durable abstractions to develop and optimize applications.

November

02 / 05

GPU Programming with Julia

A four-day course with lectures and hands-on sessions is offered to discover both basic and advanced topics relevant for single and multi-GPU computing with Julia. The programming language Julia is more and more prevalent in HPC due to its unique way of combining performance with simplicity and interactivity, in turn enabling unprecedented productivity in HPC development.

05

Read the article

USI joins first European master's program in high-performance computing

A consortium of European partners led by the University of Luxembourg are selected by the EuroHPC Joint Undertaking to design and implement the first pan-European HPC pilot master's program. As members of the consortium, USI and CSCS will together offer courses starting in autumn 2022 that will provide students with outstanding career perspectives in the rapidly expanding field of HPC, high-performance data analytics (HPDA), or artificial intelligence.

12

Webinar: "FirecREST: Enabling programmatic access of HPC resources"

The webinar focuses on introduction to the core concepts and architecture of FirecREST, especially from the system administrator's point of view. Additionally, participants look into the internals of FirecREST, like the integration with the authentication and authorization infrastructure of the site and data transfers.

12

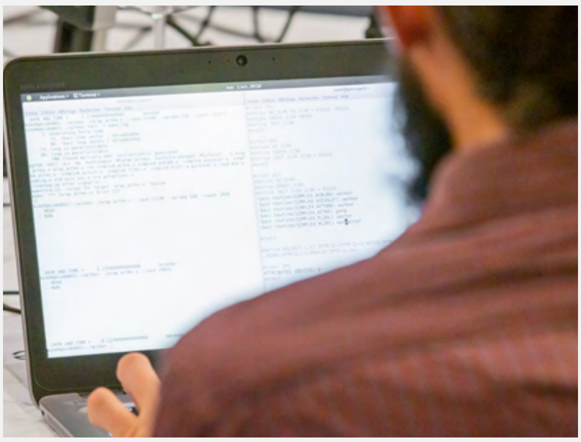
Webinar: "Sarus: Toward HPC Performance for Portable Containers"

The webinar aims at providing insights about Sarus's modular architecture, highlights some HPC-specific features, and illustrates the advantages that hook programs adopting the OCI specifications bring to users, system administrators and developers alike. The training also covers a quick installation and setup procedure for Sarus. Basic Sarus usage and container customization capabilities are also showcased including comparative performance results with native applications at scale.

22/24

Distributed training with PyTorch on "Piz Daint"

A three-day course on distributed training with PyTorch is organized to address the use of this tool on "Piz Daint". Attendees have the chance to observe how to run distributed deep learning workloads with PyTorch. The main focus of the course is training modules with PyTorch taking advantage of "Piz Daint" and its setup of multiple single-GPU nodes.



December

01

Kick-off at the project to increasing office space in Lugano

To support the staff growth in Lugano, new offices are rented by ETH Zurich in a building 450 meters away from CSCS headquarters. The new offices have a total of 54 workplaces and will be available in the first half of 2022.

Lucie Delemotte - Royal Institute of Technology KTH

“CSCS and the computer time on Piz Daint makes it possible for us to tackle problems on a much larger scale than otherwise possible. I am grateful to be able to take on ambitious project thanks to this support”!

Name
Lucie Delemotte

Position
Associate Professor

Institution
Royal Institute of Technology KTH, Stockholm

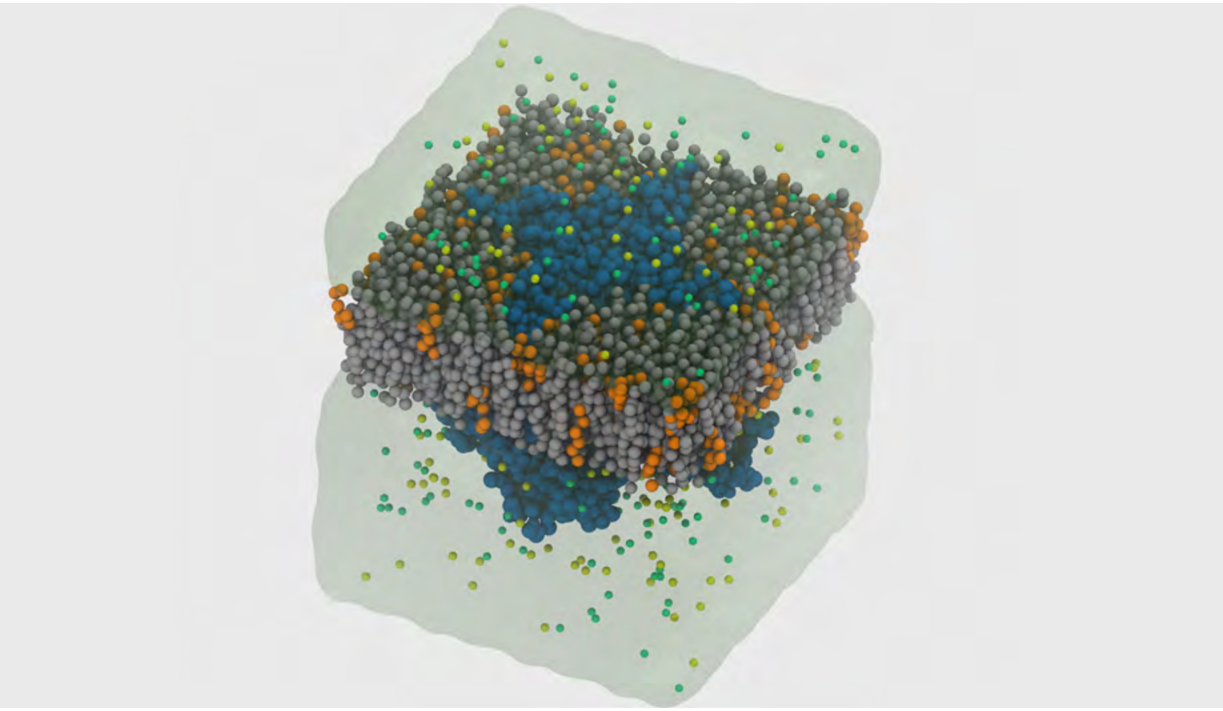
Background

2008-2011	PhD in theoretical chemistry, University of Lorraine, France
2011-2015	Postdoc and Marie Curie Fellow, Temple University, USA
2015-2016	Marie Curie Fellow, EPF Lausanne
2016-2019	Assistant Professor, Royal Institute of Technology KTH, Sweden
2019-Present	Associate Professor, Royal Institute of Technology KTH, Sweden

Area of research
Computational biophysics.

Specialised in
Molecular modeling of membrane proteins, including ion channels, transporters and G-protein coupled receptors.

HPC means for me
Molecular dynamics simulations of biological systems enable a beautifully detailed description of atomistic interactions, which is critical for applications such as structure-based drug discovery. Unfortunately, this comes with a hefty computational price tag. HPC makes it possible to run such calculations!



Current ongoing project on "Piz Daint"

Lipid modulation of membrane protein functional cycle — Ion channels are critical mediators of electrochemical signaling in neurons. Accordingly, many clinically relevant drugs act on ion channels, often via their membrane-facing domains. Such lipophilic interactions have historically been difficult to study, due to limited structural data, complexities of the nonaqueous electrostatic environment, competitive interactions with other membrane components, and other challenges to mechanistic modeling. Our large scale simulations on "Piz Daint" make it possible to understand how ion channels are regulated by the membrane, and thus how to exploit these interactions in drug discovery projects.

A new era of computing and data infrastructure: “Alps” at CSCS

Earlier this year CSCS announced a new research infrastructure: “Alps”. The first four cabinets were installed and made available to early users starting April 2021. “Alps” will enable research in a wide range of fields, from weather and climate, materials sciences, astrophysics, computational fluid dynamics, life sciences, molecular dynamics to quantum chemistry and particle physics, and it will also cover new domains like economics and social sciences.

It was a great pleasure for CSCS to have the User Lab Day in Lucerne again, albeit still as a hybrid event due to pandemic restrictions. On August 31, CSCS staff welcomed more than 40 participants at the Lucerne Culture and Congress Centre (KKL) and 45 more following online. CSCS director Thomas Schulthess explained his vision for “Alps”, stressing that this new research infrastructure will ensure continuity of the User Program but at the same time create new opportunities in Artificial Intelligence and Machine Learning. The true novelty is that “Alps”, being a service-oriented architecture, will allow CSCS to provide a flexible cloud-like infrastructure driven by software rather than hardware. Ad-hoc virtual clusters will be made available to the User Lab, to the Weather & Climate community, and to other partners and scientific communities.

CSCS was happy to attract Erik Lindahl as plenary speaker. He serves in the Scientific Advisory Committee of CSCS and is a well-known professor of Biophysics at Stockholm University and KTH. He underlined that HPC is moving toward modern hardware, the major part of compute power currently coming from accelerators. He reminded the HPC community of the need to improve software portability to be prepared for future hardware developments and to minimize dependence on specific vendor solutions. New computer architectures start to be available to researchers; they demand reformulation of scientific problems, so they fit modern hardware. Erik Lindahl concluded that scientists need to consider Artificial Intelligence and Machine Learning as strategies complementing traditional scientific computing that may help them solve problems that cannot be solved by any other means. After his talk he also stood by to answer a number of pressing questions from the audience about the reviewing process at CSCS.

Resources allocated in 2021

Usage statistics shows that Chemistry & Materials remains the best-represented field at CSCS, using 35% of the available resources. Life Science follows with 18% of the total allocation, followed by Earth & Environmental Science, Physics and Mechanics & Engineering with 12, 11 and 9% each. This year, other disciplines still account for 15% of utilization.

ETH Zurich and EPF Lausanne are the largest users among institutions with 19 and 18%, respectively. The Universities of Zurich, Bern, Geneva, and Basel (13, 7, 3, 1%), other Swiss institutions are sharing the remaining 11% of the resources. International utilization remains high at about 27%. Like in previous years, the User Lab Calls are still the primary path to resource allocation for domestic research institutions, but the majority of the international allocation has been granted in PRACE Tier-0 calls.

List of PRACE Tier-0 Projects

Principal Investigator	Organisation	Research Field	Project Title	Node h
Olaf Kaczmarek	University of Bielefeld	Physics	Scaling properties of conserved charge fluctuations in QCD	1 776 000
Massimiliano Bonomi	Institute Pasteur Paris	Life Science	ModFil – Modulating the structure and dynamics of bacterial filaments	1 582 000
Davide Modesti	Delft University of Technology	Mechanics & Engineering	INSULATE: dIrect Numerical SimULAtion of Turbulent boundary layers over acoustic linErs	1 500 000
Nikolina Ban	University of Innsbruck	Earth & Environ. Science	Mountain climate at the kilometre-scale resolution: Phase 2 (kmMountains)	1 498 000
Gabriel Włazlowski	University of Warsaw	Physics	Superfluid dynamics with oscillating currents in Fermi systems	1 235 000
Gabriele Tocci	University of Zurich	Chemistry & Materials	Ab-initio molecular dynamics for nanoscale osmotic energy conversion	1 200 000
Carlo Camilloni	University of Milan	Life Science	Protein dynamics and toxicity in light chain amyloidosis	1 000 000
Christoph Schär	ETH Zurich	Earth & Environ. Science	Kilometer-resolution climate modeling on GPUs (kmCLIM2)	1 000 000
Karl Liedl	University of Innsbruck	Life Science	Antibody ensembles in solution as a new paradigm in antibody structure prediction	1 000 000
Sandra Luber	University of Zurich	Chemistry & Materials	Water Splitting at Ruthenium Oxide/Water Interfaces: Forefront DFT-MD and machine-learning-metadynamics investigations	882 000
Constantia Alexandrou	University of Cyprus & Cyprus Institute	Physics	NPiTwist – The Nπ system using twisted mass fermions at the physical point	758 000
Raffaela Cabriolu	EPF Lausanne	Chemistry & Materials	Thermal conductivity of Metal-Organic-Frameworks (TC_MOFs)	582 000
Ville Kalia	Stockholm University	Life Science	Functional dynamics of mitochondrial supercomplexes	451 500
Francesco Gervasio	University of Geneva	Life Science	Combining and testing collective-variable-based free energy algorithms for efficient calculations of absolute binding free energies	441 200

Largest Projects (> 600 000 Node h)

Principal Investigator	Organisation	Research Field	Project Title	Node h
Petros Koumoutsakos	ETH Zurich	Mechanics & Engineering	Modeling, sensing and control of turbulent flows	2 090 000
Nicola Spaldin	ETH Zurich	Chemistry & Materials	Coupled and competing instabilities in complex oxides	990 000
Mathieu Luisier	ETH Zurich	Chemistry & Materials	Ab-initio modeling of three-terminal valence change memory cells for neuromorphic computing applications	880 000
Jürg Hutter	University of Zurich	Chemistry & Materials	Molecules at interfaces from density functional theory	840 000
Ursula Röthlisberger	EPF Lausanne	Chemistry & Materials	Towards lead-free and stable solar cells	828 832
Urs Wenger	University of Bern	Physics	A look into light pseudoscalar and vector mesons: Radiative transitions and gluon structure	823 910
Stefan Goedecker	University of Basel	Chemistry & Materials	Structure and dynamics of solids, interfaces and clusters	800 000
Sandra Luber	University of Zurich	Chemistry & Materials	Guiding the design of novel and highly efficient water reduction catalysts by ab-initio methods	707 176
Ursula Röthlisberger	EPF Lausanne	Chemistry & Materials	Computational characterization of the atomistic mechanisms involved in surface passivation: Towards perovskite based solar cells with enhanced stability	700 000
Sandra Luber	University of Zurich	Chemistry & Materials	Advancing real-time propagation methods for spectroscopy in the condensed phase	680 000
Nicola Marzari	EPF Lausanne	Chemistry & Materials	Materials for energy	650 000
Carlo A. Pignedoli	Empa	Chemistry & Materials	Characterization of on-surface reactions in the fabrication of atomically precise nanographenes with non-hexagonal rings	630 000
Ursula Röthlisberger	EPF Lausanne	Life Science	Molecular dynamics simulations of biological systems: From molecular mechanisms to medicinal chemistry	600 000
Constantia Alexandrou	Cyprus Institute & University of Cyprus	Physics	Precision nucleon structure using lattice QCD	600 000
Andreas Fichtner	ETH Zurich	Earth & Environ. Science	Full-waveform inversion of the Alpine belt	600 000

Platform for Advanced Scientific Computing

In 2021, the Platform for Advanced Scientific Computing (PASC) program entered its third cycle, marking the end for the 10 projects of the call for the period 2017 - 2020, and the beginning for 15 new projects of the call 2021 - 2024. The overarching goal for the 2021 - 2024 period is to position Swiss computational sciences in the emerging exascale era, and to ensure application readiness on CSCS' infrastructure.

Impact on the User Lab

The PASC core team of CSCS consists of research software and HPC application engineers who support PASC projects with code development and software engineering expertise.

Highlights of the applications developed this year at PASC with the CSCS core team include:

- The majority of Swiss PIs with PRACE Tier-0 allocations on "Piz Daint" and more than 30 User Lab projects are employing applications co-developed in PASC.
- Co-design of the "Alps" infrastructure with representative PASC applications significantly influenced the scale out that will be available to users in 2023.
- Enabled key applications integrated in AiiDA workflows for the Materials Cloud platform. As a pilot project on LUMI supercomputer these workflows demonstrated readiness for exascale.
- Co-design of a novel cosmological simulation code that has been scaled up to 5 300 nodes on "Piz Daint" with 88% efficiency.

Looking forward: projects 2021 – 2024

The current round of PASC started in August with 15 projects (see table on right) that cover a wide range of scientific fields including electronic structure and molecular dynamics, weather and climate, geophysics and earth sciences, cosmology, fluid dynamics and machine learning.

Since every project is different, the first task of the core team at CSCS is to work with the projects to identify how they can collaborate and contribute to these projects.

Contributions can be software development support including direct contribution to each project's source code, development of portable libraries and their integration into projects, and containerisation and workflow integration.

The core team also provides and facilitates access to HPC resources at CSCS, configuration of modern CI/CD on HPC systems, project planning, and consultation on software engineering for performance portability.

The core team's initial priority was helping the projects to configure automated testing and deployment pipelines (CI/CD). In parallel, priority has been given to porting to AMD GPUs, to give projects a head start accessing the novel system architecture of the LUMI supercomputer – with two PIs successfully applying for the early access pilot projects.

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, the 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.

The 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	EPF Lausanne	Chemistry & Materials	Spectral properties of materials on accelerated architectures	488 320.00
Jürg 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
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
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	Physics	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
Jean-Paul Kneib	EPF Lausanne	Physics	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	EPF Lausanne	Chemistry & Materials	Machine learning for materials and molecules: toward the exascale	313 525.00

List of Projects by Institution

CERN

CERN'S LINAC4 H– source beam formation study, Anna Vnuchenko (Physics, 60 000 node h)

Dalle Molle Institute for Artificial Intelligence Research IDSIA

Advancing sequence processing with neural networks, Kazuki Irie (Computer Science, 36 000 node h)

Structured models for visual perception and reasoning, Jürgen Schmidhuber (Computer Science, 100 000 node h)

Parameter-based value functions: An alternative to back-propagation through time, Jürgen Schmidhuber (Computer Science, 150 000 node h)

Meta learning general purpose reinforcement learning algorithms, Jürgen Schmidhuber (Computer Science, 50 000 node h)

EAWAG

Calibration and uncertainty quantification of stochastic models with SPUX: Applications to hydrology (Part II), Marco Bacci (Earth & Environmental Science, 72 000 node h)

Empa

Atmospheric simulations for inverse estimation of greenhouse gas emissions, Dominik Brunner (Earth & Environmental Science, 93 800 node h)

Enantioselective adsorption of 10,10'-dibromo-9,9'-bianthracene molecules on PdGa-surfaces, Daniele Passerone (Chemistry & Materials, 300 000 node h)

Designing new Mg alloys with improved ductility by understanding twin growth, Vladlyslav Turlo (Chemistry & Materials, 280 000 node h)

EPF Lausanne

Gyrokinetic studies of the low momentum diffusivity regime in tokamak plasmas, Justin Ball (Physics, 120 000 node h)

Modeling of turbulence measurements with gyrokinetic simulations and synthetic diagnostics, Stephan Brunner (Physics, 275 000 node h)

Thermal conductivity of MOFs, Raffaella Cabriolu (Chemistry & Materials, 200 000 node h)

Surface-based design of viral epitope mimetics for Influenza, Bruno Correia (Life Science, 140 000 node h)

Mesoscopic simulations of block copolymer nanocomposites, Javier Diaz Brañas (Chemistry & Materials, 250 000 node h)

Stationary and dynamical properties of topological defects in the Active Brownian Particles model, Pasquale Digregorio (Physics, 300 000 node h)

Exploring the space of high entropy alloys, from DFT to machine learning, Guillaume Fraux (Chemistry & Materials, 391 000 node h)

Global simulations of plasma fluid turbulence in stellarators, Jonathan Graves (Physics, 100 000 node h)

Dynamics of minority species in 3D fusion plasmas: Unconventional fast ion heating schemes, metallic impurity accumulation and runaway electron transport, Joaquim Loizu (Physics, 125 000 node h)

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

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

Large-Eddy simulation of large-scale wind-farm flows, Fernando Porté-Agel (Mechanics & Engineering, 130 000 node h)

Collective behavior of squirmer suspensions in viscoelastic fluids, Kai Qi (Chemistry & Materials, 300 000 node h)

Simulation of the tokamak boundary in reactor-relevant conditions, Paolo Ricci (Physics, 440 000 node h)

Three dimensional active flows from moderate to large Reynolds numbers, Cecilia Rorai (Chemistry & Materials, 300 000 node h)

Data-driven nanocrystals' phase diagrams, Kevin Rossi (Chemistry & Materials, 35 520 node h)

First-principles, real-size turbulence simulations in innovative tokamak boundary shapes, Christian Theiler (Physics, 220 000 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)

String breaking in QCD using C* boundary conditions, Marco Catillo (Physics, 150 000 node h)

Architected materials for tailored elastic wave control: From lattice-like to bio-inspired structures, Andrea Colombi (Mechanics & Engineering, 88 200 node h)

Magnetotelluric imaging of geological controls on geothermal resources from surface down to the upper mantle, Samrock Friedemann (Earth & Environmental Science, 95 000 node h)

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

Mars investigations, Domenico Giardini (Earth & Environmental Science, 60 000 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, Ilja Karlin (Mechanics & Engineering, 310 000 node h)

Optimized experimental design for 3D seismic full waveform inversion, Hansruedi Maurer (Earth & Environmental Science, 100 000 node h)

Computation of forward and inverse problems for statistical solutions of compressible fluid flow, Siddhartha Mishra (Computer Science, 200 000 node h)

Resolving cloud-circulation interactions, Sebastian Schemm (Earth & Environmental Science, 300 000 node h)

The quantum muon: Tunnelling-corrected hopping barriers in Cr_2O_3, Kane Shenton (Chemistry & Materials, 224 000 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, 65 000 node h)

Electronic, optical, and dynamical processes in mercury telluride semiconductor nanocrystals and their assemblies, Nuri Yazdani (Chemistry & Materials, 150 000 node h)

Fachhochschule Nordwestschweiz

Ping dark matter with gravitational lenses, Stefan Hackstein (Physics, 36 000 node h)

HES-SO Valais-Wallis

GPU-accelerated particle-based simulation of 6-Jet full-size pelton turbines flow including all the interactive components, Cécile Münch-Alligné (Mechanics & Engineering, 120 000 node h)

Imperial College London

Optimising rotorcraft aerofoils for martian aerodynamic conditions, Peter Vincent (Mechanics & Engineering, 375 000 node h)

Institute for Snow and Avalanche Research SLF

Blowing snow dynamics and its impact on snow cover and the atmospheric boundary layer, Michael Lehning (Earth & Environmental Science, 107 100 node h)

Simulating tree species migration: From post-glacial to future climate change, Heike Lischke (Earth & Environmental Science, 100 000 node h)

IRB Bellinzona

Effect of antibody single-point mutations on the improvement of thermodynamic stability, Andrea Cavalli (Life Science, 36 000 node h)

IRSOL

Realistic magneto-hydrodynamic simulations of solar and stellar atmospheres, Fabio Riva (Physics, 180 000 node h)

Italian Institute of Technology Genoa

Liquid-liquid phase transition and criticalpoint of sulfur using ab-initio machine learning enhanced sampling, Manyi Yang (Chemistry & Materials, 220 000 node h)

National University of Singapore

Efficient training methods for super-large deep learning models, You Yang (Computer Science, 36 000 node h)

Paul Scherrer Institute

Surface adsorption and structural incorporation of Tc and Pu by magnetite, Sergey Churakov (Earth & Environmental Science, 180 000 node h)

Ab-initio simulations of competitive cation adsorption on swelling clays, Sergey Churakov (Earth & Environmental Science, 140 000 node h)

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, 360 000 node h)

First principles characterization of the Ba0.5Sr0.5Co0.75Fe0-.25O3-δ type electrocatalysts guided by experimental electrocatalytic characterization, Monica Kosa (Chemistry & Materials, 150 000 node h)

Dynamics of porous catalytic particles in fluidized beds for biogas methanation, Ioannis Mantzaras (Mechanics & Engineering, 50 000 node h)

Resolving calcium carbonate polymorphs precipitation in porous media: A combined modeling – experimental approach with synchrotron-based tomography, Nikolaos Prasianakis (Earth & Environmental Science, 100 000 node h)

SUPSI

ANUBIS: elucidAting the molecular mechaNism of the TAT-RasGAP317-326 necrotic-like ability indUced by plasmatic memBrane permeabilizatIon apoptosiS, Gianvito Grasso (Life Science, 35 700 node h)

Modelling of light-responsive behaviour in supramolecular architectures, Giovanni M. Pavan (Chemistry & Materials, 338 000 node h)

Tata Institute of Fundamental Research Mumbai

Multi-frequency simulations of the high-redshift Lyman-alpha forest, Girish Kulkarni (Physics, 220 000 node h)

University Hospital Zurich

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

Accurate wave propagation modeling for quantitative medical ultrasound, Naiara Korta (Life Science, 35 800 node h)

Università della Svizzera italiana

Structural insight into selective ligand binding to G-protein Coupled Receptor FPR2, Vittorio Limongelli (Life Science, 148 000 node h)

A coarse grained funnel-metadynamics approach for in-silico screening, Vittorio Limongelli (Life Science, 120 000 node h)

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 Cambridge

Phase diagram of confined water using quantum Monte Carlo, Venkat Kapil (Chemistry & Materials, 100 000 node h)

Accurate modelling of metal-oxide supported nanoclusters, Myung Chang Woo (Chemistry & Materials, 60 000 node h)

A data parallel direct-adjoint looping method inside a GPU-accelerated blood flow simulation tool for patient-specific treatment optimization, Case I: Optimizing the aortic valve prosthesis size, Hadi Zolfaghari (Life Science, 12 000 node h)

University of Bern

Geometrical parameterization of the aortic wall to investigate the evolution of hydrodynamic instabilities initiating laminar-turbulent transition past bioprosthetic aortic valves, Dominik Obrist (Life Science, 64 000 node h)

Three-dimensional analysis of hemodynamic wall-parameters in the carotid bifurcation using computer-augmented 4D-flow-MRI, Dominik Obrist (Life Science, 36 000 node h)

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

University of Fribourg

Investigating the interplay of dynamics and function of Aster proteins at endoplasmic reticulum-plasma membrane contact sites, Stefano Vanni (Life Science, 400 000 node h)

The role of cholesteryl esters in intracellular lipid droplets, Stefano Vanni (Life Science, 310 000 node h)

University of Geneva

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

Monte Carlo simulations for the DArk Matter Particle Explorer (DAMPE), Maksym Deliyergiyev (Life Science, 230 000 node h)

Understanding the mechanisms of activation of class A G-protein-coupled receptors by ligands with different efficacy profiles, Francesco L. Gervasio (Life Science, 500 000 node h)

Spin-crossover iron(III) complexes encapsulated in metal-organic frameworks: Insights into novel bistable functional materials for chemosensing from metadynamics studies, Latévi Max Lawson Daku (Chemistry & Materials, 400 000 node h)

University of Lausanne

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

University of Rome 2

Geometrically induced selectivity and electroosmotic flow in uncharged nanopores, Mauro Chinappi (Chemistry & Materials, 127 700 node h)

University of Stuttgart

Merger-simulations using high-level abstractions, Dirk Pflueger (Physics, 247 000 node h)

University of Zurich

Outflows in simulated massive galaxies at high redshift, Luigi Bassini (Physics, 40 000 node h)

Tailoring Fluorescence and Absorption Spectroscopy for High-performance computing (FLASH), Jürg Hutter (Chemistry & Materials, 225 000 node h)

A thermodynamic benchmark of high-level density functional approximations, Jürg Hutter (Chemistry & Materials, 188 000 node h)

Cation effects on electrochemical interface from quantum dynamics, Marcella Iannuzzi (Chemistry & Materials, 410 000 node h)

Liquid-liquid phase separation of highly charged disordered proteins, Milos Ivanovic (Life Science, 300 000 node h)

Understanding the mechanisms and developing chemical probes for writing and reading the N6-methyladenosine modification in messenger RNA, Yaozong Li (Life Science, 55 000 node h)

Three-dimensional study of multi-fluid dust dynamics inprotoplanetary disks with embedded low-mass planets, David Velasco-Romero (Physics, 495 000 node h)

ZHAW

Development of reduced order models for the prediction of unsteady aerodynamic forces in structural dynamics and aeroelasticity using machine learning, Marcello Righi (Mechanics & Engineering, 36 000 node h)

Renewals

Aix-Marseille University

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

Cyprus Institute & University of Cyprus

Precision nucleon structure using lattice QCD, Constantia Alexandrou (Physics, 600 000 node h)

EPF Lausanne

A single-cell atlas of spinal cord injury, Quentin Barraud (Life Science, 100 000 node h)

Molecular dynamics simulations to assist the engineering of protein-based nanopores for DNA sequencing, Matteo Dal Peraro (Life Science, 381 000 node h)

ETH Zurich

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

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

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

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

Institute for Snow and Avalanche Research SLF

Small-scale simulations of drifting snow using Large Eddy Simulations and a Lagrangian stochastic model, Michael Lehning (Earth & Environmental Science, 50 000 node h)

Physical Meteorological Observatory Davos / World Radiation Centre

Past and future of the ozone layer evolution (POLE), Eugene Rozanov (Earth & Environmental Science, 94 000 node h)

University of Basel

Atomization energies from ab-initio calculations without empirical corrections, Dirk Bakowies (Chemistry & Materials, 120 000 node h)

University of Bern

A high-resolution palaeoreanalysis, Stefan Brönnimann (Earth & Environmental Science, 420 000 node h)

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

ISOCARBON-II (Modelling ISOtopes of CARBON in the Earth System), Fortunat Joos (Earth & Environmental Science, 139 200 node h)

High-resolution glacial climate conditions over the Alps (HicAp), Christoph Raible (Earth & Environmental Science, 254 000 node h)

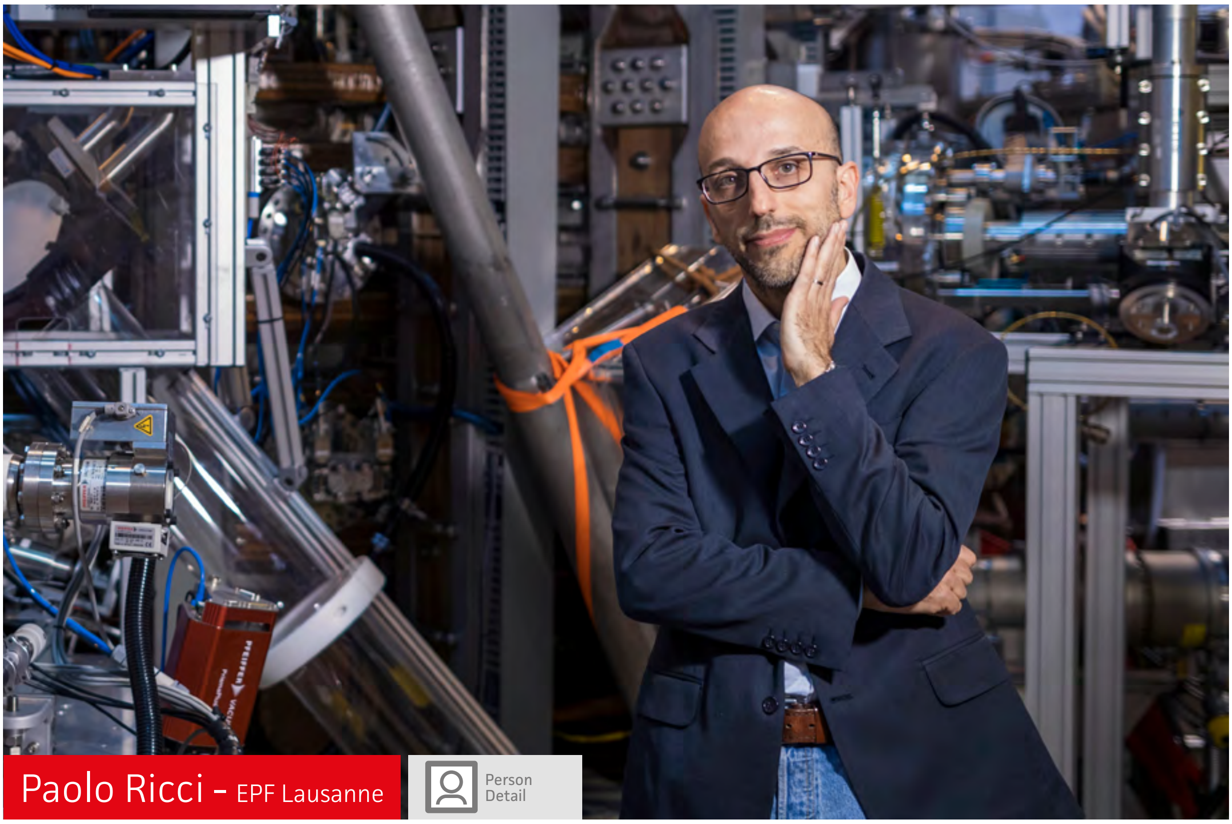
Highest-resolution simulations of climate change and land use to project the impact on water resources and human well-being in Kenya, Thomas Stocker (Earth & Environmental Science, 144 000 node h)

University of Lausanne

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

University of Zurich

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



Paolo Ricci – EPF Lausanne

"State-of-the-art facilities managed by the CSCS and its extraordinarily efficient team have enabled the Swiss Plasma Center to make fundamental advances in predicting the behavior of plasma dynamics in ITER, a necessary step to optimize the functioning of this incredibly complex experiment. Ultimately, by replicating the Sun's fusion processes, ITER will demonstrate that it is possible to create clean energy on Earth".

Name
Paolo Ricci

Position
Associate Professor

Institution
EPF Lausanne

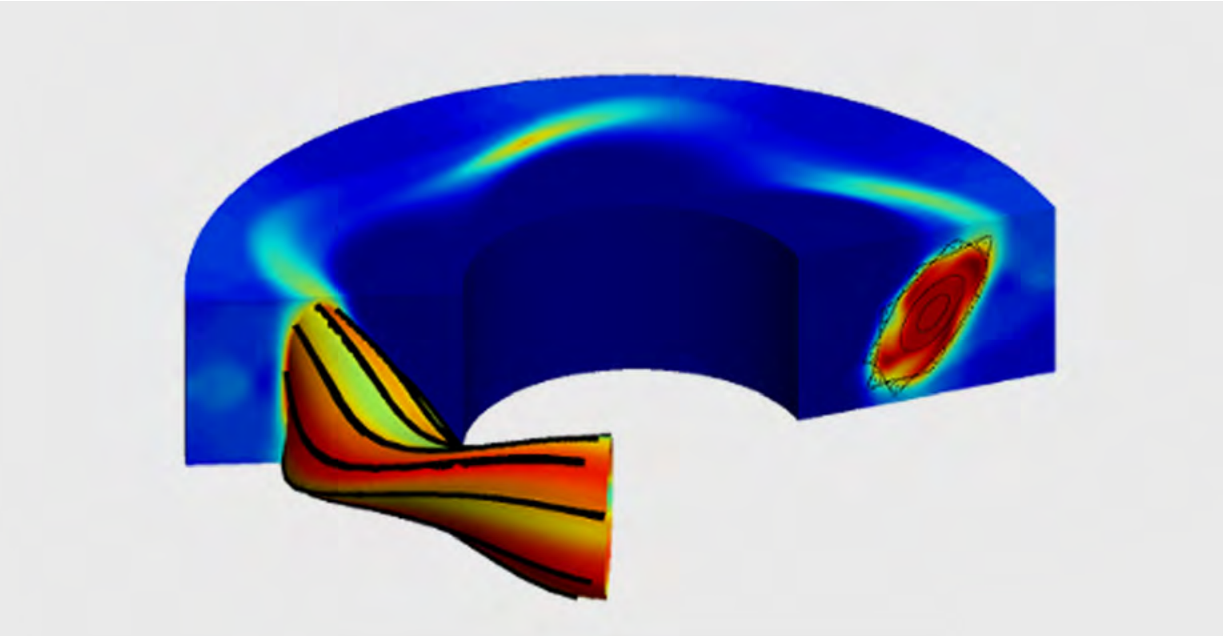
Background

2000-2004	PhD in physics, Politecnico di Torino, Italy
2004-2006	Research Associate, Dartmouth College, USA
2010-2016	Tenure Track Assistant Professor, EPF Lausanne
2016-Present	Associate Professor, EPF Lausanne

Area of research
Theoretical plasma physics.

Specialised in
Turbulent phenomena that occur in the boundary of fusion devices where, within a few centimetres, the temperature drops from values ten times as high as in the core of the sun to room temperature.

HPC means for me
An essential tool to disentangle the complex physical phenomena at play in fusion devices. This is necessary for optimal ITER operation and DEMO design.



Simulation of the tokamak boundary in reactor-relevant conditions

We address the interaction of the plasma with the neutral atoms that are injected with the goal of cooling the plasma before it reaches the solid walls of a fusion reactor.

Papers with Highest Journal Impact Factor[1)]

Nature

Impact Factor: 49.96

S. Park, L. M. Western, T. Saito, A. L. Redington, S. Henne, X. Fang, R. G. Prinn, A. J. Manning, S. A. Montzka, P. J. Fraser, A. L. Ganesan, C. M. Harth, J. Kim, P. B. Krummel, Q. Liang, J. Mühle, S. O'Doherty, H. Park, M.-K. Park, S. Reimann, P. K. Salameh, R. F. Weiss, M. Rigby, A decline in emissions of CFC-11 and related chemicals from Eastern China, Nature, DOI 10.1038/s41586-021-03277-w.

N. Gruber, P. W. Boyd, T. L. Frölicher, M. Vogt, Biogeochemical extremes and compound events in the ocean, Nature, DOI 10.1038/s41586-021-03981-7.

S. Mishra, G. Catarina, F. Wu, R. Ortiz, D. Jacob, K. Eimre, J. Ma, C. A. Pignedoli, X. Feng, P. Ruffieux, J. Fernández-Rossier, R. Fasel, Observation of fractional edge excitations in nanographene spin chains, Nature, DOI 10.1038/s41586-021-03842-3.

J. Jeong, M. Kim, J. Seo, H. Lu, P. Ahlawat, A. Mishra, Y. Yang, M. A. Hope, F. T. Eickemeyer, M. Kim, Y. Jin Yoon, I. W. Choi, B. Primera Darwich, S. J. Choi, Y. Jo, J. H. Lee, B. Walker, S. M. Zakeeruddin, L. Emsley, U. Röthlisberger, A. Hagfeldt, D. S. Kim, M. Grätzel, J. Y. Kim, Pseudo-halide anion engineering for α-$FAPbI_3$ perovskite solar cells, Nature, DOI 10.1038/s41586-021-03406-5.

Science

Impact Factor: 47.73

A. Khan, S. Ceylan, M. van Driel, D. Giardini, P. Lognonne, H. Samuel, N. C. Schmerr, S. C. Stahler, A. C. Duran, Q. C. Huang, D. Kim, A. Broquet, C. Charalambous, J. F. Clinton, P. M. Davis, M. Drilleau, F. Karakostas, V. Lekic, S. M. McLennan, R. R. Maguire, C. Michaut, M. P. Panning, W. T. Pike, B. Pinot, M. Plasman, J. R. Scholz, R. Widmer-Schnidrig, T. Spohn, S. E. Smrekar, W. B. Banerdt, Upper mantle structure of Mars from InSight seismic data, Science, DOI 10.1126/science.abf2966.

S. C. Stähler, A. Khan, B. Banerdt, P. Lognonné, D. Giardini, S. Ceylan, M. Drilleau, C. Duran, R. F. Garcia, Q. Huang, D. Kim, V. Lekic, H. Samuel, M. Schimmel, N. Schmerr, D. Sollberger, E. Stutzmann, Z. Xu, D. Antonangeli, C. Charalambous, P. M. Davis, J. C. E. Irving, T. Kawamura, M. Knapmeyer, R. Maguire, A. G. Marusiak, M. P. Panning, C. Perrin A.-C. Plesa, A. Rivoldini, C. Schmelzbach, G. Zenhäusern, E. Beucler, J. Clinton, N. Dahmen, M. van Driel T. Gudkova, A. Horleston, W. T. Pike, M. Plasman, S. E. Smrekar, Seismic detection of the Martian core, Science, DOI 10.1126/science.abi7730.

Energy & Environmental Science

Impact Factor: 38.53

A. Krishna, H. Zhang, Z. Zhou, T. Gallet, M. Dankl, O. Ouellette, F. T. Eickemeyer, F. Fu, S. Sanchez, M. Mensi, S. M. Zakeeruddin, U. Röthlisberger, G. N. M. Reddy, A. Redinger, M. Grätzel, A. Hagfeldt, Nanoscale interfacial engineering enables highly stable and efficient perovskite photovoltaics, Energy & Environmental Science, DOI 10.1039/D1EE02454J.

Nature Electronics

Impact Factor: 33.69

T. Knobloch, Y. Y. Illarionov, F. Ducry, C. Schleich, S. Wachter, T. Müller, M. Waltl, M. Lanza, M. I. Vexler, M. Luisier, T. Grasser, The performance limits of hexagonal boron nitride as an insulator for scaled CMOS devices based on two-dimensional materials, Nature Electronics, DOI 10.1038/s41928-020-00529-x.

Advanced Materials

Impact Factor: 30.85

S. Stolz, M. Danese, M. Di Giovannantonio, J. I. Urgel, Q. Sun, A. Kinikar, M. Bommert, S. Mishra, H. Brune, O. Gröning, D. Passerone, R. Widmer, Asymmetric elimination reaction on chiral metal surfaces, Advanced Materials, DOI 10.1002/adma.202104481.

Nature Methods

Impact Factor: 28.55

J. A. Alfaro, P. Bohländer, M. Dai, M. Filius, C. J. Howard. X. F. van Kooten, S. Ohayon, A. Pomorski, S. Schmid, A. Aksimentiev, E. V. Anslyn, G. Bedran, C. Cao, M. Chinappi, E. Coyaud, C. Dekker, G. Dittmar, N. Drachman, R. Eelkema, D. Goodlett, S. Hentz, U. Kalathiya, N. L. Kelleher, R. T. Kelly, Z. Kelman, S. H. Kim, B. Kuster, D. Rodriguez-Larrea, S. Lindsay, G. Maglia, E. M. Marcotte, J. P. Marino, C. Masselon, M. Mayer, P. Samaras, K. Sarthak, L. Sepiashvili, D. Stein, M. Wanunu, M. Wilhelm, P. Yin, A. Meller, C. Joo, The emerging landscape of single-molecule protein sequencing technologies, Nature Methods, DOI 10.1038/s41592-021-01143-1.

Nature Chemistry

Impact Factor: 24.43

L. Sévery, J. Szczerbiński, M. Taskin, I. Tuncay, F. Brandalise Nunes, C. Cignarella, G. Tocci, O. Blacque, J. Osterwalder, R. Zenobi, M. Iannuzzi, S. D. Tilley, Immobilization of molecular catalysts on electrode surfaces using host–guest interactions, Nature Chemistry, DOI 10.1038/s41557-021-00652-y.

[1)] Journal of Impact Factor 2021 - JCR, Web Of Science

T. Bian, A. Gardin, J. Gemen, L. Houben, C. Perego, B. Lee, N. Elad, Z. Chu, G. M. Pavan, R. Klajn, Electrostatic co-assembly of nanoparticles with oppositely charged small molecules into static and dynamic superstructures, Nature Chemistry, DOI 10.1038/s41557-021-00752-9.

S. Mishra, X. Yao, Q. Chen, K. Eimre, O. Gröning, R. Ortiz, M. Di Giovannantonio, J. C. Sancho-García, J. Fernández-Rossier, C. A. Pignedoli, K. Müllen, P. Ruffieux, A. Narita, R. Fasel, Large magnetic exchange coupling in rhombus-shaped nanographenes with zigzag periphery, Nature Chemistry, DOI 10.1038/s41557-021-00678-2.

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.

Applied Physics Review
Impact Factor: 19.16

G. Buchs, M. Marganska, J. W. González, K. Eimre, C. A. Pignedoli, D. Passerone, A. Ayuela, O. Gröning, D. Bercioux, Metallic carbon nanotube quantum dots with broken symmetries as a platform for tunable terahertz detection, Applied Physics Reviews, DOI 10.1063/5.0018944.

Nucleic Acids Research
Impact Factor: 16.97

M. D. Hoffmann, J. Mathony, J. Upmeier zu Belzen, Z. Harteveld, S. Aschenbrenner, C. Stengl, D. Grimm, B. E. Correia, R. Eils, D. Niopek, Optogenetic control of Neisseria meningitidis Cas9 genome editing using an engineered, light-switchable anti-CRISPR protein, Nucleic Acids Research, DOI 10.1093/nar/gkaa1198.

ACS Nano
Impact Factor: 15.88

E. Papadopoulou, J. Zavadlav, R. Podgornik, M. Praprotnik, P. Koumoutsakos, Tuning the dielectric response of water in nanoconfinement through surface wettability, ACS Nano, DOI 10.1021/acsnano.1c08512.

K. Portner, M. Schmuck, P. Lehmann, C. Weilenmann, C. Haffner, P. Ma, J. Leuthold, M. Luisier, A. Emboras, Analog nanoscale electro-optical synapses for neuromorphic computing applications, ACS Nano, DOI 10.1021/acsnano.1c04654.

C. Lionello, A. Gardin A. Cardellini, D. Bochicchio, M. Shivrayan, A. Fernandez, S. Thayumanavan, G. M. Pavan, Motion following specific chemical gradients to multivalency-controlled disassembly, ACS Nano, DOI 10.1021/acsnano.1c05000.

A. L. de Marco, D. Bochicchio, A. Gardin, G. Doni, G. M. Pavan, Controlling exchange pathways in dynamic supramolecular polymers by controlling defects, ACS Nano, DOI 10.1021/acsnano.1c01398.

L. Joly, R. H. Meissner, M. Iannuzzi, G. Tocci, Osmotic transport at the aqueous graphene and hBN interfaces: Scaling laws from a unified, first-principles description, ACS Nano, DOI 10.1021/acsnano.1c05931.

Nature Machine Intelligence
Impact Facture: 15.51

G. Novati, H. L. de Laroussilhe, P. Koumoutsakos, Automating turbulence modelling by multi-agent reinforcement learning, Nature Machine Intelligence, DOI 10.1038/s42256-020-00272-0.

Journal of the American Chemical Society
Impact Factor: 15.42

C. Domene, R. Ocello, M. Masetti, S. Furini, Ion conduction mechanism as a fingerprint of potassium channels, Journal of the American Chemical Society, DOI 10.1021/jacs.1c04802.

P. Knecht, B. Zhang, J. Reichert, D. A. Duncan, M. Schwarz, F. Haag, P. T. P. Ryan, Y.-L. Lee, P. S. Deimel, P. Feulner, F. Allegretti, W. Auwärter, G. Médard, A. P. Seitsonen, J. V. Barth, A. C. Papageorgiou, Assembly and manipulation of a prototypical n-heterocyclic carbene with a metalloporphyrin pedestal on a solid surface, Journal of the American Chemical Society, DOI 10.1021/jacs.1c01229.

M. F. Nüesch, M. T. Ivanović, J. B. Claude, D. Nettels, R. B. Best, J. Wenger, B. Schuler, Single-molecule detection of ultrafast biomolecular dynamics with nanophotonics, Journal of the American Chemical Society, DOI 10.1021/jacs.1c09387.

Angewandte Chemie - International Edition
Impact Factor: 15.34

P. Knecht, J. Reichert, P. S. Deimel, P. Feulner, F. Haag, F. Allegretti, M. Garnica, M. Schwarz, W. Auwärter, P. T. P. Ryan, T.-L. Lee, D. A. Duncan, A. P. Seitsonen, J. V. Barth, A. C. Papageorgiou, Conformational control of chemical reactivity for surface-confined Ru-porphyrins, Angewandte Chemie-International Edition, DOI 10.1002/anie.202104075.

A. J. Knorpp, A. B. Pinar, C. Baerlocher, L. B. McCusker, N. Casati, M. A. Newton, S. Checchia, J. Meyet, D. Palagin, J. A. van Bokhoven, Paired copper monomers in zeolite omega: The active site for methane-to-methanol conversion, Angewandte Chemie-International Edition, DOI 10.1002/anie.202014030.

K. Tashiro, K. Katayama, K. Tamaki, L. Pesce, N. Shimizu, H. Takagi, R. Haruki, M. J. Hollamby, G. M. Pavan, S. Yagai, Non-uniform photoinduced unfolding of supramolecular polymers leading to topological block nanofibers, Angewandte Chemie-International Edition, DOI 10.1002/anie.202110224.

G. Moreno-Alcántar, A. Aliprandi, R. Rouquette, L. Pesce, K. Wurst, C. Perego, P. Brüggeller, G. M. Pavan, L. De Cola, Solvent-driven supramolecular wrapping of self-assembled structures, Angewandte Chemie-International Edition, DOI 10.1002/anie.202013474.

Nature Chemical Biology

Impact Factor: 15.04

C. Yang, F. Sesterhenn, J. Bonet, E. A. van Aalen, L. Scheller, L. A. Abriata, J. T. Cramer, X. Wen, S. Rosset, S. Georgeon, T. Jardetzky, T. Krey, M. Fussenegger, M. Merkx, B. E. Correia, Bottom-up de novo design of functional proteins with complex structural features, Nature Chemical Biology, DOI 10.1038/s41589-020-00699-x.

Nature Communications

Impact Factor: 14.92

A. Reinhardt, B. Cheng, Quantum-mechanical exploration of the phase diagram of water, Nature Communications, DOI 10.1038/s41467-020-20821-w.

S. Shui, P. Gainza, L. Scheller, C. Yang, Y. Kurumida, S. Rosset, S. Georgeon, R. B. Di Roberto, R. Castellanos-Rueda, S. T. Reddy, B. E. Correia, A rational blueprint for the design of chemically-controlled protein switches, Nature Communications, DOI 10.1038/s41467-021-25735-9.

E. Cignoni, M. Lapillo, L. Cupellini, S. Acosta-Gutiérrez, F. L. Gervasio, B. Mennucci, A different perspective for nonphotochemical quenching in plant antenna complexes, Nature Communications, DOI 10.1038/s41467-021-27526-8.

T. W. Ko, J. A. Finkler, S. Goedecker, J. Behler, A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer, Nature Communication, DOI 10.1038/s41467-020-20427-2.

J. Lan, V. Kapil, P. Gasparotto, M. Ceriotti, M. Iannuzzi, V. V. Rybkin, Simulating the Ghost: Quantum dynamics of the solvated electron, Nature Communications, DOI 10.1038/s41467-021-20914-0.

E. Grifoni, G. M. Piccini, J. A. Lercher, V.-A. Glezakou, R. Rousseau, M. Parrinello, Confinement effects and acid strength in zeolites, Nature Communications, DOI 10.1038/s41467-021-22936-0.

O. Shyshov, S. V. Haridas, L. Pesce, H. Qi, A. Gardin, D. Bochicchio, U. Kaiser, G. M. Pavan, M. von Delius, Living supramolecular polymerization of fluorinated cyclohexanes, Nature Communications, DOI 10.1038/s41467-021-23370-y.

S. E. Ammerman, V. Jelic, Y. Wei, V. N. Breslin, M. Hassan, N. Everett, S. Lee, Q. Sun, C. A. Pignedoli, P. Ruffieux, R. Fasel, T. L. Cocker, Lightwave-driven scanning tunnelling spectroscopy of atomically precise graphene nanoribbons, Nature Communications, DOI 10.1038/s41467-021-26656-3.

C. Zeni, K. Rossi, T. Pavloudis, J. Kioseoglou, S. de Gironcoli, R. E. Palmer, F. Baletto, Data-driven simulation and characterisation of gold nanoparticle melting, Nature Communications, DOI 10.1038/s41467-021-26199-7.

H. Zhang, F. T. Eickemeyer, Z. Zhou, M. Mladenović, F. Jahanbakhshi, L. Merten, A. Hinderhofer, M. A. Hope, O. Ouellette, A. Mishra, P. Ahlawat, D. Ren, T.-S. Su, A. Krishna, Z. Wang, Z. Dong, J. Guo, S. M. Zakeeruddin, F. Schreiber, A. Hagfeldt, L. Emsley, U. Röthlisberger, J. V. Milić, M. Grätzel, Multimodal host–guest complexation for efficient and stable perovskite photovoltaics, Nature Communications, DOI 10.1038/s41467-021-23566-2.

M. Giraldo, Q. N. Meier, A. Bortis, D. Nowak, N. A. Spaldin, M. Fiebig, M. C. Weber, T. Lottermoser, Magnetoelectric coupling of domains, domain walls and vortices in a multiferroic with independent magnetic and electric order, Nature Communications, DOI 10.1038/s41467-021-22587-1.

C. Guo, A. Alexandradinata, C. Putzke, A. Estry, T. Tu, N. Kumar, F.-R. Fan, S. Zhang, Q. Wu, O. V. Yazyev, K. R. Shirer, M. D. Bachmann, H. Peng, E. D. Bauer, F. Ronning, Y. Sun, C. Shekhar, P. J. W. Moll, Temperature dependence of quantum oscillations from non-parabolic dispersions, Nature Communications, DOI 10.1038/s41467-021-26450-1.

Nature Astronomy

Impact Factor: 14.44

H. Deng, L. Mayer, R. Helled, Formation of intermediate-mass planets via magnetically controlled disk fragmentation, Nature Astronomy, DOI 10.1038/s41550-020-01297-6.

Science Advances

Impact Factor: 14.14

S. Q. Huang, S. X. Li, L. F. Villalobos, M. Dakhchoune, M. Micari, D. J. Babu, M. T. Vahdat, M. Mensi, E. Oveisi, K. V. Agrawal, Millisecond lattice gasification for high-density CO_2- and O_2-sieving nanopores in single-layer graphene, Science Advances, DOI 10.1126/sciadv.abf0116.

W. W. L. Cheung, T. L. Frölicher, V. W. Y. Lam, M. A. Oyinlola G. Reygondeau, R. Sumaila, T. C. Tai, L. C. L. Teh, C. C. C. Wabnitz, Marine high temperature extremes amplify the impacts of climate change on fish and fisheries, Science Advances, DOI 10.1126/sciadv.abh0895.

J. Terhaar, T. L. Frölicher, F. Joos, Southern Ocean anthropogenic carbon sink constrained by sea surface salinity, Science Advances, DOI 10.1126/sciadv.abd5964.

Z. R. Gao, M. Odstrcil, S. Bocklein, D. Palagin, M. Holler, D. F. Sanchez, F. Krumeich, A. Menzel, M. Stampanoni, G. Mestl, J. A. van Bokhoven, M. Guizar-Sicairos, J. Ihli, Sparse ab-initio x-ray transmission spectrotomography for nanoscopic compositional analysis of functional materials, Science Advances, DOI 10.1126/sciadv.abf6971.

P. Ahlawat, A. Hinderhofer, E. A. Alharbi, H. Lu, A. Ummadisingu, H. Niu, M. Invernizzi, S. M. Zakeeruddin, I. Dar, F. Schreiber, A. Hagfeldt, M. Grätzel, U. Röthlisberger, M. Parrinello, A combined molecular dynamics and experimental study of two-step process enabling low-temperature formation of phase-pure α-$FAPbI_3$, Science Advances, DOI 10.1126/sciadv.abe3326.

Genome Biology

Impact Factor: 13.58

M. A. Skinnider, J. W. Squair, G. Courtine, Enabling reproducible re-analysis of single-cell data, Genome Biology, DOI 10.1186/s13059-021-02422-y.

Journal of Materials Chemistry A

Impact Factor: 12.73

A. Boucly, L. Artiglia, E. Fabbri, D. Palagin, D. Aegerter, D. Pergolesi, Z. Novotny, N. Comini, J. T. Diulus, T. Huthwelker, M. Ammann, T. J. Schmidt, Direct evidence of cobalt oxyhydroxide formation on a $La_{0.2}Sr_{0.8}CoO_3$ perovskite water splitting catalyst, Journal of Materials Chemistry A, DOI 10.1039/d1ta04957g.

X. Wang, A. Beck, J. A. van Bokhoven, D. Palagin, Thermodynamic insights into strong metal–support interaction of transition metal nanoparticles on titania: simple descriptors for complex chemistry, Journal of Materials Chemistry A, DOI 10.1039/d0ta11650e.

Developmental Cell

Impact Factor: 12.27

F. S. Mesquita, L. Abrami, O. Sergeeva, P. Turelli, E. Qing, B. Kunz, C. Raclot, J. Paz Montoya, L. A. Abriata, T. Gallagher, M. Dal Peraro, D. Trono, G. D'Angelo, F. G. van der Goot, S-acylation controls SARS-CoV-2 membrane lipid organization and enhances infectivity, Developmental Cell, DOI 10.1016/j.devcel.2021.09.016.

Nucleic Acids Research

Impact Factor: 11.50

M. D. Hoffmann, J. Mathony, J. Upmeier zu Belzen, Z. Harteveld, S. Aschenbrenner, C. Stengl, D. Grimm, B. E. Correia, R. Eils, D. Niopek, Optogenetic control of Neisseria meningitidis Cas_9 genome editing using an engineered, light-switchable anti-CRISPR protein, Nucleic Acids Research, DOI 10.1093/nar/gkaa1198.

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

Impact Factor: 11.21

R.-A. A. Garibsingh, E. Ndaru, A. A. Garaeva, Y. Shi, L. Zielewicz, P. Zakrepine, M. Bonomi, D. J. Slotboom, C. Paulino, C. Grewer, A. Schlessinger, Rational design of ASCT2 inhibitors using an integrated experimental-computational approach, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2104093118.

V. Zoni, R. Khaddaj, I. Lukmantara, W. Shinoda, H. Yang, R. Schneiter, S. Vanni, Seipin accumulates and traps diacylglycerols and triglycerides in its ring-like structure, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2017205118.

Nano Letters

Impact Factor: 11.19

D. Campi, S. Kumari, N. Marzari, Prediction of phonon-mediated superconductivity with high critical temperature in the two-dimensional topological semimetal W_2N_3, Nano Letters, DOI 10.1021/acs.nanolett.0c05125.

N. V. Tepliakov, Q.S. Wu, O. V. Yazyev, Crystal field effect and electric field screening in multilayer graphene with and without twist, Nano Letters, DOI 10.1021/acs.nanolett.1c00678.

Global Change Biology

Impact Factor: 10.86

C. M. Duarte, C. R. Voolstra, Integrating environmental variability to broaden the research on coral responses to future ocean conditions, Global Change Biology, DOI 10.1111/gcb.15840.

Remote Sensing of Environment

Impact Factor: 10.16

M. Kim, D. Brunner, G. Kuhlmann, Importance of satellite observations for high-resolution mapping of near-surface NO_2 by machine learning, Remote Sensing of Environment, DOI 10.1016/j.rse.2021.112573.

Chemical Science

Impact Factor: 9.83

L. M. Mateo, Q. Sun, K. Eimre, C. A. Pignedoli, T. Torres, R. Fasel, G. Bottari, On-surface synthesis of singly and doubly porphyrin-capped graphene nanoribbon segments, Chemical Science, DOI 10.1039/D0SC04316H.

S. B. Varandili, D. Stoian, J. Vavra, K. Rossi, J. R. Pankhurst, Y. T. Guntern, N. López, R. Buonsanti, Elucidating the structure-dependent selectivity of CuZn towards methane and ethanol in CO_2 electroreduction using tailored Cu/ZnO precatalysts, Chemical Science, DOI 10.1039/D1SC04271H.

Chemistry of Materials

Impact Factor: 9.81

A. Mishra, P. Ahlawat, G. C. Fish, F. Jahanbakhshi, M. Mladenović, M. Almalki, M. A. Ruiz-Preciado, M. C. Gelvéz-Rueda, D. J. Kubicki, P. A. Schouwink, V. Dufoulon, T. Schneeberger, A. Aslanzadeh, F. C. Grozema, S. M. Zakeeruddin, J.-E. Moser, U. Röthlisberger, L. Emsley, J. V. Milić, M. Grätzel, Naphthalenediimide/formamidinium-based low-dimensional perovskites, Chemistry of Materials, DOI 10.1021/acs.chemmater.1c01635.

Chemical Science

Impact Factor: 9.83

A. Grisafi, J. Nigam, M. Ceriotti, Multi-scale approach for the prediction of atomic scale properties, Chemical Science, DOI 10.1039/d0sc04934d.

Carbon

Impact Factor: 9.59

P. P. Shinde, J. Liu, T. Dienel, O. Gröning, T. Dumslaff, M. Mühlinghaus, A. Narita, K. Müllen, C. A. Pignedoli, R. Fasel, P. Ruffieux, D. Passerone, Graphene nanoribbons with mixed cove-cape-zigzag edge structure, Carbon, DOI 10.1016/j.carbon.2020.12.069.

ACS Applied Materials & Interfaces

Impact Factor: 9.23

B. Chen, F. Qin, M. Su, Z. Zhang, Q. Pan, M. Zou, X. Yang, S. Chen, D. Derome, J. Carmeliet, Y. Song, Self-driven multiplex reaction: Reactant and product diffusion via a transpiration-inspired capillary, ACS Applied Materials & Interfaces, DOI 10.1021/acsami.1c03614.

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.

Physical Review Letters

Impact Factor: 9.16

D. E. Gökmen, Z. Ringel, S. D. Huber, M. Koch-Janusz, Statistical physics through the lens of real-space mutual information, Physical Review Letters, DOI 10.1103/PhysRevLett.127.240603.

M. H. Dehn, J. K. Shenton, D. J. Arseneau, W. A. MacFarlane, G. D. Morris, A. Maigné, N. A. Spaldin, R. F. Kiefl, Local electronic structure and dynamics of muon-polaron complexes in Fe_2O_3, Physical Review Letters, DOI 10.1103/PhysRevLett.126.037202.

T. Silva, L. D. Amorim, M. C. Downer, M. J. Hogan, V. Yakimenko, R. Zgadzaj, J. Vieira, Stable positron acceleration in thin, warm, hollow plasma channels, Physical Review Letters, DOI 10.1103/PhysRevLett.127.104801.

Q.S. Wu, J. Liu, Y. Guan, O. V. Yazyev, Landau levels as a probe for band topology in graphene Moiré superlattices, Physical Review Letters, DOI 10.1103/PhysRevLett.126.056401.

C. Alexandrou, S. Bacchio, G. Bergner, J. Finkenrath, A. Gasbarro, K. Hadjiyiannakou, K. Jansen, B. Kostrzewa, K. Ottnad, M. Petschlies, F. Pittler, F. Steffens, C. Urbach, U. Wenger, Quark and gluon momentum fractions in the pion from $N_f = 2 + 1 + 1$ Lattice QCD, Physical Review Letters, DOI 10.1103/PhysRevLett.127.252001.

A. Bulgac, I. Abdurrahman, S. Jin, K. Godbey, N. Schunck, I. Stetcu, Fission fragment intrinsic spins and their correlations, Physical Review Letters, DOI 10.1103/PhysRevLett.126.142502.

Nano Research

Impact Factor: 8.90

X. Xu, M. Di Giovannantonio, J. I. Urgel, C. A. Pignedoli, P. Ruffieux, K. Müllen, R. Fasel, A. Narita, On-surface activation of benzylic C-H bonds for the synthesis of pentagon-fused graphene nanoribbons, Nano Research, DOI 10.1007/s12274-021-3419-2.

eLife

Impact Factor: 8.14

I. Galdadas, L. Carlino, R. A Ward, S. J Hughes, S. Haider, F. L. Gervasio, Structural basis of the effect of activating mutations on the EGF receptor, eLife, DOI 10.7554/eLife.65824.

E. Trofimenko, G. Grasso, M. Heulot, N. Chevalier, M. A Deriu, G. Dubuis, Y. Arribat, M. Serulla, S. Michel, G. Vantomme, F. Ory, L. C. Dam, J. Puyal, F. Amati, A. Lüthi, A. Danani, C. Widmann, Genetic, cellular, and structural characterization of the membrane potential-dependent cell-penetrating peptide translocation pore, eLife, DOI 10.7554/eLife.69832.

S. Vullo, N. Ambrosio, J. P. Kucera, O. Bignucolo, S. Kellenberger, Kinetic analysis of ASIC1a delineates conformational signaling from proton-sensing domains to the channel gate, eLife, DOI 10.7554/eLife.66488.

J. Jordan, M. Schmidt, W. Senn, M. A. Petrovici, Evolving interpretable plasticity for spiking networks, eLife, DOI 10.7554/eLife.66273.

V. Zoni, R. Khaddaj, P. Campomanes, A. R. Thiam, R. Schneiter, S. Vanni, Pre-existing bilayer stresses modulate triglyceride accumulation in the ER versus lipid droplets, eLife, DOI 10.7554/eLife.62886.


INDUPRO
044-835 30 70
K-FLEX

Papers Published in 2021 by Principal Investigator

Julian Adamek, University of Zurich

F. Lepori, J. Adamek, R. Durrer, Cosmological simulations of number counts, Journal of Cosmology and Astroparticle Physics, DOI 10.1088/1475-7516/2021/12/021.

Donat J. Adams, University of Bern

D. J. Adams, L. Wang, G. Steinle-Neumann, D. Passerone, S. V. Churakov, Anharmonic effects on the dynamics of solid aluminum from ab-initio simulations, Journal of Physics: Condensed Matter, DOI 10.1088/1361-648X/abc972.

Andreas Adelmann, Paul Scherrer Institute

M. Frey, A. Adelmann, Global sensitivity analysis on numerical solver parameters of Particle-In-Cell models in particle accelerator systems, Computer Physics Communications, DOI 10.1016/j.cpc.2020.107577.

Alex Aiken, Stanford University

R. Soi, M. Bauer, S. Treichler, M. Papadakis, W. Lee, P. McCormick, A. Aiken, E. Slaughter, Index launches: Scalable, flexible representation of parallel task groups, Proceedings of the International Conference on Supercomputing, DOI 10.1145/3458817.3476175.

M. Bauer, W. Lee, E. Slaughter, Z. Jia, M. Di Renzo, M. Papadakis, G. Shipman, P. McCormick, M. Garland, A. Aiken, Scaling implicit parallelism via dynamic control replication, Proceedings of Principles and Practice of Parallel Programming, DOI 10.1145/3437801.3441587.

Sebnem Aksoyoglu, Paul Scherrer Institute

J. Jiang, I. El Haddad, S. Aksoyoglu, G. Stefenelli, A. Bertrand, N. Marchand, F. Canonaco, J.-E. Petit, O. Favez, S. Gilardoni, U. Baltensperger, A. S. H. Prévôt, Influence of biomass burning vapor wall loss correction on modeling organic aerosols in Europe by CAMx v6.50, Geoscientific Model Development, DOI 10.5194/gmd-14-1681-2021.

Kumar Varoon Agrawal, EPF Lausanne

S. Q. Huang, S. X. Li, L. F. Villalobos, M. Dakhchoune, M. Micari, D. J. Babu, M. T. Vahdat, M. Mensi, E. Oveisi, K. V. Agrawal, Millisecond lattice gasification for high-density CO_2- and O_2-sieving nanopores in single-layer graphene, Science Advances, DOI 10.1126/sciadv.abf0116.

Constantia Alexandrou, University of Cyprus & Cyprus Institute

C. Alexandrou, S. Bacchio, M. Constantinou, P. Dimopoulos, J. Finkenrath, K. Hadjiyiannakou, K. Jansen, G. Koutsou, B. Kostrzewa, T. Leontiou, C. Urbach, Nucleon axial and pseudoscalar form factors from lattice QCD at the physical point, Physical Review D, DOI 10.1103/PhysRevD.103.034509.

C. Alexandrou, A. Athenodorou, K. Hadjiyiannakou, A. Todaro, Neutron electric dipole moment using lattice QCD simulations at the physical point, Physical Review D, DOI 10.1103/PhysRevD.103.054501.

C. Alexandrou, S. Bacchio, M. Constantinou, K. Hadjiyiannakou, K. Jansen, G. Koutsou, Quark flavor decomposition of the nucleon axial form factors, Physical Review D, DOI 10.1103/PhysRevD.104.074503.

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, E. Papadiofantous, F. Pittler, G. C. Rossi, F. Sanfilippo, S. Simula, C. Tarantino, A. Todaro, C. Urbach, U. Wenger, Quark masses using twisted-mass fermion gauge ensembles, Physical Review D, DOI 10.1103/PhysRevD.104.074515.

Ulrich Aschauer, University of Bern

C. Ricca, U. Aschauer, Interplay between polarization, strain, and defect pairs in Fe-doped $SrMnO_{3-\delta}$, Physical Review Research, DOI 10.1103/PhysRevResearch.3.033237.

C. Ricca, D. Berkowitz, U. Aschauer, Ferroelectricity promoted by cation/anion divacancies in $SrMnO_3$, Journal of Materials Chemistry C, DOI 10.1039/D1TC02317A.

J. Franklin, B. Xu, D. Davino, A. Mahabir, A. V. Balatsky, U. Aschauer, I. Sochnikov, Giant Grüneisen parameter in a superconducting quantum paraelectric, Physical Review B, DOI 10.1103/PhysRevB.103.214511.

V. Stotskyi, U. Aschauer, Water oxidation catalysis on the nitrogen-deficient $SrNbO_2N(001)$ surface, The Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.0c09445.

M. Bouri, S. Ninova, H. Ouhbia, N. Vonrüti, U. Aschauer, Surface chemistry of perovskite oxynitride photocatalysts: A computational perspective, Chimia, DOI 10.2533/chimia.2021.202.

Dirk Bakowies, University of Basel

D. Bakowies, O. A. von Lilienfeld, Density functional geometries and zero-point energies in ab-initio thermochemical treatments of compounds with first-row atoms (H, C, N, O, F), Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.1c00474.

Justin Ball, EPF Lausanne

J. Ball, S. Brunner, A non-twisting flux tube for local gyrokinetic simulations, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/abf8f4.

C. J. Ajay, S. Brunner, J. Ball, Effect of collisions on non-adiabatic electron dynamics in ITG-driven microturbulence, Physics of Plasmas, DOI 10.1063/5.0055303.

Nikolina Ban, University of Innsbruck

N. Ban, C. Caillaud, E. Coppola, E. Pichelli, S. Sobolowski, M. Adinolfi, B. Ahrens, A. Alias, I. Anders, S. Bastin, D. Belušić, S. Berthou, E. Brisson, R. M. Cardoso, S. C. Chan, O. Bøssing Christensen, J. Fernández, Lluís Fita, T. Frisius, G. Gašparac, F. Giorgi, K. Goergen, J. E. Haugen, Ø. Hodnebrog, S. Kartsios, E. Katragkou, E. J. Kendon, K. Keuler, A. Lavin-Gullon, G. Lenderink, D. Leutwyler, T. Lorenz, D. Maraun, P. Mercogliano, J. Milovac, H.-J. Panitz, M. Raffa, A. Reca Remedio, C. Schär, P. M. M Soares, L. Srnec, B. M. Steensen, P. Stocchi, M. H. Tölle, H. Truhetz, J. Vergara-Temprado, H. de Vries, K. Warrach-Sagi, V. Wulfmeyer, M. J. Zander, The first multi-model ensemble of regional climate simulations at kilometer-scale resolution, part I: Evaluation of precipitation, Climate Dynamics, DOI 10.1007/s00382-021-05708-w.

A. Serifi, T. Günther, N. Ban, Spatio-temporal downscaling of climate data using convolutional and error-predicting neural networks, Frontiers in Climate, DOI 10.3389/fclim.2021.656479.

Quentin Barraud, EPF Lausanne

M. A. Skinnider, J. W. Squair, G. Courtine, Enabling reproducible re-analysis of single-cell data, Genome Biology, DOI 10.1186/s13059-021-02422-y.

Dmitry Bocharov, University of Latvia

D. Bocharov, I. Pudza, K. Klementiev, M. Krack, A. Kuzmin, Study of high-temperature behaviour of ZnO by ab-initio molecular dynamics simulations and X-ray absorption spectroscopy, Materials, DOI 10.3390/ma14185206.

Massimiliano Bonomi, Institute Pasteur Paris

Y. Karami, A. López-Castilla, A. Ori, J. L. Thomassin, B. Bardiaux, T. Malliavin, N. Izadi-Pruneyre, O. Francetic, M. Nilges, Computational and biochemical analysis of type IV pilus dynamics and stability, Structure, DOI 10.1016/j.str.2021.07.008.

R.-A. A. Garibsingh, E. Ndaru, A. A. Garaeva, Y. Shi, L. Zielewicz, P. Zakrepine, M. Bonomi, D. J. Slotboom, C. Paulino, C. Grewer, A. Schlessinger, Rational design of ASCT2 inhibitors using an integrated experimental-computational approach, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2104093118.

Dominik Brunner, Empa

M. Kim, D. Brunner, G. Kuhlmann, Importance of satellite observations for high-resolution mapping of near-surface NO_2 by machine learning, Remote Sensing of Environment, DOI 10.1016/j.rse.2021.112573.

G. Kuhlmann, S. Henne, Y. Meijer, D. Brunner, Quantifying CO_2 emissions of power plants with CO_2 and NO_2 imaging satellites, Frontiers in Remote Sensing, DOI 10.3389/frsen.2021.689838.

S. Park, L. M. Western, T. Saito, A. L. Redington, S. Henne, X. Fang, R. G. Prinn, A. J. Manning, S. A. Montzka, P. J. Fraser, A. L. Ganesan, C. M. Harth, J. Kim, P. B. Krummel, Q. Liang, J. Mühle, S. O'Doherty, H. Park, M.-K. Park, S. Reimann, P. K. Salameh, R. F. Weiss, M. Rigby, A decline in emissions of CFC-11 and related chemicals from Eastern China, Nature, DOI 10.1038/s41586-021-03277-w.

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.

Amedeo Caflisch, University of Zurich

E. V. Moroz-Omori, D. Huang, R. K. Bedi, S. J. Cheriyamkunnel, E. Bochenkova, A. Dolbois, M. D. Rzeczkowski, Y. Li, L. Wiedmer, A. Caflisch, METTL3 inhibitors for epitranscriptomic modulation of cellular processes, ChemMedChem, DOI 10.1002/cmdc.202100291.

Y. Li, R. K. Bedi, L. Wiedmer, X. Sun, D. Huang, A. Caflisch, Atomistic and thermodynamic analysis of N6-Methyladenosine (m^6A) recognition by the reader domain of YTHDC1, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.0c01136.

C. Camilloni, University of Milan

C. Paissoni, C. Camilloni, How to determine accurate conformational ensembles by metadynamics metainference: A chignolin study case, Frontiers in Molecular Biosciences, DOI 10.3389/fmolb.2021.694130.

D. Saad, C. Paissoni, A. Chaves-Sanjuan, M. Nardini, R. Mantovani, N. Gnesutta, C. Camilloni, High conformational flexibility of the E2F1/DP1/DNA complex, Journal of Molecular Biology, DOI 10.1016/j.jmb.2021.167119.

Jan Carmeliet, ETH Zurich

F. Qin, J. Zhao, Q. Kang, D. Derome, J. Carmeliet, Lattice Boltzmann modeling of drying of porous media considering contact angle hysteresis, Transport in Porous Media, DOI 10.1007/s11242-021-01644-9.

J. Zhao, F. Qin, Q. Kang, D. Derome, J. Carmeliet, Pore-scale simulation of drying in porous media using a hybrid lattice Boltzmann: Pore network model, Drying Technology, DOI 10.1080/07373937.2021.1933017.

B. Chen, F. Qin, M. Su, Z. Zhang, Q. Pan, M. Zou, X. Yang, S. Chen, D. Derome, J. Carmeliet, Y. Song, Self-driven multiplex reaction: Reactant and product diffusion via a transpiration-inspired capillary, ACS Applied Materials & Interfaces, DOI 10.1021/acsami.1c03614.

F. Qin, J. Zhao, Q. Kang, T. Brunschwiler, J. Carmeliet, D. Derome, Three influential factors on colloidal nanoparticle deposition for heat conduction enhancement in 3D chip stacks, Applied Thermal Engineering, DOI 10.1016/j.applthermaleng.2021.116585.

T. C. de Goede, A. M. Moqaddam, K. C. M. Limpens, S. A. Kooij, D. Derome, J. Carmeliet, N. Shahidzadeh, D. Bonn, Droplet impact of Newtonian fluids and blood on simple fabrics: Effect of fabric pore size and underlying substrate, Physics of Fluids, DOI 10.1063/5.0037123.

F. Qin, J. Zhao, Q. Kang, T. Brunschwiler, D. Derome, J. Carmeliet, Lattice Boltzmann modeling of heat conduction enhancement by colloidal nanoparticle deposition in microporous structures, Physical Review E, DOI 10.1103/PhysRevE.103.023311.

J. Zhao, F. Qin, R. Fischer, Q. Kang, D. Derome, J. Carmeliet, Spontaneous imbibition in a square tube with corner films: Theoretical model and numerical simulation, Water Resources Research, DOI 10.1029/2020WR029190.

Michele Ceriotti, EPF Lausanne

R. K. Cersonsky, B. A. Helfrecht, E. A. Engel, S. Kliavinek, M. Ceriotti, Improving sample and feature selection with principal covariates regression, Machine Learning: Science and Technology, DOI 10.1088/2632-2153/abfe7c.

E. A. Engel, V. Kapil, M. Ceriotti, Importance of Nuclear Quantum Effects for NMR Crystallography, The Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.1c01987.

A. Grisafi, J. Nigam, M. Ceriotti, Multi-scale approach for the prediction of atomic scale properties, Chemical Science, DOI 10.1039/d0sc04934d.

Bingqing Cheng, University of Cambridge

A. Reinhardt, B. Cheng, Quantum-mechanical exploration of the phase diagram of water, Nature Communications, DOI 10.1038/s41467-020-20821-w.

Mauro Chinappi, University of Rome Tor Vergata

A. Shahmardi, O. Tammisola, M. Chinappi, L. Brandt, Effects of surface nanostructure and wettability on pool boiling: A molecular dynamics study, International Journal of Thermal Sciences, DOI 10.1016/j.ijthermalsci.2021.106980.

J. A. Alfaro, P. Bohländer, M. Dai, M. Filius, C. J. Howard. X. F. van Kooten, S. Ohayon, A. Pomorski, S. Schmid, A. Aksimentiev, E. V. Anslyn, G. Bedran, C. Cao, M. Chinappi, E. Coyaud, C. Dekker, G. Dittmar, N. Drachman, R. Eelkema, D. Goodlett, S. Hentz, U. Kalathiya, N. L. Kelleher, R. T. Kelly, Z. Kelman, S. H. Kim, B. Kuster, D. Rodriguez-Larrea, S. Lindsay, G. Maglia, E. M. Marcotte, J. P. Marino, C. Masselon, M. Mayer, P. Samaras, K. Sarthak, L. Sepiashvili, D. Stein, M. Wanunu, M. Wilhelm, P. Yin, A. Meller, C. Joo, The emerging landscape of single-molecule protein sequencing technologies, Nature Methods, DOI 10.1038/s41592-021-01143-1.

Bastien Chopard, University of Geneva

C. Kotsalos, J. Latt, J. Beny, B. Chopard, Digital blood in massively parallel CPU/GPU systems for the study of platelet transport, Interface Focus, DOI 10.1098/rsfs.2019.0116.

J. Latt, O. Malaspinas, D. Kontaxakis, A. Parmigiani, D. Lagrava, F. Brogi, M. B. Belgacem, Y. Thorimbert, S. Leclaire, S. Li, F. Marson, J. Lemus, C. Kotsalos, R. Conradin, C. Coreixas, R. Petkantchin, F. Raynaud, J. Beny, B. Chopard, Palabos: Parallel lattice Boltzmann solver, Computers & Mathematics with Applications, DOI 10.1016/j.camwa.2020.03.022.

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

D. P. Roos, A. C. Scheinost, S. V. Churakov, M. Nagashima, G. Cametti, On the nature of Pb species in Pb-exchanged zeolite stellerite (STI): A combined experimental and theoretical study, Microporous and Mesoporous Materials, DOI 10.1016/j.micromeso.2021.111444.

K. Karalis, D. Zahn, N. I. Prasianakis, B. Niceno, S. V. Churakov, Deciphering the molecular mechanism of water boiling at heterogeneous interfaces, Scientific Reports, DOI 10.1038/s41598-021-99229-5.

R. Schliemann, S. V. Churakov, Pyrophyllite dissolution at elevated pressure conditions: An ab-initio study, Geochimica et Cosmochimica Acta, DOI 10.1016/j.gca.2021.05.017.

R. Schliemann, S. V. Churakov, Atomic scale mechanism of clay minerals dissolution revealed by ab-initio simulations, Geochimica et Cosmochimica Acta, DOI 10.1016/j.gca.2020.10.026.

G. Cametti, A. C. Scheinost, S. V. Churakov, Cd^{2+} incorporation in small-pore LEV/ERI intergrown zeolites: A multi-methodological study, Microporous and Mesoporous Materials, DOI 10.1016/j.micromeso.2020.110835.

Florina M. Ciorba, University of Basel

A. Eleliemy, F. M. Ciorba, A distributed chunk calculation approach for self-scheduling of parallel applications on distributed-memory systems, Journal of Computational Science, DOI 10.1016/j.jocs.2020.101284.

Andrea Colombi, ETH Zurich

P. Martakis, G. Aguzzi, V. K. Dertimanis, E. N. Chatzi, A. Colombi, Nonlinear periodic foundations for seismic protection: Practical design, realistic evaluation and stability considerations, Soil Dynamics and Earthquake Engineering, DOI 10.1016/j.soildyn.2021.106934.

Bruno E. Correia, EPF Lausanne

C. Yang, F. Sesterhenn, J. Bonet, E. A. van Aalen, L. Scheller, L. A. Abriata, J. T. Cramer, X. Wen, S. Rosset, S. Georgeon, T. Jardetzky, T. Krey, M. Fussenegger, M. Merkx, B. E. Correia, Bottom-up de novo design of functional proteins with complex structural features, Nature Chemical Biology, DOI 10.1038/s41589-020-00699-x.

G. Sormani, Z. Harteveld, S. Rosset, B. Correia, A. Laio, A Rosetta-based protein design protocol converging to natural sequences, The Journal of Chemical Physics, DOI 10.1063/5.0039240.

M. D. Hoffmann, J. Mathony, J. Upmeier zu Belzen, Z. Harteveld, S. Aschenbrenner, C. Stengl, D. Grimm, B. E. Correia, R. Eils, D. Niopek, Optogenetic control of Neisseria meningitidis Cas9 genome editing using an engineered, light-switchable anti-CRISPR protein, Nucleic Acids Research, DOI 10.1093/nar/gkaa1198.

S. Shui, P. Gainza, L. Scheller, C. Yang, Y. Kurumida, S. Rosset, S. Georgeon, R. B. Di Roberto, R. Castellanos-Rueda, S. T. Reddy, B. E. Correia, A rational blueprint for the design of chemically-controlled protein switches, Nature Communications, DOI 10.1038/s41467-021-25735-9.

Matteo Dal Peraro, EPF Lausanne

F. S. Mesquita, L. Abrami, O. Sergeeva, P. Turelli, E. Qing, B. Kunz, C. Raclot, J. Paz Montoya, L. A. Abriata, T. Gallagher, M. Dal Peraro, D. Trono, G. D'Angelo, F. G. van der Goot, S-acylation controls SARS-CoV-2 membrane lipid organization and enhances infectivity, Developmental Cell, DOI 10.1016/j.devcel.2021.09.016.

A. Chiki, Z. Zhang, K. Rajasekhar, L. A. Abriata, I. Rostami, L. F. Krapp, D. Boudeffa, M. Dal Peraro, H. A. Lashuel, Investigating crosstalk among PTMs provides novel insight into the structural basis underlying the differential effects of Nt17 PTMs on mutant Httex1 aggregation, Frontiers in Molecular Biosciences, DOI 10.3389/fmolb.2021.686086.

L. A. Abriata, M. Dal Peraro, Assessment of transferable force-fields for protein simulations attests improved description of disordered states and secondary structure propensities, and hints at multi-protein systems as the next challenge for optimization, Computational and Structural Biotechnology Journal, DOI 10.1016/j.csbj.2021.04.050.

Carmen Domene, University of Bath

C. Domene, R. Ocello, M. Masetti, S. Furini, Ion conduction mechanism as a fingerprint of potassium channels, Journal of the American Chemical Society, DOI 10.1021/jacs.1c04802.

S. Gonzalez-Resines, P. J. Quinn, R. J. Naftalin, C. Domene, Multiple interactions of glucose with the extra-membranous loops of GLUT1 aid transport, Journal of Chemical Information and Modeling, DOI 10.1021/acs.jcim.1c00310.

Robert Feldmann, University of Zurich

L. Liang, R. Feldmann, C. C. Hayward, D. Narayanan, O. Çatmabacak, D. Kereš, C.-A. Faucher Giguère, P. F. Hopkins, The IRX–β relation of high-redshift galaxies, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab096.

E. Rohr, R. Feldmann, J. S Bullock, O. Çatmabacak, M. Boylan-Kolchin, C.-A. Faucher-Giguère, D. Kereš, L. Liang, J. Moreno, A. Wetzel, The galaxy–halo size relation of low–mass galaxies in FIRE, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab3625.

Andreas Fichtner, ETH Zurich

Y. Gao, X. Yuan, B. Heit, F. Tilmann, D.-P. van Herwaarden, S. Thrastarson, A. Fichtner, B. Schurr, Impact of the Juan Fernandez Ridge on the pampean flat subduction inferred from full waveform inversion, Geophysical Research Letters, DOI 10.1029/2021GL095509.

S.-S. Chen, S.-G. Lee, S. Simutė, A. Fichtner, T. J. Lee, Y.-S. Lee, J.-Q. Liu, R. Gao,Geochemical and seismic tomography constraints of two-layer magma chambers beneath the bimodal volcanism: A case study of late Cenozoic volcanic rocks from Ulleung Island and Mt. Changbai (Paektu), Chemical Geology, DOI 10.1016/j.chemgeo.2021.120386.

J. K. H. Igel, L. A. Ermert, A. Fichtner, Rapid finite-frequency microseismic noise source inversion at regional to global scales, Geophysical Journal International, DOI 10.1093/gji/ggab210.

Y. Gao, F. Tilmann, D.-P. van Herwaarden, S. Thrastarson, A. Fichtner, B. Heit, X. Yuan, B. Schurr, Full waveform inversion beneath the central Andes: Insight into the dehydration of the Nazca slab and delamination of the back-arc lithosphere, Journal of Geophysical Research-Solid Earth, DOI 10.1029/2021JB021984.

L. A. Ermert, K. Sager, T. Nissen-Meyer, A. Fichtner, Multifrequency inversion of global ambient seismic sources, Geophysical Journal International, DOI 10.1093/gji/ggab050.

D. P. van Herwaarden, M. Afanasiev, S. Thrastarson, A. Fichtner, Evolutionary full-waveform inversion, Geophysical Journal International, DOI 10.1093/gji/ggaa459.

V. Hapla, M. G. Knepley, M. Afanasiev, C. Boehm, M. van Driel, L. Krischer, A. Fichtner, Fully parallel mesh I/O using PETSc DMPlex with an application to waveform modeling, SIAM Journal on Scientific Computing, DOI 10.1137/20M1332748.

P. Marty, C. Boehm, A. Fichtner, Acoustoelastic full-waveform inversion for transcranial ultrasound computed tomography, Medical Imaging 2021: Ultrasonic Imaging and Tomography, DOI 10.1117/12.2581029.

Carlo Fiorina, EPF Lausanne

S. Radman, C. Fiorina, A. Pautz, Development of a novel two-phase flow solver for nuclear reactor analysis: Validation against sodium boiling experiments, Nuclear Engineering and Design, DOI 10.1016/j.nucengdes.2021.111422.

S. Radman, C. Fiorina, A. Pautz, Development of a novel two-phase flow solver for nuclear reactor analysis: Algorithms, verification and implementation in OpenFOAM, Nuclear Engineering and Design, DOI 10.1016/j.nucengdes.2021.111178.

A. Scolaro, P. Van Uffelen, C. Fiorina, A. Schubert, I. Clifford, A. Pautzac, Investigation on the effect of eccentricity for fuel disc irradiation tests, Nuclear Engineering and Technology, DOI 10.1016/j.net.2020.11.003.

Samrock Friedemann, ETH Zurich

F. Samrock, A. V. Grayver, O. Bachmann, Ö. Karakas, M. O. Saar, Integrated magnetotelluric and petrological analysis of felsic magma reservoirs: Insights from Ethiopian rift volcanoes, Earth and Planetary Science Letters, DOI 10.1016/j.epsl.2021.116765.

Thomas Frölicher, University of Bern

N. Gruber, P. W. Boyd, T. L. Frölicher, M. Vogt, Biogeochemical extremes and compound events in the ocean, Nature, DOI 10.1038/s41586-021-03981-7.

W. W. L. Cheung, T. L. Frölicher, V. W. Y. Lam, M. A. Oyinlola G. Reygondeau, R. Sumaila, T. C. Tai, L. C. L. Teh, C. C. C. Wabnitz, Marine high temperature extremes amplify the impacts of climate change on fish and fisheries, Science Advances, DOI 10.1126/sciadv.abh0895.

M. Ziegler, A. Anton, S. G. Klein, N. Rädecker, N. R. Geraldi, S. Schmidt-Roach, V. Saderne, P. J. Mumby, M. J. Cziesielski, C. Martin, T. L. Frölicher, J. M. Pandolfi, D. J. Suggett, M. Aranda, C. M. Duarte, C. R. Voolstra, Integrating environmental variability to broaden the research on coral responses to future ocean conditions, Global Change Biology, DOI 10.1111/gcb.15840.

T. M. Clarke, C. C. C. Wabnitz, S. Striegel, T. L. Frölicher, G. Reygondeau, W. W. L. Cheung, Aerobic growth index (AGI): An index to understand the impacts of ocean warming and deoxygenation on global marine fisheries resources, Progress in Oceanography, DOI 10.1016/j.pocean.2021.102588.

Oliver Fuhrer, Vulcan Inc.

S. Westerhuis, O. Fuhrer, A locally smoothed terrain-following vertical coordinate to improve the simulation of fog and low stratus in numerical weather prediction models, Journal of Advances in Modeling Earth Systems, DOI 10.1029/2020MS002437.

Thomas Gehrmann, University of Zurich

A. Buckley, X. Chen, J. Cruz-Martinez, S. Ferrario Ravasio, T. Gehrmann, E. W. N. Glover, S. Höche, A. Huss, J. Huston, J. M. Lindert, S. Plätzer, M. Schönherr, A comparative study of Higgs boson production from vector-boson fusion, Journal of High Energy Physics, DOI 10.1007/JHEP11(2021)108.

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

S. Ilmjärv, F. Abdul, S. Acosta-Gutiérrez, C. Esrarellas, I. Galdadas, M. Casimir, M. Alessandrini, F. L. Gervasio, K.-H. Krause, Concurrent mutations in RNA-dependent RNA polymerase and spike protein emerged as the epidemiologically most successful SARS-CoV-2 variant, Scientific Reports, DOI 10.1038/s41598-021-91662-w.

I. Galdadas, L. Carlino, R. A Ward, S. J Hughes, S. Haider, F. L. Gervasio, Structural basis of the effect of activating mutations on the EGF receptor, eLife, DOI 10.7554/eLife.65824.

C. Noble Jesus, R. Evans, J. Forth, C. Estarellas, F. L. Gervasio, G. Battaglia, Amphiphilic histidine-based oligopeptides exhibit pH-reversible fibril formation, ACS Macro Letters, DOI 10.1021/acsmacrolett.1c00142.

E. Cignoni, M. Lapillo, L. Cupellini, S. Acosta-Gutiérrez, F. L. Gervasio, B. Mennucci, A different perspective for nonphotochemical quenching in plant antenna complexes, Nature Communications, DOI 10.1038/s41467-021-27526-8.

Marco Gibertini, University of Geneva

M. Gibertini, Magnetism and stability of all primitive stacking patterns in bilayer chromium Trihalides, Journal of Physics D: Applied Physics, DOI 10.1088/1361-6463/abc2f4.

L. Rademaker, M. Gibertini, Gate-tunable imbalanced Kane-Mele model in encapsulated bilayer jacutingaite, Physical Review Materials, DOI 10.1103/PhysRevMaterials.5.044201.

Stefan Goedecker, University of Basel

S. Rostami, S. A. Ghasemi, S. Goedecker, Novel polymorphs and polytypes of lithium chloride from structure predictions based on charge equilibration via neural network technique, Physical Review Materials, DOI 10.1103/PhysRevMaterials.5.123603.

B. Parsaeifard, D. S. De, J. A. Finkler, S. Goedecker, Fingerprint-based detection of non-local effects in the electronic structure of a simple single component covalent system, Condensed Matter, DOI 10.3390/condmat6010009.

T. W. Ko, J. A. Finkler, S. Goedecker, J. Behler, A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer, Nature Communication, DOI 10.1038/s41467-020-20427-2.

Gianvito Grasso, SUPSI

E. Trofimenko, G. Grasso, M. Heulot, N. Chevalier, M. A Deriu, G. Dubuis, Y. Arribat, M. Serulla, S. Michel, G. Vantomme, F. Ory, L. C. Dam, J. Puyal, F. Amati, A. Lüthi, A. Danani, C. Widmann, Genetic, cellular, and structural characterization of the membrane potential-dependent cell-penetrating peptide translocation pore, eLife, DOI 10.7554/eLife.69832.

G. Grasso, A. Di Gregorio, B. Mavkov, D. Piga, G. F. D'Urso Labate, A. Danani, M. A. Deriu, Fragmented blind docking: a novel protein–ligand binding prediction protocol, Journal of Biomolecular Structure and Dynamics, DOI 10.1080/07391102.2021.1988709.

Jonathan P. Graves, EPF Lausanne

Y. I. Kolesnichenko, H. Patten, V. V. Lutsenko, J. P. Graves, T. S. Rudenko, JET Contributors, Ion cyclotron resonance heating with shifted separatrix, Nuclear Fusion, DOI 10.1088/1741-4326/abdfdc.

M. Machielsen, J. P. Graves, W. A. Cooper, ICRF modelling in 2D and 3D magnetic configurations using a hot plasma model, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/ac11b2.

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

P. Knecht, J. Reichert, P. S. Deimel, P. Feulner, F. Haag, F. Allegretti, M. Garnica, M. Schwarz, W. Auwärter, P. T. P. Ryan, T.-L. Lee, D. A. Duncan, A. P. Seitsonen, J. V. Barth, A. C. Papageorgiou, Conformational control of chemical reactivity for surface-confined ru-porphyrins, Angewandte Chemie-International Edition, DOI 10.1002/anie.202104075.

P. Knecht, B. Zhang, J. Reichert, D. A. Duncan, M. Schwarz, F. Haag, P. T. P. Ryan, Y.-L. Lee, P. S. Deimel, P. Feulner, F. Allegretti, W. Auwärter, G. Médard, A. P. Seitsonen, J. V. Barth, A. C. Papageorgiou, Assembly and manipulation of a prototypical n-heterocyclic carbene with a metalloporphyrin pedestal on a solid surface, Journal of the American Chemical Society, DOI 10.1021/jacs.1c01229.

Torsten Hoefler, ETH Zurich

J. de Fine Licht, A. Kuster, T. De Matteis, Tal Ben-Nun, D. Hofer, T. Hoefler, StencilFlow: Mapping large stencil programs to distributed spatial computing systems, 2021 IEEE/ACM International Symposium on Code Generation and Optimization (CGO), DOI 10.1109/CGO51591.2021.9370315.

P. Grönquist, C. Yao, T. Ben-Nun, N. Dryden, P. Dueben, S. Li, T. Hoefler, Deep learning for post-processing ensemble weather forecasts, Philosophical Transactions of the Royal Society a-Mathematical Physical and Engineering Sciences, DOI 10.1098/rsta.2020.0092.

J. de Fine Licht, M. Besta, S. Meierhans, T. Hoefler, Transformations of high-level synthesis codes for high-performance computing, IEEE Transactions on Parallel and Distributed Systems, DOI 10.1109/Tpds.2020.3039409.

S. Li, T. Ben-Nun, G. Nadiradze, S. Di Girolamo, N. Dryden, D. Alistarh, T. Hoefler, Breaking (global) barriers in parallel stochastic optimization with wait-avoiding group averaging, IEEE Transactions on Parallel and Distributed Systems, DOI 10.1109/Tpds.2020.3040606.

N. Dryden, R. Böhringer, T. Ben-Nun, T. Hoefler, Clairvoyant prefetching for distributed machine learning I/O, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC21), DOI 10.1145/3458817.3476181.

M. Copik, A. Calotoiu, T. Grosser, N. Wicki, F. Wolf, T. Hoefler, Extracting clean performance models from tainted programs, Proceedings of the 26th ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming (PPoPP 21), DOI 10.1145/3437801.3441613.

A. N. Ziogas, T. Ben-Nun, T. Schneider, T. Hoefler, NPBench: A benchmarking suite for high-performance NumPy, Proceedings of the ACM International Conference on Supercomputing (ICS 21), DOI 10.1145/3447818.3460360.

M. Besta, Z. Vonarburg-Shmaria, Y. Schaner, L. Schwarz, G. Kwasniewski, L. Gianinazzi, J. Beranek, K. Janda, T. Holenstein, S. Leisinger, P. Tatkowski, E. Ozdemir, A. Balla, M. Copik, P. Lindenberger, M. Konieczny, O. Mutlu, T. Hoefler, GraphMineSuite: Enabling high-performance and programmable graph mining algorithms with set algebra, Proceedings of the VLDB Endowment, DOI 10.14778/3476249.3476252.

G. Kwasniewski, T. Ben-Nun, L. Gianinazzi, A. Calotoiu, T. Schneider, A. N. Ziogas, M. Besta, T. Hoefler, Pebbles, graphs, and a pinch of combinatorics: Towards tight I/O lower bounds for statically analyzable programs, Proceedings of the 33rd ACM Symposium on Parallelism in Algorithms and Architectures (SPAA 21), DOI 10.1145/3409964.3461796.

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. Li, T. Hoefler, Chimera: Efficiently training large-scale neural networks with bidirectional pipelines, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC21), DOI 10.1145/3458817.3476145.

G. Kwasniewski, M. Kabic, T. Ben-Nun, A. N. Ziogas, J. E. Saethre, A. Gaillard, T. Schneider, M. Besta, A. Kozhevnikov, J. VandeVondele, T. Hoefler, On the parallel I/O optimality of linear algebra kernels: Near-optimal matrix factorizations, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC21), DOI 10.1145/3458817.3476167.

A. N. Ziogas, T. Schneider, T. Ben-Nun, A. Calotoiu, T. De Matteis, J. de Fine Licht, L. Lavarini, T. Hoefler, Productivity, portability, performance: Data-centric python, Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC21), DOI 10.1145/3458817.3476176.

Sebastian Huber, ETH Zurich

D. E. Gökmen, Z. Ringel, S. D. Huber, M. Koch-Janusz, Symmetries and phase diagrams with real-space mutual information neural estimation, Physical Review E, DOI 10.1103/PhysRevE.104.064106.

D. E. Gökmen, Z. Ringel, S. D. Huber, M. Koch-Janusz, Statistical physics through the lens of real-space mutual information, Physical Review Letters, DOI 10.1103/PhysRevLett.127.240603.

Andrew Hung, RMIT University, Melbourne

L. Zhao, L. M. Barber, A. Hung, Structural and dynamical effects of targeted mutations on μO-Conotoxin MfVIA: Molecular simulation studies, Journal of Molecular Graphics and Modelling, DOI 10.1016/j.jmgm.2020.107777.

L. M. Barber, Z. Hussain, M. Thomas, A. Hung, Dimeric phosphorylation of glyoxalase I alters its symmetry and substrate binding mechanism: Simulation studies, Journal of Biomolecular Structure and Dynamics, DOI 10.1080/07391102.2021.1873186.

E. Pitsillou, J. Liang, K. Ververis, A. Hung, T. C. Karagiannis, Interaction of small molecules with the SARS-CoV-2 papain-like protease: *In-silico* studies and *in-vitro* validation of protease activity inhibition using an enzymatic inhibition assay, Journal of Molecular Graphics and Modelling, DOI 10.1016/j.jmgm.2021.107851.

E. Pitsillou, J. Liang, A. Hung, T. C. Karagiannis, Inhibition of interferon-stimulated gene 15 and lysine 48-linked ubiquitin binding to the SARS-CoV-2 papain-like protease by small molecules: *In-silico* studies, Chemical Physics Letters, DOI 10.1016/j.cplett.2021.138468.

J. Liang, E. Pitsillou, L. Burbury, A. Hung, T. C. Karagiannis, *In-silico* investigation of potential small molecule inhibitors of the SARS-CoV-2 nsp10-nsp16 methyltransferase complex, Chemical Physics Letters, DOI 10.1016/j.cplett.2021.138618.

K. K. Darmawan, T. C. Karagiannis, J. G. Hughes, D. M. Small, A. Hung, In-silico modelling of apo-lactoferrin under simulated gastric conditions: Structural dynamics, binding with β-lactoglobulin and α-lactalbumin, and functional implications, LWT, DOI 10.1016/j.lwt.2021.111726.

E. Pitsillou, J. Liang, H. Yu, M. Huang, A. Hung, T. C. Karagiannis, *In-silico* investigation to identify potential small molecule inhibitors of the RNA-dependent RNA polymerase (RdRp) nidovirus RdRp-associated nucleotidyltransferase domain, Chemical Physics Letters, DOI 10.1016/j.cplett.2021.138889.

A. Hung, I. C. Forster, C. E. Mckenzie, G. Berecki, S. Petrou, A. Kathirvel, M. S. Soh, C. A. Reid, Biophysical analysis of an HCN1 epilepsy variant suggests a critical role for S5 helix Met-305 in voltage sensor to pore domain coupling, Progress in Biophysics and Molecular Biology, DOI 10.1016/j.pbiomolbio.2021.07.005.

R. C. Beh, E. Pitsillou, J. J. Liang, A. Hung, T. C. Karagiannis, *In-silico* investigation of DNA minor groove binding bibenzimidazoles in the context of UVA phototherapy, Royal Society of Chemistry, DOI 10.1039/d1cp04841d.

Jürg Hutter, University of Zurich

J. Lan, V. Kapil, P. Gasparotto, M. Ceriotti, M. Iannuzzi, V. V. Rybkin, Simulating the Ghost: Quantum dynamics of the solvated electron, Nature Communications, DOI 10.1038/s41467-021-20914-0.

A. Bussy, J. Hutter, Efficient and low-scaling linear-response time-dependent density functional theory implementation for core-level spectroscopy of large and periodic systems, Physical Chemistry Chemical Physics, DOI 10.1039/D0CP06164F.

Marcella Iannuzzi, University of Zurich

N. Baumann, J. Lan, M. Iannuzzi, CO_2 adsorption on the pristine and reduced CeO_2 (111) surface: Geometries and vibrational spectra by first principles simulations, AIP The Journal of Chemical Physics, DOI 10.1063/5.0042435.

L. Sévery, J. Szczerbiński, M. Taskin, I. Tuncay, F. Brandalise Nunes, C. Cignarella, G. Tocci, O. Blacque, J. Osterwalder, R. Zenobi, M. Iannuzzi, S. D. Tilley, Immobilization of molecular catalysts on electrode surfaces using host–guest interactions, Nature Chemistry, DOI 10.1038/s41557-021-00652-y.

M. Pauletti, V. V. Rybkin, M. Iannuzzi, Subsystem density functional theory augmented by a delta learning approach to achieve Kohn-Sham accuracy, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.1c00592.

Anela Ivanova, University of Sofia

C. G. Wilson, L. Aarons, P. Augustijns, J. Brouwers, A. S. Darwich, T. De Waal, G. Garbacz, S. Hansmann, D. Hoc, A. Ivanova, M. Koziolek, C. Reppas, P. Schick, M. Vertzoni, J. A. García-Horsman, Integration of advanced methods and models to study drug absorption and related processes: An UNGAP perspective, European Journal of Pharmaceutical Sciences, DOI 10.1016/j.ejps.2021.106100.

Andrew Jackson, ETH Zurich

Y. Lin, A. Jackson, Large-scale vortices and zonal flows in spherical rotating convection, Journal of Fluid Mechanics, DOI 10.1017/jfm.2020.1151.

Fortunat Joos, University of Bern

J. Terhaar, T. L. Frölicher, F. Joos, Southern Ocean anthropogenic carbon sink constrained by sea surface salinity, Science Advances, DOI 10.1126/sciadv.abd5964.

Olaf Kaczmarek, University of Bielefeld

O. Kaczmarek, L. Mazur, S. Sharma, Eigenvalue spectra of QCD and the fate of $U_A(1)$ breaking towards the chiral limit, Physical Review D, DOI 10.1103/PhysRevD.104.094518.

D. A. Clarke, O. Kaczmarek, F. Karsch, A. Lahiri, M. Sarkar, Sensitivity of the Polyakov loop and related observables to chiral symmetry restoration, Physical Review D, DOI 10.1103/PhysRevD.103.L011501.

S. Dentinger, Screening meson masses towards the chiral limit, Bielefeld - Universität Bielefeld, DOI 10.4119/unibi/2960222.

Tomasz Kacprzak, ETH Zurich

R. Sgier, J. Fluri, J. Herbel, A. Réfrégier, A. Amara, T. Kacprzak, A. Nicola, Fast lightcones for combined cosmological probes, Journal of Cosmology and Astroparticle Physics, DOI 10.1088/1475-7516/2021/02/047.

Venkat Kapil, University of Cambridge

S. Shepherd, J. Lan, D. M. Wilkins, V. Kapil, Efficient quantum vibrational spectroscopy of water with high-order path integrals: From bulk to interfaces, The Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.1c02574.

Ilya V. Karlin, ETH Zurich

N. Sawant, B. Dorschner, I. V. Karlin, A lattice Boltzmann model for reactive mixtures, Philosophical Transactions of the Royal Society A, DOI 10.1098/rsta.2020.0402.

A. Bhadauria, B. Dorschner, I. V. Karlin, Lattice Boltzmann method for fluid–structure interaction in compressible flow, Physics of Fluids, DOI 10.1063/5.0062117.

N. G. Kallikounis, B. Dorschner, I. V. Karlin, Multiscale semi-Lagrangian lattice Boltzmann method, Physical Review E, DOI 10.1103/PhysRevE.103.063305.

M. H. Saadat, S. A. Hosseini, B. Dorschner, I. V. Karlin, Extended lattice Boltzmann model for gas dynamics, Physics of Fluids, DOI 10.1063/5.0048029.

M. H. Saadat, B. Dorschner, I. V. Karlin, Extended lattice Boltzmann model, Entropy, DOI 10.3390/e23040475.

E. Reyhanian, B. Dorschner, I. V. Karlin, Kinetic Simulations of Compressible Non-Ideal Fluids: From Supercritical Flows to Phase-Change and Exotic Behavior, Computation, DOI 10.3390/computation9020013.

Stephan Kellenberger, University of Lausanne

S. Vullo, N. Ambrosio, J. P. Kucera, O. Bignucolo, S. Kellenberger, Kinetic analysis of ASIC1a delineates conformational signaling from proton-sensing domains to the channel gate, eLife, DOI 10.7554/eLife.66488.

Himanshu Khandelia, University of Southern Denmark

A. S. Busk Heitmann, A. A. Hakami Zanjani, M. Berg Klenow, A. Mularski, S. L. Sønder, F. W. Lund, T. L. Boye, C. Dias, P. M. Bendix, A. Cohen Simonsen, H. Khandelia, J. Nylandsted, Phenothiazines alter plasma membrane properties and sensitize cancer cells to injury by inhibiting annexin-mediated repair, Journal of Biological Chemistry, DOI 10.1016/j.jbc.2021.101012.

V. Dubey, D. L. Stokes, B. Panyella Pedersen, H. Khandelia, An intracellular pathway controlled by the N-terminus of the pump subunit inhibits the bacterial KdpFABC ion pump in high K^+ conditions, Journal of Molecular Biology, DOI 10.1016/j.jmb.2021.167008.

Harald Köstler, Friedrich-Alexander University of Erlangen-Nürmberg

M. Holzer, M. Bauer, H. Köstler, U. Rüde, Highly efficient lattice Boltzmann multiphase simulations of immiscible fluids at high-density ratios on CPUs and GPUs through code generation, The International Journal of High Performance Computing Applications, DOI 10.1177/10943420211016525.

M. Bauer, H. Köstler, U. Rüde, lbmpy: Automatic code generation for efficient parallel lattice Boltzmann methods, Journal of Computational Science, DOI 10.1016/j.jocs.2020.101269.

M. Bauer, S. Eibl, C. Godenschwager, N. Kohl, M. Kuron, C. Rettinger, F. Schornbaum, C. Schwarzmeier, D. Thönnes, H. Köstler, U. Rüde, waLBerla: A block-structured high-performance framework for multiphysics simulations, Computers & Mathematics with Applications, DOI 10.1016/j.camwa.2020.01.007.

Petros Koumoutsakos, ETH Zurich & Harvard University

E. Papadopoulou, J. Zavadlav, R. Podgornik, M. Praprotnik, P. Koumoutsakos, Tuning the dielectric response of water in nanoconfinement through surface wettability, ACS Nano, DOI 10.1021/acsnano.1c08512.

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

G. Novati, H. L. de Laroussilhe, P. Koumoutsakos, Automating turbulence modelling by multi-agent reinforcement learning, Nature Machine Intelligence, DOI 10.1038/s42256-020-00272-0.

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.

K. Larson, G. Arampatzis, C. Bowman, Z. Chen, P. Hadjidoukas, C. Papadimitriou, P. Koumoutsakos, A. Matzavinos, Data-driven prediction and origin identification of epidemics in population networks, Royal Society Open Science, DOI 10.1098/rsos.200531.

A. Economides, G. Arampatzis, D. Alexeev, S. Litvinov, L. Amoudruz, L. Kulakova, C. Papadimitriou, P. Koumoutsakos, Hierarchical bayesian uncertainty quantification for a model of the red blood cell, Physical Review Applied, DOI 10.1103/PhysRevApplied.15.034062.

P. R. Vlachas, J. Zavadlav, M. Praprotnik, P. Koumoutsakos, Accelerated simulations of molecular systems through learning of effective dynamics, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.1c00809.

Martin Kröger, ETH Zurich

M. Kröger, R. Schlickeiser, Verification of the accuracy of the SIR model in forecasting based on the improved SIR model with a constant ratio of recovery to infection rate by comparing with monitored second wave data, Royal Society Open Science, DOI 10.1098/rsos.211379.

A. Moghimikheirabadi, M. Kröger, A. V. Karatrantos, Insights from modeling into structure, entanglements, and dynamics in attractive polymer nanocomposites, Soft Matter, DOI 10.1039/D1SM00683E.

Z. Shen, H. Ye, Q. Wang, M. Kröger, Y. Li, Sticky rouse time features the self-adhesion of supramolecular polymer networks, Macromolecules, DOI 10.1021/acs.macromol.1c00335.

M. Pourali, M. Kröger, J. Vermant, P. D. Anderson, N. O. Jaensson, Drag on a spherical particle at the air–liquid interface: Interplay between compressibility, Marangoni flow, and surface viscosities, Physics of Fluids, DOI 10.1063/5.0050936.

Girish Kulkarni, Tata Institute of Fundamental Research, Mumbai

J. Raste, G. Kulkarni, L. C. Keating, M. G. Haehnelt, J. Chardin, D. Aubert, Implications of the z>5 Lyman-α forest for the 21-cm power spectrum from the epoch of reionization, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab2424.

Martin Kunz, University of Geneva

F. Hassani, P. Shi, J. Adamek, M. Kunz, P. Wittwer, New nonlinear instability for scalar fields, Physical Review D, DOI 10.1103/PhysRevD.105.L021304.

L. Coates, J. Adamek, P. Bull, C. Guandalin, C. Clarkson, Observing relativistic features in large-scale structure surveys – II. Doppler magnification in an ensemble of relativistic simulations, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab1076.

Michael Lehning, WSL Institute for Snow and Avalanche Research SLF

A. Sigmund, J. Dujardin, F. Comola, V. Sharma, H. Huwald, D. Brito Melo, N. Hirasawa, K. Nishimura, M. Lehning, Evidence of strong flux underestimation by bulk parametrizations during drifting and blowing snow, Boundary-Layer Meteorology, DOI 10.1007/s10546-021-00653-x.

David Leutwyler, Max Planck Institute for Meteorology

D. Leutwyler, C. Hohenegger, Weak cooling of the troposphere by tropical islands in simulations of the radiative-convective equilibrium, Quarterly Journal of the Royal Meteorological Society, DOI 10.1002/qj.3995.

Yaakov Levy, Weizmann Institute of Science

L. S. Bigman, Y. Levy, Modulating microtubules: A molecular perspective on the effects of tail modifications, Journal of Molecular Biology, DOI 10.1016/j.jmb.2021.166988.

Vittorio Limongelli, Università della Svizzera italiana

B. Fiorillo, V. Sepe, P. Conflitti, R. Roselli, M. Biagioli, S. Marchianò, P. De Luca, G. Baronissi, P. Rapacciuolo, C. Cassiano, B. Catalanotti, A. Zampella, V. Limongelli, S. Fiorucci, Structural basis for developing multitarget compounds acting on cysteinyl leukotriene receptor 1 and G-protein-coupled bile acid receptor 1, Journal of Medicinal Chemistry, DOI 10.1021/acs.jmedchem.1c01078.

S. Raniolo, V. Limongelli, Improving small-molecule force field parameters in ligand binding studies, Frontiers in Molecular Biosciences, DOI 10.3389/fmolb.2021.760283.

A. de Felice, S. Aureli, V. Limongelli, Drug repurposing on g protein-coupled receptors using a computational profiling approach, Frontiers in Molecular Biosciences, DOI 10.3389/fmolb.2021.673053.

P. C. T. Souza, V. Limongelli, S. Wu, S. J. Marrink, L. Monticelli, Perspectives on high-throughput ligand/protein docking with Martini MD simulations, Frontiers in Molecular Biosciences, DOI 10.3389/fmolb.2021.657222.

Ulrike Lohmann, ETH Zurich

Z. Dedekind, A. Lauber, S. Ferrachat, U. Lohmann, Sensitivity of precipitation formation to secondary ice production in winter orographic mixed-phase clouds, Atmospheric Chemistry and Physics, DOI 10.5194/acp-21-15115-2021.

Detlef Lohse, University of Twente

A. Blass, P. Tabak, R. Verzicco, R. J. A. M. Stevens, D. Lohse, The effect of Prandtl number on turbulent sheared thermal convection, Journal of Fluid Mechanics, DOI 10.1017/jfm.2020.1019.

Sandra Luber, University of Zurich

R. Ketkaew, F. Creazzo, S. Luber, Closer look at inverse electron demand Diels–Alder and nucleophilic addition reactions on s-tetrazines using enhanced sampling methods, Topics in Catalysis, DOI 10.1007/s11244-021-01516-y.

L. Schreder, S. Luber, Local approaches for electric dipole moments in periodic systems and their application to real-time time-dependent density functional theory, The Journal of Chemical Physics, DOI 10.1063/5.0058793.

F. Creazzo, S. Luber, Explicit solvent effects on (1 1 0) ruthenium oxide surface wettability: Structural, electronic and mechanical properties of rutile RuO_2 by means of spin-polarized DFT-MD, Applied Surface Science, DOI 10.1016/j.apsusc.2021.150993.

F. Creazzo, S. Luber, Water-assisted chemical route towards the oxygen evolution reaction at the hydrated (110) ruthenium oxide surface: Heterogeneous catalysis via DFT-MD & metadynamics simulations, Chemistry A European Journal, DOI 10.1002/chem.202102356.

R. Han, S. Luber, Fast estimation of Møller–Plesset correlation energies based on atomic contributions, The Journal of Physical Chemistry, DOI 10.1021/acs.jpclett.1c00900.

E. Ditler, C. Kumar, S.Luber, Analytic calculation and analysis of atomic polar tensors for molecules and materials using the Gaussian and plane waves approach, The Journal of Chemical Physics, DOI 10.1063/5.0041056.

M. Mališ, S. Luber, ΔSCF with subsystem density embedding for efficient nonadiabatic molecular dynamics in condensed-phase systems, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.0c01200.

J. Mattiat, S. Luber, Time domain simulation of (resonance) Raman spectra of liquids in the short time approximation, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.0c00755.

R. Han, M. Rodríguez-Mayorga, S. Luber, A machine learning approach for MP2 correlation energies and its application to organic compounds, Journal of Chemical Theory and Computation, DOI 10.1021/acs.jctc.0c00898.

Mathieu Luisier, ETH Zurich

K. Portner, M. Schmuck, P. Lehmann, C. Weilenmann, C. Haffner, P. Ma, J. Leuthold, M. Luisier, A. Emboras, Analog nanoscale electro-optical synapses for neuromorphic computing applications, ACS Nano, DOI 10.1021/acsnano.1c04654.

X. Wen, A. Arabhavi, W. Quan, O. Ostinelli, C. Mukherjee, M. Deng, S. Frégonèse, T. Zimmer, C. Maneux, C. R. Bolognesi, M. Luisier, Performance prediction of InP/GaAsSb double heterojunction bipolar transistors for THz applications, Journal of Applied Physics, DOI 10.1063/5.0054197.

T. Knobloch, Y. Y. Illarionov, F. Ducry, C. Schleich, S. Wachter, T. Müller, M. Waltl, M. Lanza, M. I. Vexler, M. Luisier, T. Grasser, The performance limits of hexagonal boron nitride as an insulator for scaled CMOS devices based on two-dimensional materials, Nature Electronics, DOI 10.1038/s41928-020-00529-x.

C. Klinkert, S. Fiore, J. Backman, Y. Lee, M. Luisier, Impact of orientation misalignment on black phosphorus ultrascaled field-effect transistors, IEEE Electron Device Letters, DOI 10.1109/LED.2021.3055287.

Y. Lee, T. Agarwal, M. Luisier, Ab-initio modelling framework for Majorana transport, 2D Materials: Towards topological quantum computing, Proceedings of the IEDM, DOI 10.1109/IEDM13553.2020.9371923.

Carlos J. A. P. Martins, University of Porto

J. R. C. C. C. Correia, C. J. A. P. Martins, High resolution calibration of the cosmic strings velocity dependent one-scale model, Physical Review D, DOI 10.1103/PhysRevD.104.063511.

J. R. C. C. C. Correia, C. J. A. P. Martins, Abelian–Higgs cosmic string evolution with multiple GPUs, Astronomy and Computing, DOI 10.1016/j.ascom.2020.100438.

Nicola Marzari, EPF Lausanne

M. T. Vahdat, D. Campi, N. Colonna, N. Marzari, K. V. Agrawal, Gas transport across Carbon nitride nanopores: A comparison of van der Waals functionals against the random-phase Approximation, The Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.1c03822.

M. Uhrin, S. P. Huber, J. Yuc, N. Marzari, G. Pizzi, Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows, Computational Materials Science, DOI 10.1016/j.commatsci.2020.110086.

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.

R. Mahajan, I. Timrov, N. Marzari, A. Kashyap, Importance of intersite Hubbard interactions in β-MnO_2: A first-principles DFT+U+V study, Physical Review Materials, DOI 10.1103/PhysRevMaterials.5.104402.

D. Campi, S. Kumari, N. Marzari, Prediction of phonon-mediated superconductivity with high critical temperature in the two-dimensional topological semimetal W_2N_3, NanoLetters, DOI 10.1021/acs.nanolett.0c05125.

G. Materzanini, L. Kahle, A. Marcolongo, N. Marzari, High Li-ion conductivity in tetragonal LGPO: A comparative first-principles study against known LISICON and LGPS phases, Physical Review Materials, DOI 10.1103/PhysRevMaterials.5.035408.

I. Timrov, N. Marzari, M. Cococcioni, Self-consistent Hubbard parameters from density-functional perturbation theory in the ultrasoft and projector-augmented wave formulations, Physical Review B, DOI 10.1103/PhysRevB.103.045141.

Lucio Mayer, University of Zurich

T. Tamfal, L. Mayer, T. R. Quinn, P. R. Capelo, S. Kazantzidis, A. Babul, D. Potter, Revisiting dynamical friction: The role of global modes and local wakes, The Astrophysical Journal, DOI 10.3847/1538-4357/ac0627.

H. Deng, L. Mayer, R. Helled, Formation of intermediate-mass planets via magnetically controlled disk fragmentation, Nature Astronomy, DOI 10.1038/s41550-020-01297-6.

H. Deng, G. I. Ogilvie, L. Mayer, Parametric instability in a free-evolving warped protoplanetary disc, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/staa3504.

MeteoSwiss

A. Burgstall, S. Kotlarski, A. Casanueva, E. Hertig, E. Fischer, R. Knutti, Urban multi-model climate projections of intense heat in Switzerland, Climate Services, DOI 10.1016/j.cliser.2021.100228.

Dominik Obrist, University of Bern

D. De Marinis, D. Obrist, Data assimilation by stochastic ensemble Kalman filtering to enhance turbulent cardiovascular flow data from under-resolved observations, Frontiers in Cardiovascular Medicine, DOI 10.3389/fcvm.2021.742110.

H. Zolfaghari, D. Obrist, A high-throughput hybrid task and data parallel Poisson solver for large-scale simulations of incompressible turbulent flows on distributed GPUs, Journal of Computational Physics, DOI 10.1016/j.jcp.2021.110329.

Pierre Ocvirk, University of Strasbourg

M. Gronke, P. Ocvirk, C. Mason, J. Matthee, S. E. I. Bosman, J. G. Sorce, J. Lewis, K. Ahn, D. Aubert, T. Dawoodbhoy, I. T. Iliev, P. R. Shapiro, G. Yepes, Lyman-α transmission properties of the intergalactic medium in the CoDaII simulation, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab2762.

Dennis Palagin, Paul Scherrer Institute

A. Boucly, L. Artiglia, E. Fabbri, D. Palagin, D. Aegerter, D. Pergolesi, Z. Novotny, N. Comini, J. T. Diulus, T. Huthwelker, M. Ammann, T. J. Schmidt, Direct evidence of cobalt oxyhydroxide formation on a $La_{0.2}Sr_{0.8}CoO_3$ perovskite water splitting catalyst, Journal of Materials Chemistry A, DOI 10.1039/d1ta04957g.

D. Palagin, V. L. Sushkevich, A. J. Knorpp, M. Ranocchiari, J. A. van Bokhoven, Mapping vibrational spectra to the structures of copper species in zeolites based on calculated stretching frequencies of adsorbed nitrogen and carbon monoxides, The Journal of Physical Chemistry C, DOI 10.1021/acs.jpcc.1c01649.

Z. R. Gao, M. Odstrcil, S. Bocklein, D. Palagin, M. Holler, D. F. Sanchez, F. Krumeich, A. Menzel, M. Stampanoni, G. Mestl, J. A. van Bokhoven, M. Guizar-Sicairos, J. Ihli, Sparse ab-initio x-ray transmission spectrotomography for nanoscopic compositional analysis of functional materials, Science Advances, DOI 10.1126/sciadv.abf6971.

X. Wang, A. Beck, J. A. van Bokhoven, D. Palagin, Thermodynamic insights into strong metal–support interaction of transition metal nanoparticles on titania: Simple descriptors for complex chemistry, Journal of Materials Chemistry A, DOI 10.1039/d0ta11650e.

A. J. Knorpp, A. B. Pinar, C. Baerlocher, L. B. McCusker, N. Casati, M. A. Newton, S. Checchia, J. Meyet, D. Palagin, J. A. van Bokhoven, Paired copper monomers in zeolite omega: the active site for methane-to-methanol conversion, Angewandte Chemie-International Edition, DOI 10.1002/anie.202014030.

Michele Parrinello, Università della Svizzera italiana

E. Grifoni, G. M. Piccini, J. A. Lercher, V.-A. Glezakou, R. Rousseau, M. Parrinello, Confinement effects and acid strength in zeolites, Nature Communications, DOI 10.1038/s41467-021-22936-0.

T. Karmakar, M. Invernizzi, V. Rizzi, M. Parrinello, Collective variables for the study of crystallization, Molecular Physics, DOI 10.1080/00268976.2021.1893848.

Daniele Passerone, Empa

S. Stolz, M. Danese, M. Di Giovannantonio, J. I. Urgel, Q. Sun, A. Kinikar, M. Bommert, S. Mishra, H. Brune, O. Gröning, D. Passerone, R. Widmer, Asymmetric elimination reaction on chiral metal surfaces, Advanced Materials, DOI 10.1002/adma.202104481.

P. P. Shinde, J. Liu, T. Dienel, O. Gröning, T. Dumslaff, M. Mühlinghaus, A. Narita, K. Müllen, C. A. Pignedoli, R. Fasel, P. Ruffieux, D. Passerone, Graphene nanoribbons with mixed cove-cape-zigzag edge structure, Carbon, DOI 10.1016/j.carbon.2020.12.069.

Alfredo Pasquarello, EPF Lausanne

P. Gono, A. Pasquarello, High-performance NiOOH/FeOOH electrode for OER catalysis, Journal of Chemical Physics, DOI 10.1063/5.0036019.

T. Bischoff, I. Reshetnyak, A. Pasquarello, Band gaps of liquid water and hexagonal ice through advanced electronic-structure calculations, Physical Review Research, DOI 10.1103/PhysRevResearch.3.023182.

A. Bouzid, A. Pasquarello, Atomic-scale modelling of electrochemical interfaces through constant Fermi level molecular dynamics, Atomic-Scale Modelling of Electrochemical Systems, DOI 10.1002/9781119605652.ch7.

A. Tal, W. Chen, A. Pasquarello, Vertex function compliant with the Ward identity for quasiparticle self-consistent calculations beyond GW, Physical Review B, DOI 10.1103/PhysRevB.103.L161104.

Giovanni M. Pavan, SUPSI

K. Tashiro, K. Katayama, K. Tamaki, L. Pesce, N. Shimizu, H. Takagi, R. Haruki, M. J. Hollamby, G. M. Pavan, S. Yagai, Non-uniform photoinduced unfolding of supramolecular polymers leading to topological block nanofibers, Angewandte Chemie-International Edition, DOI 10.1002/anie.202110224.

C. Lionello, A. Gardin A. Cardellini, D. Bochicchio, M. Shivrayan, A. Fernandez, S. Thayumanavan, G. M. Pavan, Motion following specific chemical gradients to multivalency-controlled disassembly, ACS Nano, DOI 10.1021/acsnano.1c05000.

A. L. de Marco, D. Bochicchio, A. Gardin, G. Doni, G. M. Pavan, Controlling exchange pathways in dynamic supramolecular polymers by controlling defects, ACS Nano, DOI 10.1021/acsnano.1c01398.

T. Bian, A. Gardin, J. Gemen, L. Houben, C. Perego, B. Lee, N. Elad, Z. Chu, G. M. Pavan, R. Klajn, Electrostatic co-assembly of nanoparticles with oppositely charged small molecules into static and dynamic superstructures, Nature Chemistry, DOI 10.1038/s41557-021-00752-9.

R. Capelli, A. Gardin, C. Empereur-mot, G. Doni, G. M. Pavan, A data-driven dimensionality reduction approach to compare and classify lipid force fields, The Journal of Physical Chemistry B, DOI 10.1021/acs.jpcb.1c02503.

H. Liu, C. Lionello, J. Westley, A. Cardellini, U. Huynh, G. M. Pavan, S. Thayumanavan, Understanding functional group and assembly dynamics in temperature responsive systems leads to design principles for enzyme responsive assemblies, Nanoscale, DOI 10.1039/D1NR02000E.

O. Shyshov, S. V. Haridas, L. Pesce, H. Qi, A. Gardin, D. Bochicchio, U. Kaiser, G. M. Pavan, M. von Delius, Living supramolecular polymerization of fluorinated cyclohexanes, Nature Communications, DOI 10.1038/s41467-021-23370-y.

C. Perego, L. Pesce, R. Capelli, S. J. George, G. M. Pavan, Multiscale molecular modelling of ATP-fueled supramolecular polymerisation and depolymerization, ChemSystemsChem, DOI 10.1002/syst.202000038.

G. Moreno-Alcántar, A. Aliprandi, R. Rouquette, L. Pesce, K. Wurst, C. Perego, P. Brüggeller, G. M. Pavan, L. De Cola, Solvent-driven supramolecular wrapping of self-assembled structures, Angewandte Chemie-International Edition, DOI 10.1002/anie.202013474.

Mihai Petrovici, University of Bern

J. Jordan, M. Schmidt, W. Senn, M. A. Petrovici, Evolving interpretable plasticity for spiking networks, eLife, DOI 10.7554/eLife.66273.

Simone Pezzuto, Università della Svizzera italiana

L. Gander, R. Krause, M. Multerer, S. Pezzuto, Space-time shape uncertainty in the forward and inverse problem of electrocardiography, International Journal for Numerical Methods in Biomedical Engineering, DOI 10.1002/cnm.3522.

A. Gharaviri, S. Pezzuto, M. Potse, G. Conte, S. Zeemering, V. Sobota, S. Verheule, R. Krause, A. Auricchio, U. Schotten, Synergistic antiarrhythmic effect of inward rectifier current inhibition and pulmonary vein isolation in a 3d computer model for atrial fibrillation, EP Europace, DOI 10.1093/europace/ euaa413.

A. Gharaviri, S. Pezzuto, M. Potse, S. Verheule, G. Conte, R. Krause, U. Schotten, A. Auricchio, Left atrial appendage electrical isolation reduces atrial fibrillation recurrences: A simulation study, Circulation - Arrhythmia and Electrophysiology, DOI 10.1161/CIR- CEP.120.009230.

T. Grandits, A. Effland, T. Pock, R. Krause, G. Plank, S. Pezzuto, GEASI: Geodesic-based Earliest Activation Sites Identification in cardiac models, International Journal for Numerical Methods in Biomedical Engineering, DOI 10.1002/cnm.3505.

J. M. Lubrecht, T. Grandits, A. Gharaviri, U. Schotten, T. Pock, G. Plank, R. Krause, A. Auricchio, S. Pezzuto, Automatic reconstruction of the left atrium activation from sparse intracardiac contact recordings by inverse estimate of fiber structure and anisotropic conduction in a patient-specific model, EP Europace, DOI 10.1093/europace/euaa392.

S. Pezzuto, F. W. Prinzen, M. Potse, F. Maffessanti, F. Regoli, M. L. Caputo, G. Conte, R. Krause, A. Auricchio, Reconstruction of three-dimensional biventricular activation based on the 12-lead electrocardiogram via patient-specific modelling, EP Europace, DOI 10.1093/europace/euaa330.

T. Grandits, S. Pezzuto, J. M. Lubrecht, T. Pock, G. Plank, R. Krause, PIEMAP: Personalized inverse eikonal model from cardiac electro-anatomical maps, Lecture Notes in Computer Science, DOI 10.1007/978-3-030- 68107-4_8.

Carlo A. Pignedoli, Empa

S. Mishra, G. Catarina, F. Wu, R. Ortiz, D. Jacob, K. Eimre, J. Ma, C. A. Pignedoli, X. Feng, P. Ruffieux, J. Fernández-Rossier, R. Fasel, Observation of fractional edge excitations in nanographene spin chains, Nature, DOI 10.1038/s41586-021-03842-3.

G. Buchs, M. Marganska, J. W. González, K. Eimre, C. A. Pignedoli, D. Passerone, A. Ayuela, O. Gröning, D. Bercioux, Metallic carbon nanotube quantum dots with broken symmetries as a platform for tunable terahertz detection, Applied Physics Reviews, DOI 10.1063/5.0018944.

A. V. Yakutovich, K. Eimre, O. Schütt, L. Talirz, C. S. Adorf, C. W. Andersen, E. Ditler, D. Du, D. Passerone, B. Smit, N. Marzari, G. Pizzi, C. A. Pignedoli, AiiDAlab – an ecosystem for developing, executing, and sharing scientific workflows, Computational Materials Science, DOI 10.1016/j.commatsci.2020.110165.

L. M. Mateo, Q. Sun, K. Eimre, C. A. Pignedoli, T. Torres, R. Fasel, G. Bottari, On-surface synthesis of singly and doubly porphyrin-capped graphene nanoribbon segments, Chemical Science, DOI 10.1039/D0SC04316H.

S. Mishra, X. Yao, Q. Chen, K. Eimre, O. Gröning, R. Ortiz, M. Di Giovannantonio, J. C. Sancho-García, J. Fernández-Rossier, C. A. Pignedoli, K. Müllen, P. Ruffieux, A. Narita, R. Fasel, Large magnetic exchange coupling in rhombus-shaped nanographenes with zigzag periphery, Nature Chemistry, DOI 10.1038/s41557-021-00678-2.

X. Xu, M. Di Giovannantonio, J. I. Urgel, C. A. Pignedoli, P. Ruffieux, K. Müllen, R. Fasel, A. Narita, On-surface activation of benzylic C-H bonds for the synthesis of pentagon-fused graphene nanoribbons, Nano Research, DOI 10.1007/s12274-021-3419-2.

J. I. Urgel, J. Bock, M. Di Giovannantonio, P. Ruffieux, C. A. Pignedoli, M. Kivala, R. Fasel, On-surface synthesis of π-conjugated ladder-type polymers comprising nonbenzenoid moieties, RSC Advances, DOI 10.1039/D1RA03253D.

E. Turco, S. Mishra, J. Melidonie, K. Eimre, S. Obermann, C. A. Pignedoli, R. Fasel, X. Feng, P. Ruffieux, On-surface synthesis and characterization of super-nonazethrene, The Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.1c02381.

S. E. Ammerman, V. Jelic, Y. Wei, V. N. Breslin, M. Hassan, N. Everett, S. Lee, Q. Sun, C. A. Pignedoli, P. Ruffieux, R. Fasel, T. L. Cocker, Lightwave-driven scanning tunnelling spectroscopy of atomically precise graphene nanoribbons, Nature Communications, DOI 10.1038/s41467-021-26656-3.

Fernando Porté-Agel, EPF Lausanne

T. Revaz, F. Porté-Agel, Large-Eddy simulation of wind turbine flows: A new evaluation of actuator disk models, Energies, DOI 10.3390/en14133745.

Nikolaos I. Prasianakis, Paul Scherrer Institute

M. Khatoonabadi, M. A. Safi, N. I. Prasianakis, J. Roth, J. Mantzaras, N. Kirov, F. N. Büchi, Insights on the interaction of serpentine channels and gas diffusion layer in an operating polymer electrolyte fuel cell: Numerical modeling across scales, International Journal of Heat and Mass Transfer, DOI 10.1016/j.ijheatmasstransfer.2021.121859.

M. Khatoonabadi, N. I. Prasianakis, J. Mantzaras, Lattice Boltzmann model with generalized wall boundary conditions for arbitrary catalytic reactivity, Physical Review E, DOI 10.1103/PhysRevE.103.063303.

Christoph C. Raible, University of Bern

W. M. Kim, R. Blender, M. Sigl, C. C. Raible, Statistical characteristics of extreme daily precipitation during 1501 BCE-1849 CE in the Community Earth System Model, Climate of the Past, DOI 10.5194/cp-17-2031-2021.

P. Velasquez, J. O. Kaplan, P. Ludwig, M. Messmer, C. C. Raible, The role of land cover on the climate of glacial Europe, Climate of the Past, DOI 10.5194/cp-17-1161-2021.

W. M. Kim, C. C. Raible, Dynamics of the Mediterranean droughts from 850 to 2099 AD in the Community Earth System Model, Climate of the Past, DOI 10.5194/cp-17-887-2021.

J. Zscheischler, P. Naveau, O. Martius, S. Engelke, C. C. Raible, Evaluating the dependence structure of compound precipitation and wind speed extremes, Earth System Dynamics, DOI 10.5194/esd-12-1-2021.

Paolo Ricci, EPF Lausanne

B. J. Frei, J. Ball, A. C. D. Hoffmann, R. Jorge, P. Ricci, L. Stenger, Development of advanced linearized gyrokinetic collision operators using a moment approach, Journal of Plasma Physics, DOI 10.1017/S0022377821000830.

D. Mancini, P. Ricci, N. Vianello, M. Giacomin, A. Coroado, Investigation of the density shoulder formation by using self-consistent simulations of plasma turbulence and neutral kinetic dynamics, Nuclear Fusion, DOI 10.1088/1741-4326/ac30c9.

M. Giacomin, A. Stagni, P. Ricci, J. A. Boedo, J. Horacek, H. Reimerdes, C. K. Tsui, Theory-based scaling laws of near and far scrape-off layer widths in single-null L-mode discharges, Nuclear Fusion, DOI 10.1088/1741-4326/abf8f6.

A. Coroado, P. Ricci, Moving toward mass-conserving simulations of plasma turbulence and kinetic neutrals in the tokamak boundary with the GBS code, Physics of Plasmas, DOI 10.1063/5.0027977.

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. L. 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.

Marcello Righi, ZHAW

M. Righi, D. Anderegg, M. Sonderegger, S. Mandrà, Multi-disciplinary optimization of HAPS in formation flight, AIAA Aviation 2021 Forum, DOI 10.2514/6.2021-2569.

M. Righi, Uncertainties quantification in flutter prediction of a wind tunnel model exhibiting large displacements, AIAA Scitech 2021 Forum, DOI 10.2514/6.2021-1037.

M. Righi, P. Greco, A. Da Ronch, Uncertainties quantification of CFD-based flutter prediction, AIAA Aviation 2021 Forum, DOI 10.2514/6.2021-2569.

Kevin Rossi, EPF Lausanne

C. Zeni, K. Rossi, T. Pavloudis, J. Kioseoglou, S. de Gironcoli, R. E. Palmer, F. Baletto, Data-driven simulation and characterisation of gold nanoparticle melting, Nature Communications, DOI 10.1038/s41467-021-26199-7.

S. B. Varandili, D. Stoian, J. Vavra, K. Rossi, J. R. Pankhurst, Y. T. Guntern, N. López, R. Buonsanti, Elucidating the structure-dependent selectivity of CuZn towards methane and ethanol in CO_2 electroreduction using tailored Cu/ZnO precatalysts, Chemical Science, DOI 10.1039/D1SC04271H.

Ursula Röthlisberger, EPF Lausanne

A. Krishna, H. Zhang, Z. Zhou, T. Gallet, M. Dankl, O. Ouellette, F. T. Eickemeyer, F. Fu, S. Sanchez, M. Mensi, S. M. Zakeeruddin, U. Röthlisberger, G. N. M. Reddy, A. Redinger, M. Grätzel, A. Hagfeldt, Nanoscale interfacial engineering enables highly stable and efficient perovskite photovoltaics, Energy & Environmental Science, DOI 10.1039/D1EE02454J.

A. Mishra, P. Ahlawat, G. C. Fish, F. Jahanbakhshi, M. Mladenović, M. Almalki, M. A. Ruiz-Preciado, M. C. Gelvéz-Rueda, D. J. Kubicki, P. A. Schouwink, V. Dufoulon, T. Schneeberger, A. Aslanzadeh, F. C. Grozema, S. M. Zakeeruddin, J.-E. Moser, U. Röthlisberger, L. Emsley, J. V. Milić, M. Grätzel, Naphthalenediimide/formamidinium-based low-dimensional perovskites, Chemistry of Materials, DOI 10.1021/acs.chemmater.1c01635.

H. Zhang, F. T. Eickemeyer, Z. Zhou, M. Mladenović, F. Jahanbakhshi, L. Merten, A. Hinderhofer, M. A. Hope, O. Ouellette, A. Mishra, P. Ahlawat, D. Ren, T.-S. Su, A. Krishna, Z. Wang, Z. Dong, J. Guo, S. M. Zakeeruddin, F. Schreiber, A. Hagfeldt, L. Emsley, U. Röthlisberger, J. V. Milić, M. Grätzel, Multimodal host–guest complexation for efficient and stable perovskite photovoltaics, Nature Communications, DOI 10.1038/s41467-021-23566-2.

P. Ahlawat, A. Hinderhofer, E. A. Alharbi, H. Lu, A. Ummadisingu, H. Niu, M. Invernizzi, S. M. Zakeeruddin, I. Dar, F. Schreiber, A. Hagfeldt, M. Grätzel, U. Röthlisberger, M. Parrinello, A combined molecular dynamics and experimental study of two-step process enabling low-temperature formation of phase-pure α-$FAPbI_3$, Science Advances, DOI 10.1126/sciadv.abe3326.

J. Jeong, M. Kim, J. Seo, H. Lu, P. Ahlawat, A. Mishra, Y. Yang, M. A. Hope, F. T. Eickemeyer, M. Kim, Y. Jin Yoon, I. W. Choi, B. Primera Darwich, S. J. Choi, Y. Jo, J. H. Lee, B. Walker, S. M. Zakeeruddin, L. Emsley, U. Röthlisberger, A. Hagfeldt, D. S. Kim, M. Grätzel, J. Y. Kim, Pseudo-halide anion engineering for α-$FAPbI_3$ perovskite solar cells, Nature, DOI 10.1038/s41586-021-03406-5.

A. Boziki, M. I. Dar, G. Jacopin, M. Grätzel, U. Röthlisberger, Molecular origin of the asymmetric photoluminescence spectra of $CsPbBr_3$ at low temperature, The Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.1c00263.

D. Narzi, S. C. van Keulen, U. Röthlisberger, $G\alpha_{i1}$ inhibition mechanism of ATP-bound adenylyl cyclase type 5, PLOS ONE, DOI 10.1371/journal.pone.0245197.

Eugene Rozanov, PMO-DWRC

T. Sukhodolov, T. Egorova, A. Stenke, W. T. Ball, C. Brodowsky, G. Chiodo, A. Feinberg, M. Friedel, A. Karagodin-Doyennel, T. Peter, J. Sedlacek, S. Vattioni, E. Rozanov, Atmosphere-Ocean-Aerosol-Chemistry-Climate Model SOCOLv4.0: Description and evaluation, Geoscientific Model Development, DOI 10.5194/gmd-14-5525-2021.

E. Rozanov, T. Egorova, L. Egli, A. Karagodin-Doyennel, T. Sukhodolov, H. Schill, R. Stübi, J. Gröbner, Representativeness of the Arosa/Davos measurements for the analysis of the global total column ozone behavior, Frontiers in Earth Science, DOI 10.3389/feart.2021.675084.

Andrei V. Ruban, KTH Royal Institute of Technology

A. Forslund, X. Zhang, B. Grabowski, A. V. Shapeev, A. V. Ruban, Ab-initio simulations of the surface free energy of TiN(001), Physical Review B, DOI 10.1103/PhysRevB.103.195428.

Richard Sandberg, University of Melbourne

Y. M. Zhao, R. D. Sandberg, High-fidelity simulations of a high-pressure turbine vane subject to large disturbances: Effect of exit Mach number on losses, Journal of Turbomachinery, DOI 10.1115/1.4050453.

J. J. Otero-Pérez, R. D. Sandberg, S. Mizukami, K. Tanimoto, High-fidelity simulations of multi-jet impingement cooling flows, Journal of Turbomachinery, DOI 10.1115/1.4050446.

Christoph Schär, ETH Zurich

C. Heim, L. Hengten, N. Ban, C. Schär, Inter-model variability in convection-resolving simulations of subtropical marine low clouds, Journal of the Meteorological Society of Japan, DOI 10.2151/jmsj.2021-062.

C. Zeman, N. P. Wedi, P. D. Dueben, N. Ban, C. Schär, Model intercomparison of COSMO 5.0 and IFS 45r1 at kilometer-scale grid spacing, Geoscientific Model Development, DOI 10.5194/gmd-14-4617-2021.

J. Vergara-Temprado, N. Ban, C. Schär, Extreme sub-hourly precipitation intensities scale close to the Clausius-Clapeyron rate over Europe, Geophysical Research Letters, DOI 10.1029/2020GL089506.

E. Pichelli, E. Coppola, S. Sobolowski, N. Ban, F. Giorgi, P. Stocchi, A. Alias, D. Belušić, S. Berthou, C. Caillaud, R. M. Cardoso, S. Chan, O. Bøssing Christensen, A. Dobler, H. de Vries, K. Goergen, E. J. Kendon, K. Keuler, G. Lenderink, T. Lorenz, A. N. Mishra, H.-J. Panitz, C. Schär, P. M. M. Soares, H. Truhetz, J. Vergara-Temprado, The first multi-model ensemble of regional climate simulations at kilometer-scale resolution part 2: Historical and future simulations of precipitation, Climate Dynamics, DOI 10.1007/s00382-021-05657-4.

S. Ubbiali, C. Schär, L. Schlemmer, T. C. Schulthess, A numerical analysis of six physics-dynamics coupling schemes for atmospheric models, Journal of Advances in Modeling Earth Systems, DOI 10.1029/2020MS002377.

S. L. Sørland, R. Brogli, P. K. Pothapakula, E. Russo, J. Van de Walle, B. Ahrens, I. Anders, E. Bucchignani, E. L. Davin, M.-E. Demory, A. Dosio, H. Feldmann, B. Früh, B. Geyer, K. Keuler, D. Lee, D. Li, N. P. M. van Lipzig, S.-K. Min, H.-J. Panitz, B. Rockel, C. Schär, C. Steger, W. Thiery, COSMO-CLM regional climate simulations in the Coordinated Regional Climate Downscaling Experiment (CORDEX) framework: A review, Geoscientific Model Development, DOI 10.5194/gmd-14-5125-2021.

R. Brogli, S. L. Sørland, N. Kröner, C. Schär, Future summer warming pattern under climate change is affected by lapse-rate changes, Weather and Climate Dynamics, DOI 10.5194/wcd-2-1093-2021.

E. Coppola, R. Nogherotto, J. M. Ciarlo, Filippo Giorgi, E. van Meijgaard, N. Kadygrov, C. Iles, L. Corre, M. Sandstad, S. Somot, P. Nabat, R. Vautard, G. Levavasseur, C. Schwingshackl, J. Sillmann, E. Kjellström, G. Nikulin, E. Aalbers, G. Lenderink, O.B. Christensen, F. Boberg, S.L. Sørland, M.-E. Demory, K. Bülow, C. Teichmann, K. Warrach-Sagi, V. Wulfmeyer, Assessment of the European climate projections as simulated by the large EURO-CORDEX regional and global climate model ensemble, Journal of Geophysical Research Atmospheres, DOI 10.1029/2019JD032356.

D. Leutwyler, A. Imamovic, C. Schär, The continental-scale soil-moisture precipitation feedback in Europe with parameterized and explicit convection, Journal of Climate, DOI 10.1175/JCLI-D-20-0415.1.

D. Regenass, L. Schlemmer, O. Fuhrer, J.-M. Bettems, M. Arpagaus, C. Schär, Validation of a high resolution numerical weather prediction land-surface scheme using catchment water balances, Journal of Hydrometeorology, DOI 10.1175/JHM-D-20-0273.1.

R. Vautard, N. Kadygrov, C. Iles, F. Boberg, E. Buonomo, E. Coppola, K. Bülow, L. Corre, E. van Meijgaard, R. Nogherotto, M. Sandstad, C. Schwingshackl, S. Somot, E. Aalbers, O. B Christensen, J. M. Ciarlo, M.-E. Demory, F. Giorgi, D. Jacob, R. G. Jones, K. Keuler, E. Kjellström, G. Lenderink, G. Levavasseur, G. Nikulin, J. Sillmann, C. Solidoro, S. L. Sørland, C. Steger, C. Teichmann, K. Warrach-Sagi, V. Wulfmeyer, Assessment of the large EURO-CORDEX regional climate simulation ensemble, Journal of Geophysical Research-Atmospheres, DOI 10.1029/2019JD032344.

Simon Scheidegger, University of Lausanne

S. Scheidegger, A. Treccani, Pricing American options under high-dimensional models with recursive adaptive sparse expectations, Journal of Financial Econometrics, DOI 10.1093/jjfinec/nby024.

L. Kotlikoff, F. Kubler, A. Polbin, S. Scheidegger, Pareto-improving carbon-risk taxation, Economic Policy, DOI 10.1093/epolic/eiab008.

L. Kotlikoff, F. Kubler, A. Polbin, J. Sachs, S. Scheidegger, Making carbon taxation a generational win win, International Economic Review, DOI 10.1111/iere.12483.

Sebastian Schemm, ETH Zurich

A. Oertel, S. Schemm, Quantifying the circulation induced by convective clouds in kilometer-scale simulations, Quarterly Journal of the Royal Meteorological Society, DOI 10.1002/qj.3992.

Olaf Schenk, Università della Svizzera italiana

A. Eftekharia, D. Pasadakisa, M. Bollhöfer, S. Scheidegger, O. Schenk, Block-enhanced precision matrix estimation for large-scale datasets, Journal of Computational Science, DOI 10.1016/j.jocs.2021.101389.

Benjamin Schuler, University of Zurich

M. F. Nüesch, M. T. Ivanović, J. B. Claude, D. Nettels, R. B. Best, J. Wenger, B. Schuler, Single-molecule detection of ultrafast biomolecular dynamics with nanophotonics, Journal of the American Chemical Society, DOI 10.1021/jacs.1c09387.

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.

Nicola A. Spaldin, ETH Zurich

A. Mansouri Tehrani, N. A. Spaldin, Untangling the structural, magnetic dipole, and charge multipolar orders in Ba_2MgReO_6, Physical Review Materials, DOI 10.1103/PhysRevMaterials.5.104410.

M. Giraldo, Q. N. Meier, A. Bortis, D. Nowak, N. A. Spaldin, M. Fiebig, M. C. Weber, T. Lottermoser, Magnetoelectric coupling of domains, domain walls and vortices in a multiferroic with independent magnetic and electric order, Nature Communications, DOI 10.1038/s41467-021-22587-1.

B. F. Grosso, N. A. Spaldin, Prediction of low-energy phases of $BiFeO_3$ with large unit cells and complex tilts beyond Glazer notation, Physical Review Materials, DOI 10.1103/PhysRevMaterials.5.054403.

J. Souto-Casares, N. A. Spaldin, C. Ederer, Oxygen vacancies in strontium titanate: A DFT+DMFT study, Physical Review Research, DOI 10.1103/PhysRevResearch.3.023027.

M. J. Neugebauer, D. M. Juraschek, M. Savoini, P. Engeler, L. Boie, E. Abreu, N. A. Spaldin, S. L. Johnson, Comparison of coherent phonon generation by electronic and ionic Raman scattering in $LaAlO_3$, Physical Review Research, DOI 10.1103/PhysRevResearch.3.013126.

M. H. Dehn, J. K. Shenton, D. J. Arseneau, W. A. MacFarlane, G. D. Morris, A. Maigné, N. A. Spaldin, R. F. Kiefl, Local electronic structure and dynamics of muon-polaron complexes in Fe_2O_3, Physical Review Letters, DOI 10.1103/PhysRevLett.126.037202.

I. Efe, N. A. Spaldin, C. Gattinoni, On the happiness of ferroelectric surfaces and its role in water dissociation: The example of bismuth ferrite, The Journal of Chemical Physics, DOI 10.1063/5.0033897.

M. E. Merkel, C. Ederer, Charge disproportionation and Hund's insulating behavior in a five-orbital Hubbard model applicable to d^4 perovskites, Physical Review B, DOI 10.1103/PhysRevB.104.165135.

Joachim Stadel, University of Zurich

Euclid Collaboration, M. Knabenhans, J. Stadel, D. Potter, J. Dakin, S. Hannestad, T. Tram, S. Marelli, A. Schneider, R. Teyssier, P. Fosalba, S. Andreon, N. Auricchio, C. Baccigalupi, A. Balaguera-Antolínez, M. Baldi, S. Bardelli, P. Battaglia, R. Bender, A. Biviano, C. Bodendorf, E. Bozzo, E. Branchini, M. Brescia, C. Burigana, R. Cabanac, S. Camera, V. Capobianco, A. Cappi, C. Carbone, J. Carretero, C. S. Carvalho, R. Casas, S. Casas, M. Castellano, G. Castignani, S. Cavuoti, R. Cledassou, C. Colodro-Conde, G. Congedo, C. J. Conselice, L. Conversi, Y. Copin, L. Corcione, J. Coupon, H. M. Courtois, A. Da Silva, S. de la Torre, D. Di Ferdinando, C. A. J. Duncan, X. Dupac, G. Fabbian, S. Farrens, P. G. Ferreira, F. Finelli, M. Frailis, E. Franceschi, S. Galeotta, B. Garilli, C. Giocoli, G. Gozaliasl, J. Graciá-Carpio, F. Grupp, L. Guzzo, W. Holmes, F. Hormuth, H. Israel, K. Jahnke, E. Keihanen, S. Kermiche, C. C. Kirkpatrick, B. Kubik, M. Kunz, H. Kurki-Suonio, S. Ligori, P. B. Lilje, I. Lloro, D. Maino, O. Marggraf, K. Markovic, N. Martinet, F. Marulli, R. Massey, N. Mauri, S. Maurogordato, E. Medinaceli, M. Meneghetti, B. Metcalf, G. Meylan, M. Moresco, B. Morin, L. Moscardini, E. Munari, C. Neissner, S. M. Niemi, C. Padilla, S. Paltani, F. Pasian, L. Patrizii, V. Pettorino, S. Pires, G. Polenta, M. Poncet, F. Raison, A. Renzi, J. Rhodes, G. Riccio, E. Romelli, M. Roncarelli, R. Saglia, A. G. Sánchez, D. Sapone, P. Schneider, V. Scottez, A. Secroun, S. Serrano, C. Sirignano, G. Sirri, L. Stanco, F. Sureau, P. Tallada Crespí, A. N. Taylor, M. Tenti, I. Tereno, R. Toledo-Moreo, F. Torradeflot, L. Valenziano, J. Valiviita, T. Vassallo, M. Viel, Y. Wang, N. Welikala, L. Whittaker, A. Zacchei, E. Zucca, Euclid preparation: IX. EuclidEmulator2-power spectrum emulation with massive neutrinos and self-consistent dark energy perturbations, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab1366.

Thomas Stocker, University of Bern

M. Messmer, S. J. González-Rojí, C. C. Raible, T. F. Stocker, Sensitivity of precipitation and temperature over the Mount Kenya area to physics parameterization options in a high-resolution model simulation performed with WRFV3.8.1, Geoscientific Model Development, DOI 10.5194/gmd-14-2691-2021.

Judit Szulágyi, ETH Zurich

F. Binkert, J. Szulágyi, T. Birnstiel, First 3D grid-based gas-dust simulations of circumstellar discs with an embedded planet, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab2075.

J. Szulágyi, A. Garufi, Observability of forming planets and their circumplanetary discs – III. Polarized scattered light in near-infrared, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab1723.

Romain Teyssier, University of Zurich

M. Han Veiga, D. A. Velasco-Romero, Q. Wenger, R. Teyssier, An arbitrary high-order spectral difference method for the induction equation, Journal of Computational Physics, DOI 10.1016/j.jcp.2021.110327.

O. Attia, R. Teyssier, H. Katz, T. Kimm, S. Martin-Alvarez, P. Ocvirk, J. Rosdahl, Cosmological magnetogenesis: The Biermann battery during the Epoch of reionization, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab1030.

Gabriele Tocci, University of Zurich

L. Joly, R. H. Meissner, M. Iannuzzi, G. Tocci, Osmotic transport at the aqueous graphene and hBN interfaces: Scaling laws from a unified, first-principles description, ACS Nano, DOI 10.1021/acsnano.1c05931.

Martin van Driel, ETH Zurich

M. van Driel, J. Kemper, C. Boehm, On the modelling of self-gravitation for full 3-D global seismic wave propagation, Geophysical Journal International, DOI 10.1093/gji/ggab237.

A. Khan, S. Ceylan, M. van Driel, D. Giardini, P. Lognonne, H. Samuel, N. C. Schmerr, S. C. Stahler, A. C. Duran, Q. C. Huang, D. Kim, A. Broquet, C. Charalambous, J. F. Clinton, P. M. Davis, M. Drilleau, F. Karakostas, V. Lekic, S. M. McLennan, R. R. Maguire, C. Michaut, M. P. Panning, W. T. Pike, B. Pinot, M. Plasman, J. R. Scholz, R. Widmer-Schnidrig, T. Spohn, S. E. Smrekar, W. B. Banerdt, Upper mantle structure of Mars from InSight seismic data, Science, DOI 10.1126/science.abf2966.

S. C. Stähler, A. Khan, B. Banerdt, P. Lognonné, D. Giardini, S. Ceylan, M. Drilleau, C. Duran, R. F. Garcia, Q. Huang, D. Kim, V. Lekic, H. Samuel, M. Schimmel, N. Schmerr, D. Sollberger, E. Stutzmann, Z. Xu, D. Antonangeli, C. Charalambous, P. M. Davis, J. C. E. Irving, T. Kawamura, M. Knapmeyer, R. Maguire, A. G. Marusiak, M. P. Panning, C. Perrin A.-C. Plesa, A. Rivoldini, C. Schmelzbach, G. Zenhäusern, E. Beucler, J. Clinton, N. Dahmen, M. van Driel T. Gudkova, A. Horleston, W. T. Pike, M. Plasman, S. E. Smrekar, Seismic detection of the Martian core, Science, DOI 10.1126/science.abi7730.

N. Brinkman, S. C. Stähler, D. Giardini, C. Schmelzbach, A. Khan, A. Jacob, N. Fuji, C. Perrin, P. Lognonné, E. Beucler, M. Böse, S. Ceylan, C. Charalambous, J. F. Clinton, M. van Driel, F. Euchner, A. Horleston, T. Kawamura, B. Knapmeyer-Endrun, G. Mainsant, M. P. Panning, W. T. Pike, J.-R. Scholz, J. O. A. Robertsson, W. B. Banerdt, First focal mechanisms of Marsquakes, Journal of Geophysical Research-Planets, DOI 10.1029/2020JE006546.

M. van Driel, S. Ceylan, J. F. Clinton, D. Giardini, A. Horleston, L. Margerin, S. C. Stähler, M. Böse, C. Charalambous, T. Kawamura, A. Khan, G. Orhand-Mainsant, J.-R. Scholz, F. Euchner, M. Knapmeyer, N. Schmerr, W. T. Pike, P. Lognonné, W. B. Banerdt, High-frequency seismic events on Mars observed by InSight, Journal of Geophysical Research-Planets, DOI 10.1029/2020JE006670.

Harry van Lenthe, ETH Zurich

A. Malhotra, M. Walle, G. R. Paul, G. A. Kuhn, R. Müller, Application of subject-specific adaptive mechanical loading for bone healing in a mouse tail vertebral defect, Scientific Reports, DOI 10.1038/s41598-021-81132-8.

G. R. Paul, E. Wehrle, D. C. Tourolle, G. A. Kuhn, R. Müller, Real-time finite element analysis allows homogenization of tissue scale strains and reduces variance in a mouse defect healing model, Scientific Reports, DOI 10.1038/s41598-021-92961-y.

M. Walle, F. C. Marques, N. Ohs, M. Blauth, R. Müller, C. J. Collins, Bone mechanoregulation allows subject-specific load estimation based on time-lapsed micro-CT and HR-pQCT in vivo, Frontiers in Bioengineering and Biotechnology, DOI 10.3389/fbioe.2021.677985.

H. Hemmatian, A. D. Bakker, J. Klein-Nulend, G. H. van Lenthe, Alterations in osteocyte lacunar morphology affect local bone tissue strains, Journal of the Mechanical Behavior of Biomedical Materials, DOI 10.1016/j.jmbbm.2021.104730.

K. Mys, P. Varga, F. Stockmans, B. Gueorguiev, V. Neumann, O. Vanovermeire, C. E. Wyers, J. P. van den Bergh, G. H. van Lenthe, High-resolution cone-beam computed tomography is a fast and promising technique to quantify bone microstructure and mechanics of the distal radius, Calcified Tissue International, DOI 10.1007/s00223-020-00773-5.

Stefano Vanni, University of Fribourg

V. Zoni, P. Campomanes, S. Vanni, Investigating the structural properties of hydrophobic solvent-rich lipid bilayers, Soft Matter, DOI 10.1039/D0SM02270E.

V. Zoni, R. Khaddaj, I. Lukmantara, W. Shinoda, H. Yang, R. Schneiter, S. Vanni, Seipin accumulates and traps diacylglycerols and triglycerides in its ring-like structure, Proceedings of the National Academy of Sciences of the United States of America, DOI 10.1073/pnas.2017205118.

V. Zoni, R. Khaddaj, P. Campomanes, A. R. Thiam, R. Schneiter, S. Vanni, Pre-existing bilayer stresses modulate triglyceride accumulation in the ER versus lipid droplets, eLife, DOI 10.7554/eLife.62886.

Franco Vazza, University of Bologna

N. Locatelli, F. Vazza, A. Bonafede, S. Banfi, G. Bernardi, C. Gheller, A. Botteon, T. Shimwell, New constraints on the magnetic field in cosmic web filaments, Astronomy & Astrophysics, DOI 10.1051/0004-6361/202140526.

T. Vernstrom, G. Heald, F. Vazza, T. J. Galvin, J. L. West, N. Locatelli, N. Fornengo, E. Pinetti, Discovery of magnetic fields along stacked cosmic filaments as revealed by radio and X-ray emission, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab1301.

T. Hodgson, F. Vazza, M. Johnston-Hollitt, B. McKinley, FIGARO simulation: FIlaments & GAlactic RadiO simulation, Publications of the Astronomical Society of Australia, DOI 10.1017/pasa.2021.32.

A. Simionescu, S. Ettori, N. Werner, D. Nagai, F. Vazza, H. Akamatsu, C. Pinto, J. de Plaa, N. Wijers, D. Nelson, E. Pointecouteau, G. W. Pratt, D. Spiga, G. Vacanti, E. Lau, M. Rossetti, F. Gastaldello, V. Biffi, E. Bulbul, M. J. Collon, J.-W. den Herder, D. Eckert, F. Fraternali, B. Mingo, G. Pareschi, G. Pezzulli, T. H. Reiprich, J. Schaye, S. A. Walker, J. Werk, Voyage through the hidden physics of the cosmic web, Experimental Astronomy, DOI 10.1007/s10686-021-09720-0.

S. Banfi, F. Vazza, C. Gheller, On the alignment of haloes, filaments and magnetic fields in the simulated cosmic web, Monthly Notices of the Royal Astronomical Society, DOI 10.1093/mnras/stab655.

Jorge Vieira, University of Lisbon

T. Silva, L. D. Amorim, M. C. Downer, M. J. Hogan, V. Yakimenko, R. Zgadzaj, J. Vieira, Stable positron acceleration in thin, warm, hollow plasma channels, Physical Review Letters, DOI 10.1103/PhysRevLett.127.104801.

J. P. Palastro, B. Malaca, J. Vieira, D. Ramsey, T. T. Simpson, P. Franke, J. L. Shaw, D. H. Froula, Laser-plasma acceleration beyond wave breaking, Physics of Plasmas, DOI 10.1063/5.0036627.

Laurent Villard, EPF Lausanne

A. Jocksch, N. Ohana, E. Lanti, E. Koutsaniti, V. Karakasis, L. Villard, An optimisation of allreduce communication in message-passing systems, Parallel Computing, DOI 10.1016/j.parco.2021.102812.

P. Donnel, J. Cazabonne, L. Villard, S. Brunner, S. Coda, J. Decker, M. Murugappan, M. Sadr, Quasilinear treatment of wave–particle interactions in the electron cyclotron range and its implementation in a gyrokinetic code, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/abf53f.

N. Ohana, C. Gheller, E. Lanti, A. Jocksch, S. Brunner, L. Villard, Gyrokinetic simulations on many- and multi-core architectures with the global electromagnetic particle-in-cell code ORB5, Computer Physics Communications, DOI 10.1016/j.cpc.2020.107208.

P. Donnel, C. Gheller, S. Brunner, L. Villard, E. Lanti, N. Ohana, M. Murugappan, Moment approach of the multi-species non-linear Coulomb collision operator adapted to particle-in-cell codes, Plasma Physics and Controlled Fusion, DOI 10.1088/1361-6587/abc92b.

Peter E. Vincent, Imperial College London

G. Giangaspero, F. Witherden, P. Vincent, Synthetic turbulence generation for high-order scale-resolving simulations on unstructured grids, AIAA Journal, DOI 10.2514/1.J061046.

Viola Vogel, ETH Zurich

L. Braun, I. Schoen, V. Vogel, PIP_2-induced membrane binding of the vinculin tail competes with its other binding partners, Biophysical Journal, DOI 10.1016/j.bpj.2021.08.018.

Olaf Yazyev, EPF Lausanne

C. Guo, A. Alexandradinata, C. Putzke, A. Estry, T. Tu, N. Kumar, F.-R. Fan, S. Zhang, Q. Wu, O. V. Yazyev, K. R. Shirer, M. D. Bachmann, H. Peng, E. D. Bauer, F. Ronning, Y. Sun, C. Shekhar, P. J. W. Moll, Temperature dependence of quantum oscillations from non-parabolic dispersions, Nature Communications, DOI 10.1038/s41467-021-26450-1.

G. Gatti, D. Gosálbez-Martínez, Q. S. Wu, J. Hu, S. N. Zhang, G. Autès, M. Puppin, D. Bugini, H. Berger, L. Moreschini, I. Vobornik, J. Fujii, J.- P. Ansermet, O. V. Yazyev, A. Crepaldi, Origin of large magnetoresistance in the topological nonsymmorphic semimetal $TaSe_3$, Physical Review B, DOI 10.1103/PhysRevB.104.155122.

Q. Chen, Z. Lou, S.N. Zhang, Y. Zhou, B. Xu, H. Chen, S. Chen, J. Du, H. Wang, J. Yang, Q.S. Wu, O. V. Yazyev, M. Fang, Extremely large magnetoresistance in the “ordinary” metal ReO_3, Physical Review B, DOI 10.1103/PhysRevB.104.115104.

M. Pizzochero, K. Čerņevičs, G. Borin Barin, S. Wang, P. Ruffieux, R. Fasel, O. V. Yazyev, Quantum electronic transport across 'bite' defects in graphene nanoribbons, 2D Materials, DOI 10.1088/2053-1583/abf716.

N. V. Tepliakov, Q.S. Wu, O. V. Yazyev, Crystal field effect and electric field screening in multilayer graphene with and without twist, Nano Letters, DOI 10.1021/acs.nanolett.1c00678.

M. Pizzochero, G. Borin Barin, K. Čerņevičs, S. Wang, P. Ruffieux, R. Fasel, O. V. Yazyev, Edge disorder in bottom-up zigzag graphene nanoribbons: implications for magnetism and quantum electronic transport, The Journal of Physical Chemistry Letters, DOI 10.1021/acs.jpclett.1c00921.

G. Gatti, D. Gosálbez-Martínez, S. Roth, M. Fanciulli, M. Zacchigna, M. Kalläne, K. Rossnagel, C. Jozwiak, A. Bostwick, E. Rotenberg, A. Magrez, H. Berger, I. Vobornik, J. Fujii, O. V. Yazyev, M. Grioni, A. Crepaldi, Hidden bulk and surface effects in the spin polarization of the nodal-line semimetal ZrSiTe, Communications Physics, DOI 10.1038/s42005-021-00555-x.

Q. S. Wu, J. Liu, Y. Guan, O. V. Yazyev, Landau levels as a probe for band topology in graphene Moiré superlattices, Physical Review Letters, DOI 10.1103/PhysRevLett.126.056401.

Y. Jian, Q. Wu, M. Yang, Q. Feng, J. Duan, D. Chen, Q. Wang, W. Xiao, Y. Shi, O. V. Yazyev, Y. Yao, Transport signatures of temperature-induced chemical potential shift and Lifshitz transition in layered type-II Weyl semimetal $TaIrTe_4$, 2D Materials, DOI 10.1088/2053-1583/abc13f.

Urs Wenger, University of Bern

C. Alexandrou, S. Bacchio, G. Bergner, J. Finkenrath, A. Gasbarro, K. Hadjiyiannakou, K. Jansen, B. Kostrzewa, K. Ottnad, M. Petschlies, F. Pittler, F. Steffens, C. Urbach, U. Wenger, Quark and gluon momentum fractions in the pion from $N_f = 2 + 1 + 1$ Lattice QCD, Physical Review Letters, DOI 10.1103/PhysRevLett.127.252001.

Heini Wernli, ETH Zurich

F. Aemisegger, R. Vogel, P. Graf, F. Dahinden, L. Villiger, F. Jansen, S. Bony, B. Stevens, H. Wernli, How Rossby wave breaking modulates the water cycle in the North Atlantic trade wind region, Weather and Climate Dynamics, DOI 10.5194/wcd-2-281-2021.

F. Dahinden, F. Aemisegger, H. Wernli, M. Schneider, C. J. Diekmann, B. Ertl, P. Knippertz, M. Werner, S. Pfahl, Disentangling different moisture transport pathways over the eastern subtropical North Atlantic using multi-platform isotope observations and high-resolution numerical modelling, Atmospheric Chemistry and Physics, DOI 10.5194/acp-21-16319-2021.

A. Oertel, M. Sprenger, H. Joos, M. Boettcher, H. Konow, M. Hagen, H. Wernli, Observations and simulation of intense convection embedded in a warm conveyor belt – how ambient vertical wind shear determines the dynamical impact, Weather and Climate Dynamics, DOI 10.5194/wcd-2-89-2021.

I. Thurnherr, K. Hartmuth, L. Jansing, J. Gehring, M. Boettcher, I. Gorodetskaya, M. Werner, H. Wernli, F. Aemisegger, The role of air–sea fluxes for the water vapour isotope signals in the cold and warm sectors of extratropical cyclones over the Southern Ocean, Weather and Climate Dynamics, DOI 10.5194/wcd-2-331-2021.

Gabriel Wlazłowski, Warsaw University of Technology

D. Pęcak, N. Chamel, P. Magierski, G. Wlazłowski, Properties of a quantum vortex in neutron matter at finite temperatures, Physical Review C, DOI 10.1103/PhysRevC.104.055801.

P. Magierski, B. Tüzemen, G. Wlazłowski, Dynamics of spin-polarized impurity in ultracold Fermi gas, Physical Review A, DOI 10.1103/PhysRevA.104.033304.

M. Tylutki, G. Wlazłowski, Universal aspects of vortex reconnections across the BCS-BEC crossover, Physical Review A, DOI 10.1103/PhysRevA.103.L051302.

S. Jin, K. J. Roche, I. Stetcu, I. Abdurrahman, A. Bulgac, The LISE package: Solvers for static and time-dependent superfluid local density approximation equations in three dimensions, Computer Physics Communications, DOI 10.1016/j.cpc.2021.108130.

A. Bulgac, I. Abdurrahman, S. Jin, K. Godbey, N. Schunck, I. Stetcu, Fission fragment intrinsic spins and their correlations, Physical Review Letters, DOI 10.1103/PhysRevLett.126.142502.

Savvas Zafeiropoulos, Aix Marseille University

C. Egerer, R. G. Edwards, C. Kallidonis, K. Orginos, A. V. Radyushkin, D. G. Richards, E. Romero, S. Zafeiropoulos on behalf of the HadStruc collaboration, Towards high-precision parton distributions from lattice QCD via distillation, Journal of High Energy Physics, DOI 10.1007/JHEP11(2021)148.

Sergey V. Churakov – Paul Scherrer Institute

Person Detail

“Numerical simulations are the basis for quantitative description of processes in the underground repository systems over geological time-scales. CSCS’s HPC resources have become for us an indispensable tool for interpretating and upscaling the laboratory experimental data and addressing phenomena acting at geological timescales”.

Name
Sergey V. Churakov

Position
Full Professor of mineralogy at the University of Bern

Institution
Laboratory for Waste Management, Paul Scherrer Institute

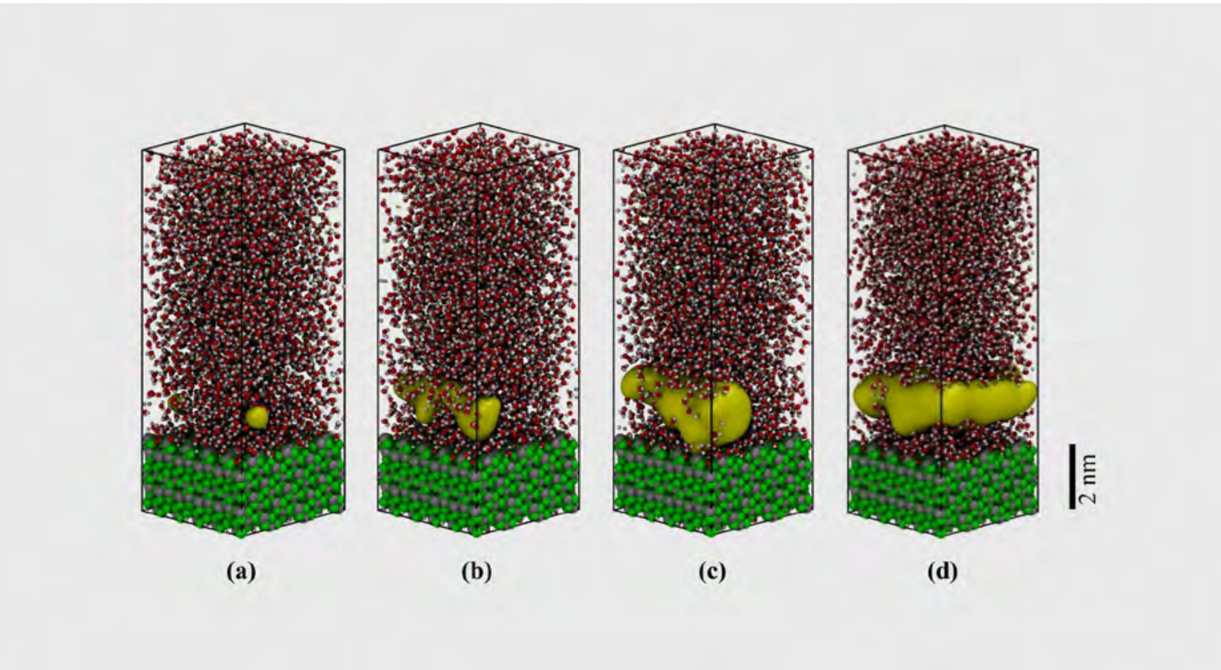
Background

1996	MSc in geochemistry, Moscow State University, Russia
1997	MSc in applied mathematics, Moscow State University, Russia
1998-2002	PhD student, GeoForschungsZentrum, Potsdam, Germany
2002-2003	Researcher, ETH Zurich & CSCS
2003-2004	Researcher, ETH Zurich & USI
2004-2006	Staff member, Paul Scherrer Institute
2008-2013	Head of the Transport Mechanisms Group, Paul Scherrer Institute
2014-2015	Titular Professor at the University of Bern
Since 2014	Head of Laboratory for Waste Management, Paul Scherrer Institute
Since 2015	Full Professor of mineralogy, University of Bern

Area of research
Mineralogy and environmental sciences.

Specialised in
Reactive transport processes in geochemical systems.

HPC means for me
I am using HPC as a powerful microscope which provides me with atomic scale insight into the mechanism of fundamental geochemical processes taking place at fluid-mineral interfaces, inside of natural materials and so to validate the models suggested by experimental laboratory observations.



Molecular scale mechanism of vapor nucleation at mineral surface interface

Nowadays, computer simulation in geosciences have become an indispensable tool for testing hypothesis and predicting geochemical evolution of natural and engineered systems used for waste disposal, CO2 sequestration or geothermal energy harvesting. Coupled geochemical reactive transport modeling is often the only way to assess possible scenarios for their evolution over geological time scales. With the HPC infrastructure and IT services offered by CSCS, we are able to create high-fidelity digital twins of natural and engineered underground systems and apply these models for system design and subsequent environmental safety assessment.

New, high-resolution models merge weather and climate

The EXCLAIM initiative is developing new, global climate models in high resolution to directly simulate regional events like thunderstorms. (Image: Shutterstock/NASA)

Torrential rain, hailstorms and flooding have dominated the weather in central and northwest Europe over summer in 2021. But how exactly are such extreme weather events connected to global warming? In fact, current climate and weather models have reached a wall, limiting the extent to which researchers can draw conclusions about how climate change affects extreme weather.

That's why ETH Zurich has teamed up with CSCS and other Swiss and international partners to launch the EXCLAIM research initiative. The project aims to develop a new generation of high-resolution weather and climate models with dramatically increased spatial resolution. Current global models typically calculate climate conditions in grid cells with a length of 50 to 100 kilometres. In the long run, EXCLAIM researchers aim to increase this resolution to a grid length of just one kilometre — the typical resolution of today's regional weather models. To achieve this, the models will have to run around 100 times faster than is currently possible.

Together with a high-performance computing infrastructure, such high-resolution models will enable scientists to forecast extreme weather events with accuracy and gain a better understanding of them in the context of global climate change.

In addition, the project will likely improve the reliability of the weather forecasts provided by the Federal Office of Meteorology and Climatology MeteoSwiss and allow scientists to predict how extreme weather events might look like in the future.

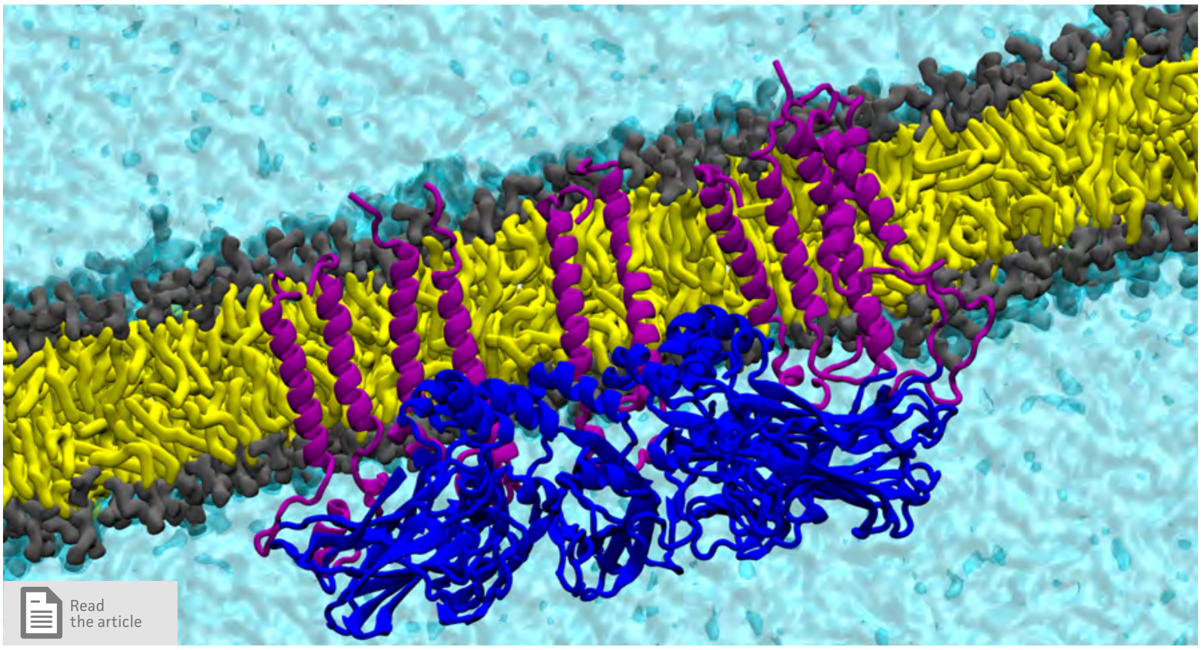
EXCLAIM will be taking a revolutionary approach by splitting the source code into two parts: a first part that represents the interface to the model developers and users; and an underlying infrastructure part in which the model's central algorithms are adapted to the respective hardware. CSCS and partner institutions have already used this approach in the current MeteoSwiss weather model with great success: They were able to accelerate the model by a factor of ten.

Also, customised computer infrastructure will be essential, which is why tailored supercomputer hardware and software is being developed in parallel — in particular, for the new CSCS "Alps" system to come in 2023.

Reference

EXCLAIM website https://exclaim.ethz.ch/

Scientists explore lipid metabolism with simulations and experiments



Multiple seipin molecules (yellow) embedded in two lipid layers, with the transmembrane domains (magenta) and luminal domains (blue). (Image: Research group Stefano Vanni, University of Fribourg)

In humans and animals, fat cells fulfil vital tasks protecting our organs and serving as a source of energy. They produce and store fat in special organelles called lipid droplets. In addition, every cell of the human organism contains lipid droplets that serve as energy suppliers and are involved in lipid metabolism inside the cells. If lipid storage is poorly regulated, this can lead to obesity and obesity-related diseases.

To better understand the mechanisms involved in lipid storage, the team of Stefano Vanni, SNSF professor at the University of Fribourg, performed molecular dynamics simulations on CSCS's "Piz Daint", and combined the simulation's outcomes with experimental results on lipid droplet formation in yeast cells.

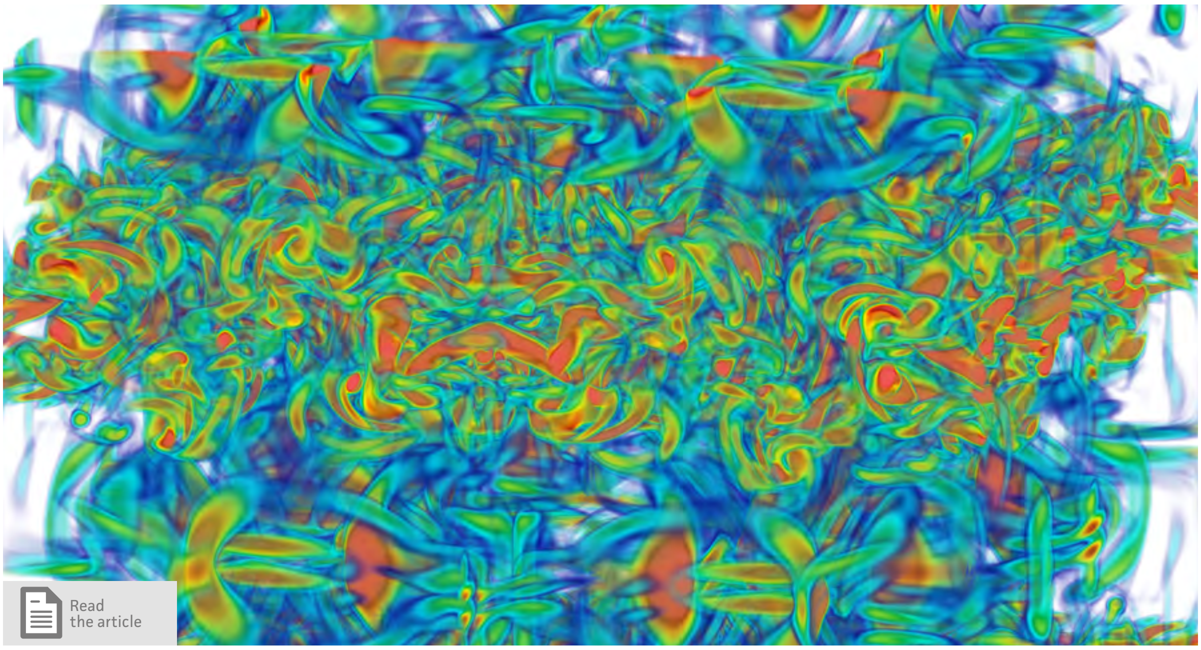
Their findings show that so-called phospholipids are involved in the regulation of lipid droplets formation in the endoplasmic reticulum, another organelle of the cell. In particular, the phospholipids regulate the aggregation of triglycerides, which are the main form of fat in lipid droplets: Phospholipids with monounsaturated fatty acids in their structure seem to favor the formation of lipid droplets, whereas short saturated fatty acids are limiting the accumulation of free triglycerides in lipid droplets. The researchers conclude that lipid droplet formation removes stress from the endoplasmic reticulum: by driving free triglycerides from the endoplasmic reticulum membrane into lipid droplets, the cells are protected from high fatty acid levels.

With further simulations, the researchers explored the role of the protein seipin, which was discovered in connection with lipodystrophy — a disease that develops in individuals who are unable to store lipids. The simulations revealed that seipin traps triglycerides within its ring-shaped structure. If, however, mutations are introduced in the trapping region, the formation of lipid droplets is hindered.

According to Vanni, these results could help to improve the understanding of metabolic diseases related to fat storage and thus aid in the development of drugs or dietary products.

Reference
Zoni et al. (2021): DOI: 10.7554/eLife.62886
Zoni et al. (2021): DOI: 10.1073/pnas.2017205118

ETH researchers compute turbulence with artificial intelligence



Vortical structures at the onset of transition to turbulence by Taylor Green vortices. (Image: CSE/lab ETH Zurich)

The modelling of turbulent flows is crucial for designing aircraft engines and heart valves, for predicting the weather, or for retracing the birth of a galaxy. Yet to this day, the complexity of fluid flows is not fully understood. Researchers at ETH Zurich have now successfully automated the modelling of turbulence by combining fluid mechanics with artificial intelligence (AI).

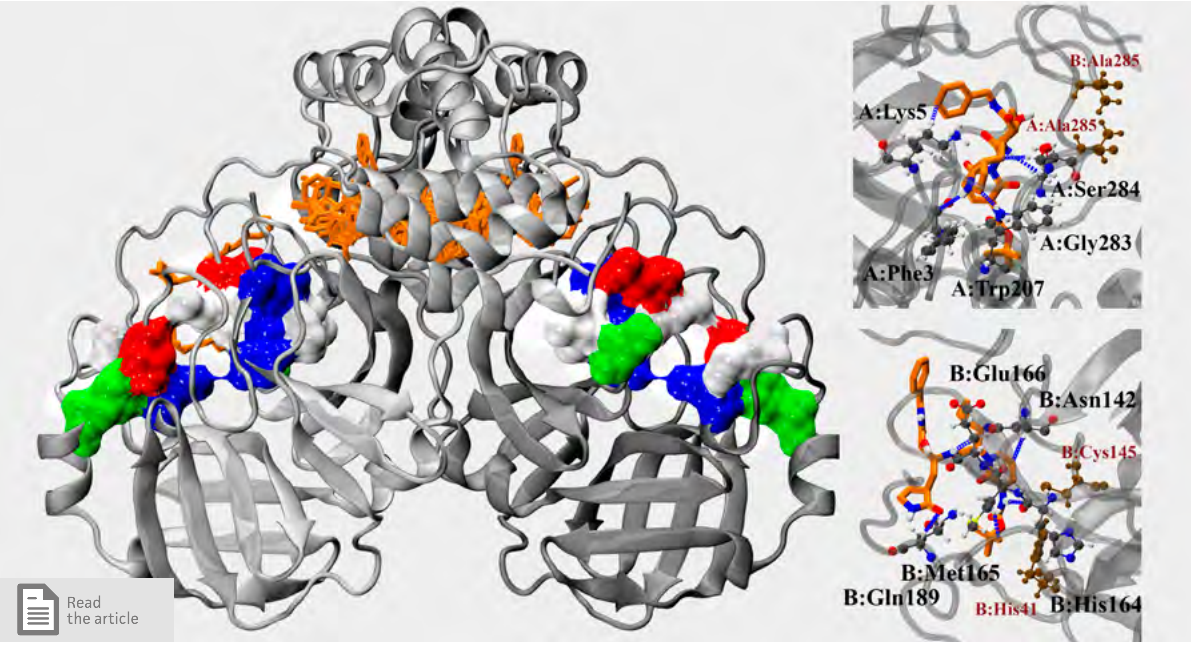
Two major approaches for simulating the complex structures of turbulence exist: One is direct numerical simulation (DNS), the other is large eddy simulation (LES). DNS is more accurate, but not practical for most real-world applications due to its massive computational cost. Using LES, computational cost is reduced, since so-called turbulence closure models account for the finer flow scales and their interactions. However, the choice of closure model is crucial for the accuracy of the results. Now, Petros Koumoutsakos, a professor at ETH Zurich, and his team have proposed to use AI to learn the best turbulent closure models from DNS and apply them to LES.

Specifically, the team developed new reinforcement learning (RL) algorithms that learn to react to patterns in the turbulent flow field. In the process, the grid points that resolve the flow field act as AI agents — they learn turbulence closure models by observing thousands of flow simulations. This happens by the algorithm playing with the flow: The AI wins if it succeeds to match LES with DNS results. Meaning, it performs the actions of the unresolved scales by observing the dynamics of the resolved large scales. This way, the method offers a powerful new way to automate multiscale modelling.

“In order to perform such large-scale simulations, it was essential to have access to the CSCS supercomputer ‘Piz Daint’”, stresses Koumoutsakos. According to him the new method not only outperforms well-established modelling approaches but can also be generalised across grid sizes and flow conditions.

Reference
Novati et al. (2021): DOI: 10.1038/s42256-020-00272-0

Scientists employ "Piz Daint" in search for drugs against COVID-19



Computational modelling predicted the binding locations of alpha-ketoamide 13b at the Mpro enzyme (left). The ligand binding at the catalytic active sites (bottom right inset) and at the dimer interface region (upper right inset) highlight the potential existence of novel sites that may be targeted by new drugs. (Image: Andrew Hung)

For people who cannot be vaccinated against COVID-19 disease due to pre-existing conditions, or have suffered a vaccine breakthrough, drugs that mitigate an infection can be lifesaving. Recently, a research group led by Andrew Hung from RMIT University, Melbourne, and Tom Karagiannis from Monash University, Melbourne, used simulations performed on the CSCS's "Piz Daint" to search for promising drug candidates against two key enzymes of the virus: the SARS-CoV-2 main protease (Mpro) and the papain-like protease (PLpro). Both enzymes process certain proteins that are essential for the virus s replication.

In their simulations, the researchers screened over 300 compounds for their properties. The results yielded a set of 30 substances showing the strongest binding affinity to Mpro. A further narrowing down revealed that above all, hypericin, a plant constituent of St. John's wort, and cyanidin-3-O-glucoside, which occurs in hibiscus and rose plants, possess the strongest binding affinity of all compounds examined.

For PLpro, the team found another compound in addition to hypericin and cyanidin-3-O-glucoside with antiviral potential: rutin, which occurs in plants and is often used as an antioxidant. PLpro is an attractive drug target because of its dual role. The enzyme is not only responsible for the replication of the virus but may also contribute to the virus ability to evade host immune responses.

In a further study, the researchers used a series of different computational methods at the molecular level to identify more drug binding regions in Mpro. Among else, the team employed so-called blind docking, a method that screens entire active region of an enzyme. This way, the researchers were able to identify a new and preferred compound binding site in Mpro.

"These results are significant because they highlight the way in which computational studies may guide lab work, potentially fast-tracking drug discovery for treating COVID-19 and other diseases," concludes Hung.

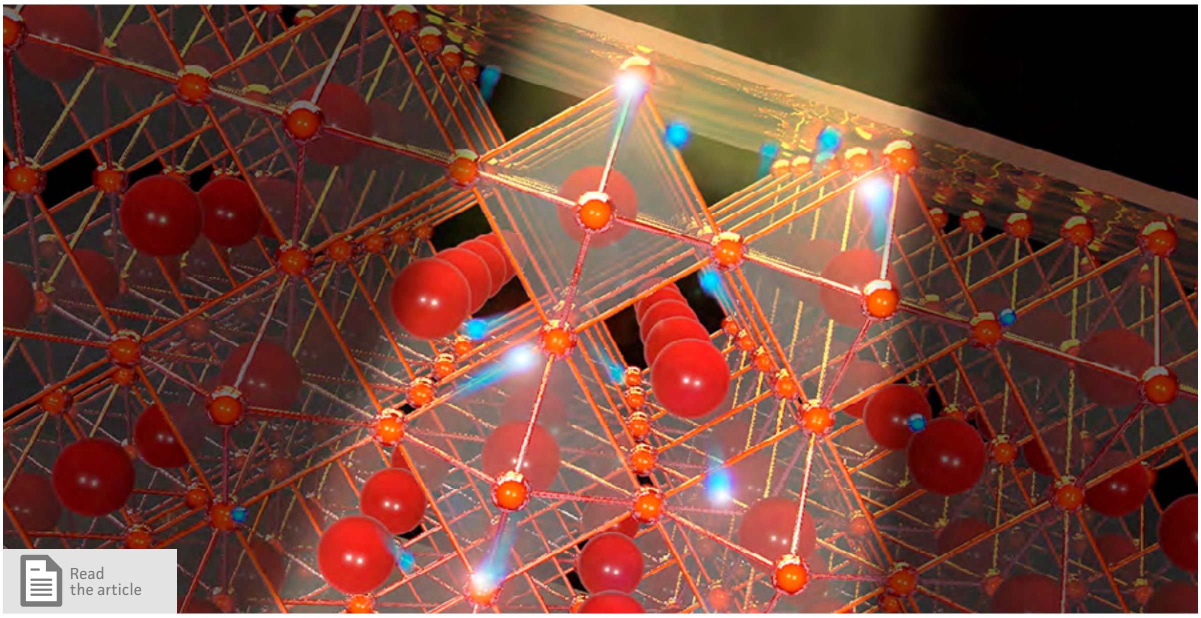
Reference

Pitsillou et al. (2020): doi.org/10.1016/j.compbiolchem.2020.107408

Pitsillou et al. (2020): doi.org/10.3389/fchem.2020.623971

Lianga et al (2020): doi.org/10.1016/j.compbiolchem.2020.107372

Computer simulations on “Piz Daint” further boost efficiency of perovskite solar cells



Highly luminescent and stable alpha-FAPbI3 perovskite via HCOO- anion engineering. (Image: Jin Young Kim, UNIST)

During the last decade, perovskite solar cells have been at the forefront of research in the race for an efficient and cost-effective new technology to harvest solar energy. In particular, researchers have focused on the cubic phase of perovskite solar cells, using so-called α-formamidinium lead triiodide (FAPbI3). Only in October 2020, the EPF Lausanne professors Michael Grätzel and Ursula Röthlisberger and their collaboration partners published a method to create thin-film solar cells based on a room-temperature stable FAPbI3 perovskite structure in Science.

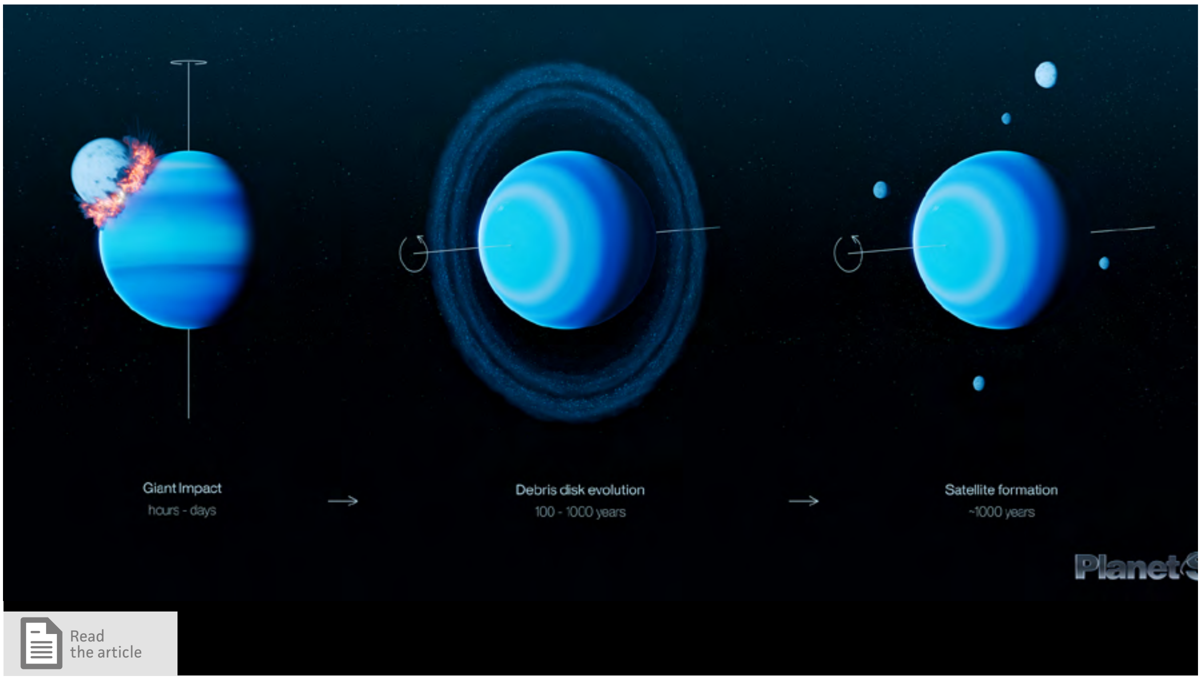
Now, the groups of Grätzel, Röthlisberger and partners have followed up on this work. In another joint experimental-computational study, the scientists succeeded to considerably increase the efficiency of FAPbI3-based perovskite solar cells through a novel chemical synthesis process.

One of the main problems in synthesis of perovskite cells stems from the halide components, in the case of FAPbI3 from iodide ions. Specifically, crystal lattice defects known as halide vacancies easily form during the production process, reducing the stability and efficiency of the cells. Based on computer simulations carried out on CSCS's “Piz Daint”, the researchers now succeeded in understanding this mechanism at atomic scale and subsequently developed an anion engineering method that suppresses the formation of such defects.

Their anion engineering approach led to an improved solar cell efficiency of up to 25.6 percent, and an operational stability of at least 450 hours. The certification value is slightly lower: “The cells achieved a certified record efficiency in power conversion of 25.21 percent, and thereby surpassed the current market-leading technology, polycrystalline silicon”, says Röthlisberger. According to her group's molecular dynamics simulations, formate anions (HCOO-) are not only best suited to suppress halide vacancy defects but also improve the morphology of the thin films.

Reference
Jeong et al. (2021): DOI: 10.1038/s41586-021-03406-5

How did the peculiar moons of Uranus form?



Artistic illustration of the formation of the largest moons of Uranus. (Image: Tobias Stierli)

While most planets rotate horizontally around their axis, Uranus does not follow this choreography. Instead, Uranus is tilted on its side and rotates vertically. The same is true for the moons of this giant, ice-rich planet, which additionally display an unusual distribution of mass between them: The five largest moons increase in mass with distance from their planet, the furthest moon being about 100 times as massive as the nearest. In a new study, a team from the University of Zurich and the NCCR PlanetS propose a reason for these peculiarities.

Moons usually form from a disc-like accumulation of ice and rocks orbiting a planet. Similar to a spinning top, the mass of such a disc concentrates towards its centre. Thus, one would expect the moons that form closer to the centre to become more massive than those further out — unlike the largest moons of Uranus. One theory is that the impact of a large celestial body created vast amounts of debris, from which the moons eventually emerged. This theory would also explain the fact that Uranus is tilted to the side.

To examine this idea, the team simulated the evolution of the planet and its moons using CSCS's "Piz Daint". The results point towards a grazing impact of an object about three times as massive as Earth. "This tilted the planet and created a disc of debris around it, from which the moons formed," says Jason Woo, first-author of the study. From their simulations, the researchers also learned that the peculiar mass distribution stems from differences in ice-evaporation. As Woo explains, "the colossal impact generated a lot of heat." Therefore, any ice debris from the planet quickly evaporated. Further out, however, the temperatures did not increase as much and more of the ice remained available as material for the moons. "Out there, the moons had more time to accumulate material and thus grew larger," Woo states.

According to the researchers, their results not only give more confidence to the idea that Uranus was indeed hit by a massive object and that this led to the formation of its largest moons, but may also help them to better understand some of the other planets in the cosmos.

Reference
Woo et al. (2022): DOI: doi.org/10.1016/j.icarus.2021.114842

Siddhartha Mishra - ETH Zurich

"I wholeheartedly thank the terrific personnel at CSCS who always work hard to keep the HPC facilities running, even in very adverse circumstances. A large part of the research of my lab cannot be performed without their dedication".

Name
Siddhartha Mishra

Position
Full Professor for applied mathematics, ETH Zurich

Institution
ETH Zurich

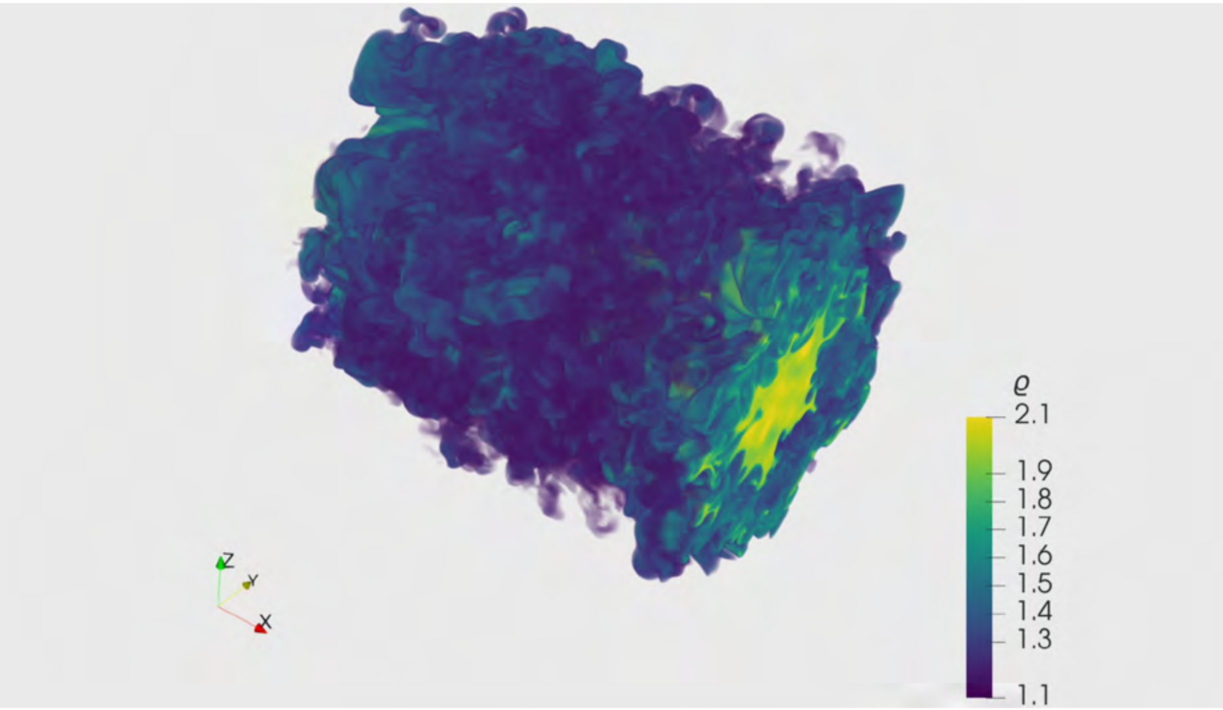
Background

2003-2005	PhD, Indian Institute of Science-Tata, Bangalore, India
2005-2009	Postdoc, University of Oslo, Norway
2009-2011	Assistant Professor, ETH Zurich
2011-2012	Associate Professor, University of Oslo, Norway
2012-Present	Professor, ETH Zurich

Area of research
Numerical analysis, scientific computing, machine learning.

Specialised in
Design and Analysis of algorithms for scientific simulations.

HPC means for me
The main resource to test my algorithms in different settings and to discover interesting and unexpected facets of the system being studied.



"Piz Daint" to study 3D compressible flows

We are using "Piz Daint" to compute statistical solutions for compressible fluids. These mathematical objects are probability measures in infinite dimensions that model all possible multi-point correlations of the flow and describe uncertainty propagation in turbulent fluid flows. We run an optimized, high-resolution, finite volume code (ALSVINN) on "Piz Daint" to compute statistical observables such as mean, variance, structure functions, etc., for three-dimensional compressible turbulent flow to discover interesting qualitative and quantitative properties of these solutions.

"Experience of users and developers is a key measure of success for us."

Sadaf Alam, Chief Technology Officer (CTO) at CSCS, was among the individuals shaping the architecture of the new "Alps" research infrastructure at CSCS. At the end of 2020, the first High Performance Computing (HPC) cluster on "Alps", called "Eiger" went into operation. Sadaf gives insights into the first experiences with the new system during 2021.

Sadaf Alam. (Image: CSCS)

Sadaf, with "Eiger", CSCS has laid the foundation stone for "Alps". The installation of "Alps" will be completed in 2023. What are the first experiences with the new system?

Sadaf Alam: Experience of users and developers is a key measure of success for us. Therefore, the CSCS team focused on ensuring a smooth transition from the "Piz Daint" multi-core HPC platform to the "Eiger" HPC platform on "Alps", primarily by maintaining the same look-n-feel for the users. There are however distinct features between the two generations of HPC platforms, notably different multi-core processors (Intel on "Piz Daint" and AMD on "Eiger"), a new high-performance network called HPE Cray SlingShot, and an innovative, cloud-like system management software stack. While the performance capabilities have improved by orders of magnitude, user interfaces for building applications and running jobs remain the same. Having said that, the underlying technology from Cray-HPE is highly innovative, which means the co-design efforts are continuing to enhance performance and quality of service. We greatly appreacite candid input from users. We have a co-designed feedback loop with the developers of key technologies at HPE Cray where our users' input is an invaluable asset for continued operational optimization and tuning efforts.

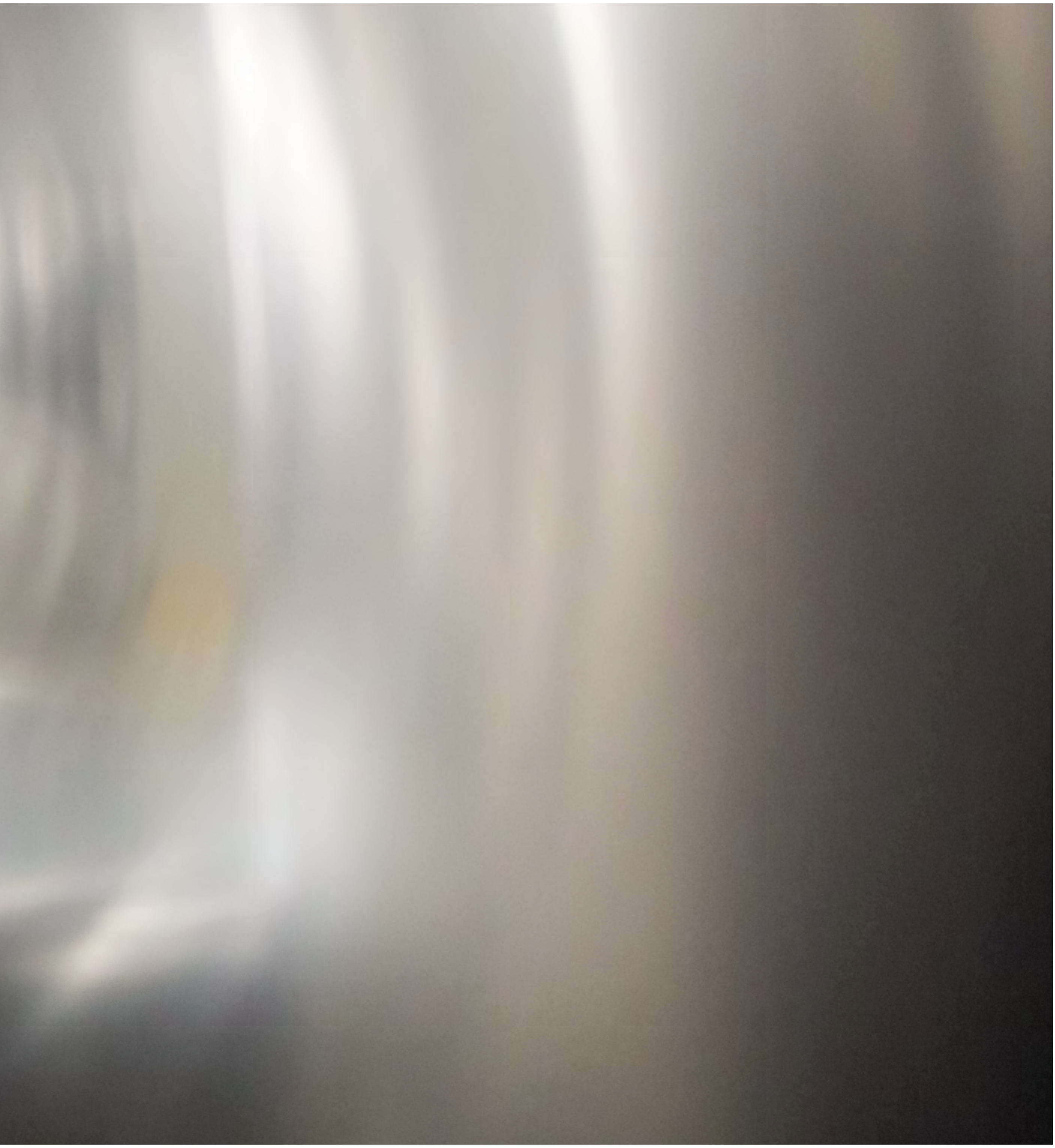
Regarding "Eiger" and "Alps" in general, what has kept you most busy this year?
CSCS has been among the first supercomputing centres going into operation on the HPE Cray EX system with an innovative, open-source software management stack called Cray System Management (CSM). This stack enables convergence of HPC and cloud technologies. "Eiger" for instance is a scalable, HPC slurm cluster on "Alps" i.e. it very closely resembles a traditional massively-parallel supercomputer, while "Alps" itself is a multi-tenant capable infrastructure that can serve different usage models. Therefore, the look-n-feel for users of "Piz Daint" hasn't changed thanks to the hard work of the development and operation teams at CSCS. Our co-design target is an extremely powerful yet highly versatile supercomputing ecosystem for users and developers of diverse research infrastructures and workflows. This ambitious design objective has been keeping the team extremely busy for the last couple of years.

Did everything go according to plan?
Partially, with some hiccups primarily due to the pandemic but also because of delays in development of some features in the system stack. Note that CSCS has been developing co-designed supercomputing platforms leveraging innovative technologies for over a decade. It is sort of in the DNA of CSCS, which helps us in planning and mitigating risks. Nevertheless, we didn't foresee the impact of the pandemic on the supply chains or on our collaborative development efforts resulting in some delays in the availability of HPC platforms for early users.

The University of Zurich is one of the institutions already using "Eiger". The possibility of creating software-defined environments is one of the special features of CSCS' new supercomputing platform. What can you tell us about the environment that was set up for UZH?
CSCS has begun leveraging software defined infrastructure technologies, which are more commonplace in cloud computing, for our HPC platforms over the past few years. Essentially, different hardware components are virtualized, without compromising performance, to configure multi-tenant virtual clusters. The University of Zurich environment is an instantiation of CSCS HPC platform, which, from a users' perspective is an HPC slurm cluster, just like "Piz Daint". For instance, the same services are available to users as before such as ssh login, slurm job submission, and interactive JupyterHub notebooks. What is unique is that "Alps" has other cluster tenants sharing the HPC network. Alongside "Eiger", there are multiple test and development HPC slurm and cloud (Kubernetes bare-metal) virtual clusters. Individual virtual clusters can be reconfigured and resized without impacting quality of service for other tenants.

I can imagine that the broader user community is already eagerly waiting to be able to use and test "Eiger". When will it become accessible for the entire User Lab?
My colleague, Maria Grazia Giuffreda who manages the User Program, is developing a roadmap for transition, which she will share with the community in a timely manner. We aim at periodically migrating the user communities over to the new infrastructure, making the transition as smooth and efficient as possible.

In a nutshell, what are the most exciting features that users can expect from the new "Alps" infrastructure?
Our objective is to maintain, sustain, and enhance the experience of our users such that wide ranging HPC workloads can exploit ever so powerful technologies. In our view, equally exciting should be the functional aspects, which are significantly revamped and are paving the way for the convergence of supercomputing and cloud technologies. Users can leverage opportunities for developing distributed IT research infrastructures for data analysis, machine learning, and simulations based workflows. I'd like to highlight two development efforts at CSCS, namely our HPC container runtime engine called Sarus and our REST API gateway to HPC resources called FirecREST. We believe that these efforts will complement the self-service, cloud-native experiences for HPC on "Alps". Stay tuned!



Finances

Expenditures in CHF

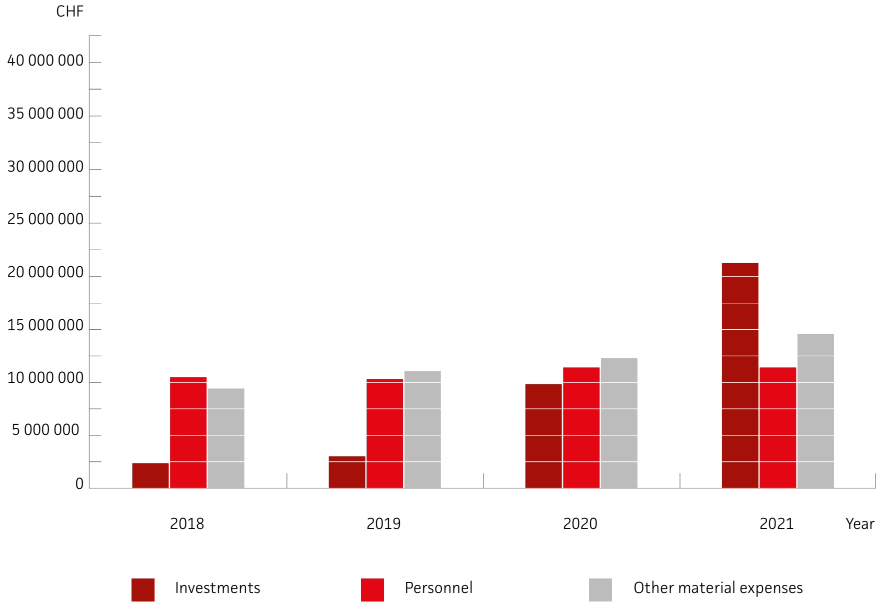
Expenditures in CHF	User Lab	Third Party	Total
HPCN-24 Investments	**24 258 475.64**	**0.00**	**24 258 475.64**
New System	20 186 443.53		20 186 443.53
Data Center	454 565.11		454 565.11
Secondary Installation	2 698 278.00		2 698 278.00
Primary Installation	919 189.00		919 189.00
IT Investments	**904 680.00**	**478 933.80**	**1 383 613.80**
Personnel	**11 640 165.36**	**5 094 967.90**	**16 735 133.26**
Payroll	11 386 612.26	5 094 967.90	16 481 580.16
Further education, Recruitment	253 553.10		253 553.10
Material expenses	**10 954 882.76**	**2 824 751.94**	**13 779 634.70**
Maintenance building & technical infrastructure	572 647.82	55 000.00	627 647.82
Energy	3 209 236.70	761 298.99	3 970 535.69
Maintenance hardware, Licenses, IT services & Telecommunication	4 841 452.79	528 751.11	5 370 203.90
Remunerations, Marketing, Workshops, Services, Travel, Membership fees	712 795.45	189 041.84	901 837.29
Granting of funds for PASC projects	1 618 750.00		1 618 750.00
Granting of funds for EuroHPC LUMI		1 290 660.00	1 290 660.00
Total expenditures	**47 758 203.76**	**8 398 653.64**	**56 156 857.40**

Income in CHF

Income in CHF	User Lab	Third Party	Total
Contribution ETH Zurich	21 529 514.83		21 529 514.83
Contribution ETH Rat - HPCN investments	32 300 000.00		32 300 000.00
Contribution ETH Rat - PASC initiative	3 250 000.00		3 250 000.00
Contribution SERI - EuroHPC LUMI		1 290 660.00	1 290 660.00
Research collaboration projects		1 753 244.00	1 753 244.00
Services for paying customers		11 302 598.55	11 302 598.55
Other income		276 062.96	276 062.96
Total income	**57 079 514.83**	**14 622 565.51**	**71 702 080.34**

User Lab Expenses Development (CHF)

	2018	2019	2020	2021
Investments	2 472 847	2 998 292	9 840 366	21 545 689
Personnel	10 479 422	10 286 088	11 378 508	11 640 165
Other material expenses	9 414 401	11 006 943	12 261 041	14 572 350



“We are thankful for the support of the CSCS team which is critical for our development and use of climate models”.

Name
Sonia I. Seneviratne

Position
Full Professor, Department of Environmental Systems Science

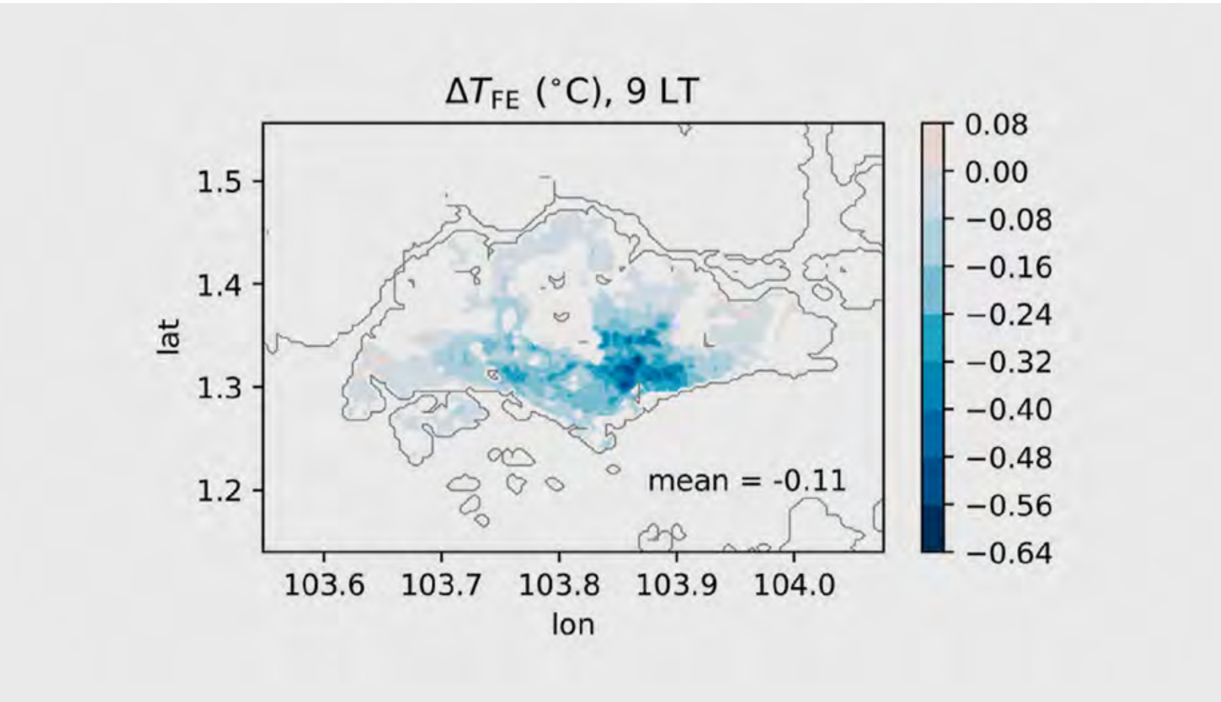
Institution
ETH Zurich

Background
1999-2002 PhD in atmospheric and climate science, ETH Zurich
2003-2004 Visiting Research Associate, NASA/GSFC, Greenbelt, USA
2005-2007 Senior Research Scientist / Oberassistentin, ETH Zurich
2007-2012 Assistant Professor, ETH Zurich
2013-2016 Associate professor, ETH Zurich
2016-Present Full professor, ETH Zurich

Area of research
Atmospheric and climate science.

Specialised in
Land-climate dynamics and climate extremes.

HPC means for me
High performance computing is an important part of the work of my team. We combine climate model experiments and statistical data analysis, based on model data, ground observations, and satellite measurements, in our research.



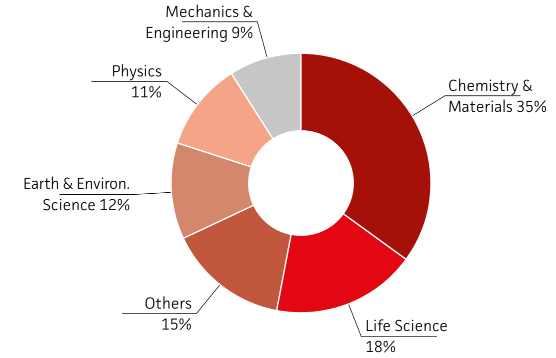
HPC for Climate Change

Sonia Seneviratne's research focuses on climate extremes and land-climate interactions. Understanding processes leading to droughts and heatwaves, the impact of land processes and land cover changes on regional climate, and their changes with global warming is a top priority to address the urgent problem of the climate change. With the help of "Piz Daint" Sonia Seneviratne and her team are investigating the role of land surface conditions, mobility and greenhouse gas emissions for regional climate and climate extremes. These studies can support policy-makers toward designing holistic solutions to address the challenge of climate change adaptation and mitigation on local to regional and global scale.

Usage Statistics

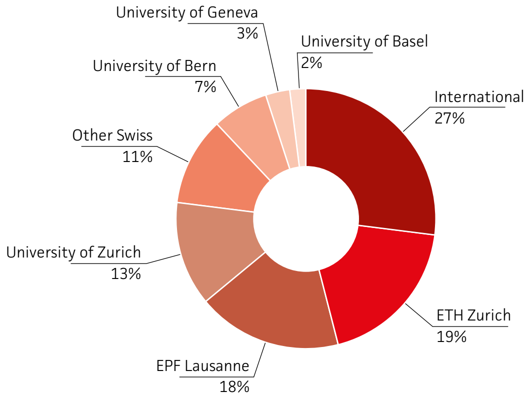
User Lab Usage by Research Field

Research Field	Node h	%
Chemistry & Materials	14 020 305	35
Life Science	7 169 159	18
Others	6 094 124	15
Earth & Environmental Science	5 041 280	12
Physics	4 535 413	11
Mechanics & Engineering	3 839 738	9
Total Usage	**40 700 019**	**100**



User Lab Usage by Institution

Institution	Node h	%
International	10 848 742	27
ETH Zurich	7 904 080	19
EPF Lausanne	7 423 572	18
University of Zurich	5 398 674	13
Other Swiss	4 356 658	11
University of Bern	2 975 721	7
University of Geneva	1 202 329	3
University of Basel	590 943	2
Total Usage	**40 700 719**	**100**



Compute Infrastructure

Computing Systems Overview

Name	Model	Installation / Upgrades	User	TFlops
Piz Daint	Cray XC50 / Cray XC40	2012 / 13 / 16 / 17	User Lab, UZH, NCCR Marvel, CHIPP	27 154 + 2 193
Grand Tavé	Cray X40	2017	Research & Development	437
Tsa / Arolla	Cray CS-Storm 500	2020	MeteoSwiss	1 169
Alps	HPE Cray EX	2020	User Lab, Research & Development	4 719

Computing Systems Specifications

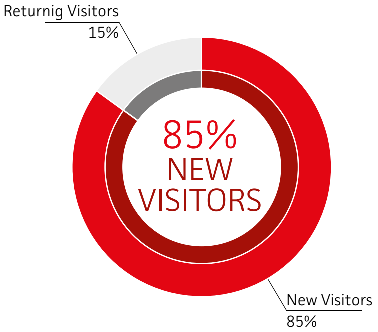
Name	Interconnect Type	CPU Type	Cores	Sockets	GPUs	Nodes
Piz Daint	Cray Aries	Intel Xeon E5-2690 v3/Nvidia Tesla P100	12	1	1	5 704
		Intel Xeon E5-2695 v4	18	2		1 813
Grand Tavé	Cray Aries	Intel Xeon Phi CPU 7230	64	1	0	164
Tsa / Arolla	100 Gb Ethernet	Intel Xeon Skylake 6143 Nvidia Tesla V100	8	2	8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

Communications Statistics

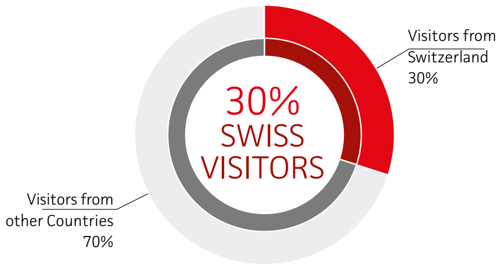
Website cscs.ch

	2020	2021
Total Website Visitors	67 360	79 907
Average Website Visits (Minutes)	1:99	2:52

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. Events www.cscs.ch/events/

Instagram

2021 creation of the CSCS page

	2021
Followers	158

Twitter

	2020	2021
Followers	1 735	2 025

LinkedIn

	2020	2021
Followers	8 678	9 496

YouTube

	2020	2021
Watch Time (Minutes)	553 764	469 866
Average View Duration (Minutes)	4:00	4:46
Number of Views	138 234	98 400

Facebook

	2020	2021
Followers	236	259

CSCS in the News

	2020	2021
News Websites	166	232
Print	97	75
Radio & TV	5	9

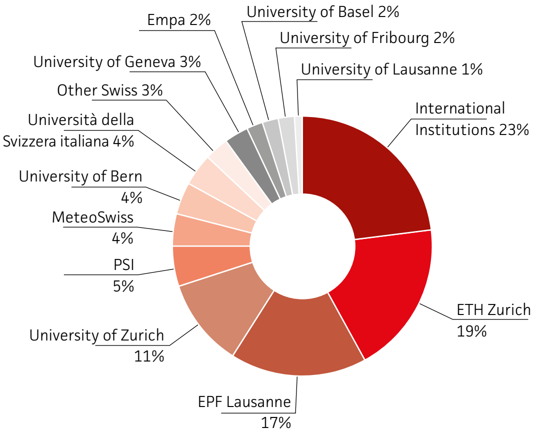
Word Cloud of News Related to CSCS

User Satisfaction

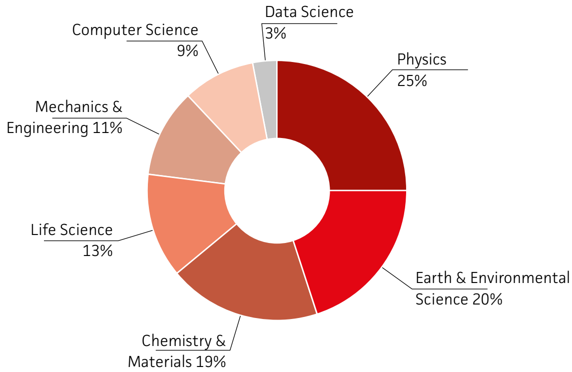
A user satisfaction survey was submitted to 2 441 users in January 2022. The response rate was of 14.7% (360 answers).

User Profile

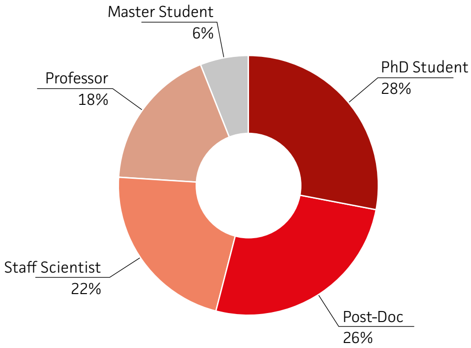
Your institution



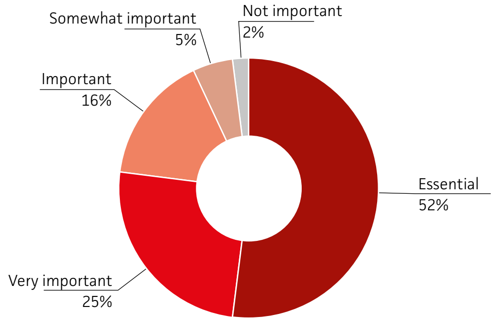
Your scientific field



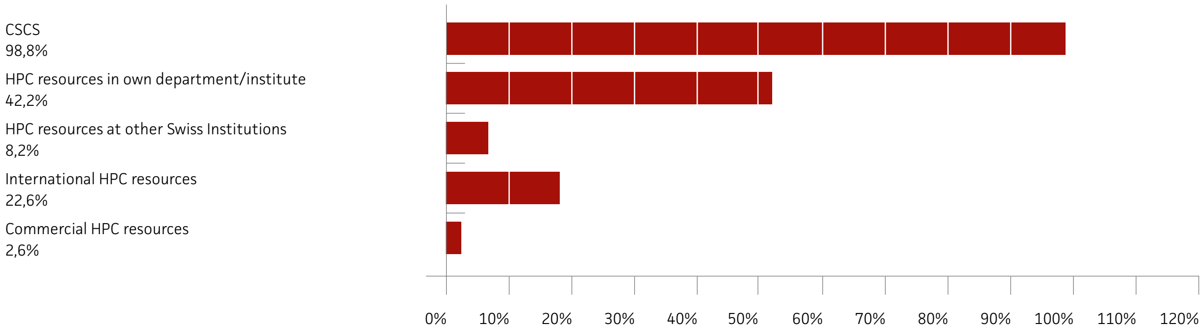
Your position



For my reserach, CSCS resources are



Which HPC resources are you using?



User Support

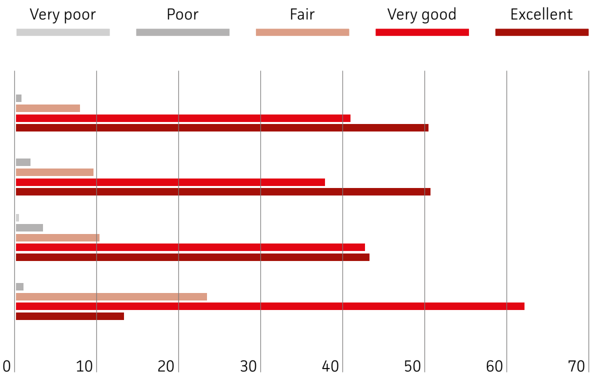
How do you rate the quality of...

Helpdesk support

System support

Application support

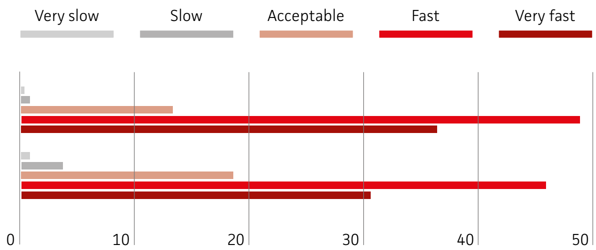
The offer of training courses and user events



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

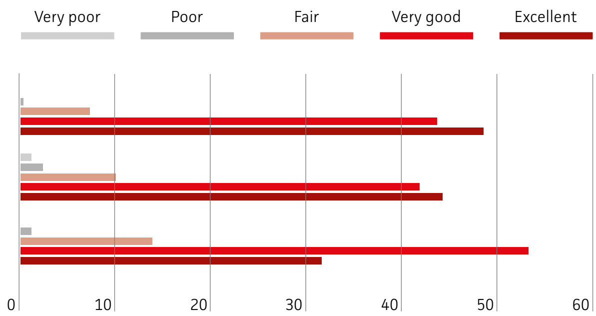
60

How you perceive...

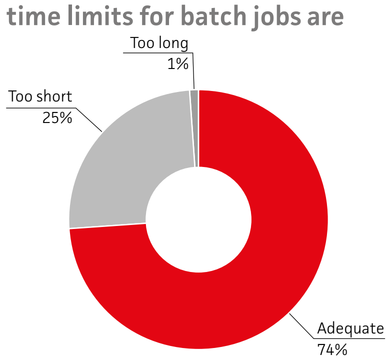
The availability of CSCS services?

The stability of CSCS services?

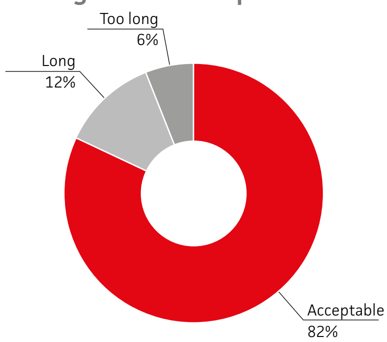
The ease of use of CSCS services?



The run time limits for batch jobs are

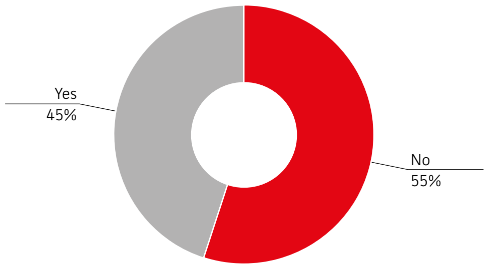


The job waiting time in the queue is

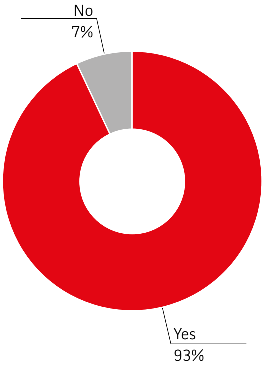


Project Proposal Process

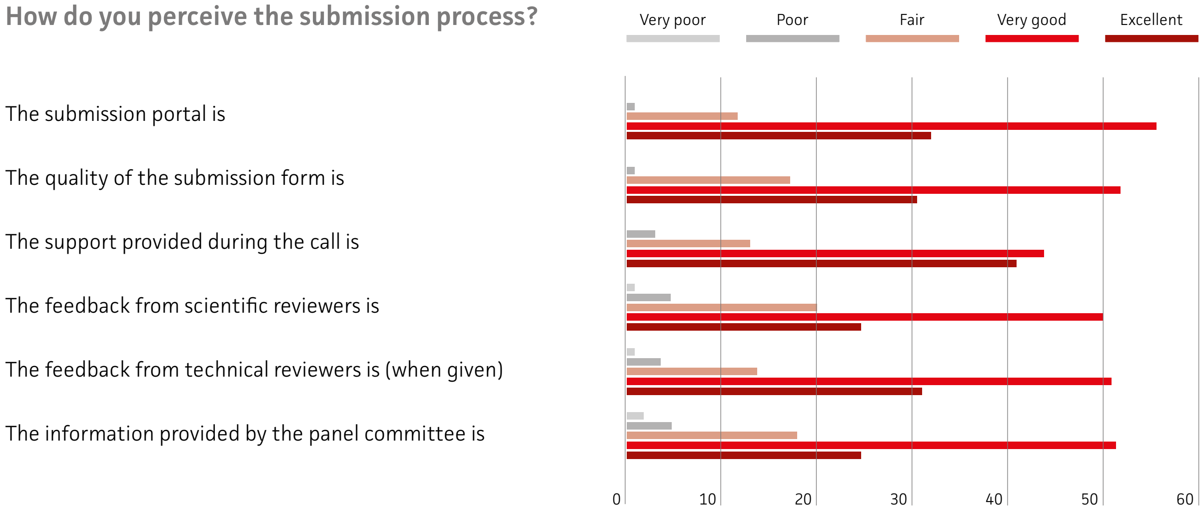
Have you been submitting project proposals to CSCS (as PI or supporting the PI?)



Is the reviewing process transparent?

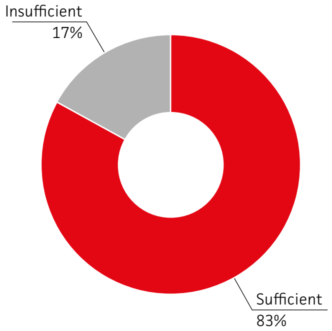


How do you perceive the submission process?

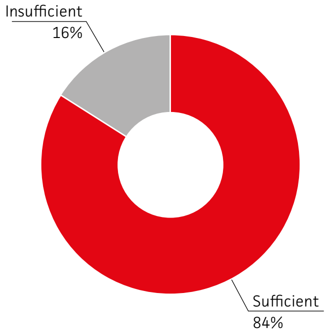


Adequacy of Allocated Resources

The resources assigned to my project are

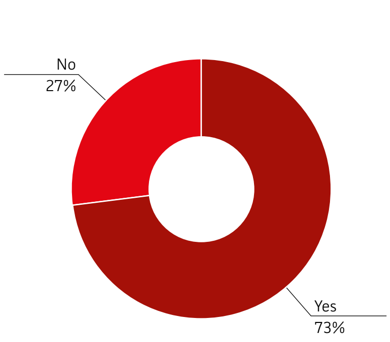


My storage allocation on "project" is

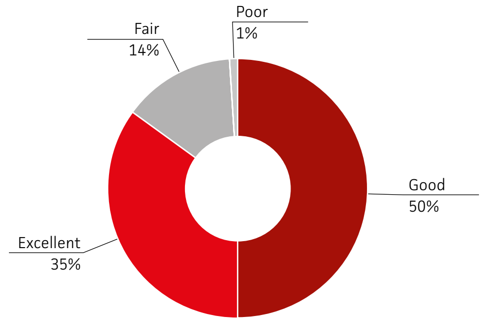


Application Development

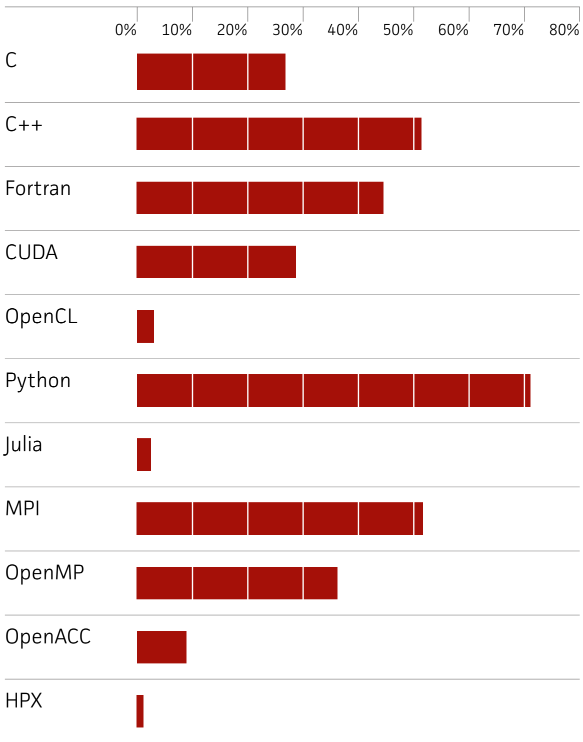
Do you develop and maintain application codes?



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



Which programming languages and parallelization paradigms are you using primarily?

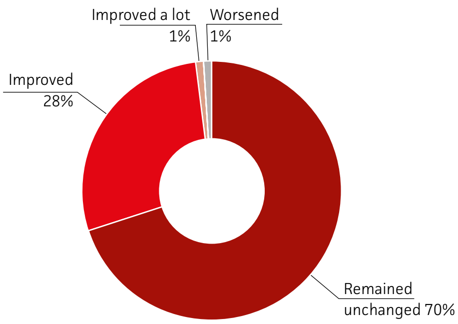


Information & Communication

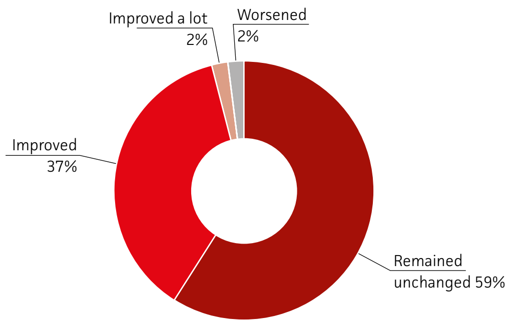
How do you feel informed about...

Perception of CSCS

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



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



Impressum

CSCS Swiss National Supercomputing Centre
Via Trevano 131
6900 Lugano
Switzerland

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

Design & Layout
Humus Brand Culture

Editorial Board
Michele De Lorenzi
Maria Grazia Giuffreda
Santina Russo
Angela Schneebeli
Simone Ulmer

Photos
CSCS, Marco Abram, Matteo Aroldi, Alessandro Della Bella
Scientists portraits: Alessandro Della Bella, Rebecca J. Howard

Printing
Lepori & Storni

Print-run
300

© CSCS 2022. All rights reserved.