Annual Report 2011

CSCS

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

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ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

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Welcome from the Director

Thomas Schulthess, Director of CSCS.

Welcome to this review of CSCS in 2011!

I have the pleasure of introducing this review of last year's most important activities and accomplishments at CSCS.

The silent but important highlight of the year 2011 was certainly the completion of the new building in Lugano. Construction started in early summer 2010, and was essentially complete by the end of 2011, leaving mainly the testing and acceptance of the complex infrastructure for 2012. On-time execution of this complex project was possible due to incredible contributions and teamwork by many participants: the real estate department and the planners at ETH; the experts from the construction planning team, and all the contributors working for the construction company Implenia as well as numerous subcontracting companies; CSCS staff, in particular Ladina Gilly; the Canton of Ticino and the municipality of Lugano. Most importantly the people of Lugano who were supportive of the project despite the disruption to their lives deserve our appreciation – after all the pipes for the lake water cooling had to be laid across the city from the lake to our new location next to the stadium in Cornaredo.

The second large project of the HPCN initiative besides the new building is the Swiss Platform for High-Performance and High-Productivity Computing (HP2C), which underwent a mid-term review in 2011. The fact that 80 scientists and developers came to this two-day review the week before Christmas is a testimony to the commitment of the community of application developers.

A panel of international reviewers recognized the high quality and pioneering contributions of the platform and its thirteen projects. A proposal for a future analogous project, to succeed HP2C, in 2013, will certainly receive a boost from this review.

Following the July 2011 meeting of ETH Board, the supercomputing systems of the HPCN initiative are now officially considered a scientific user lab with allocations carried out under a competitive peer-reviewed process. These systems are now formally a research infrastructure that will receive support as long as it is deemed important for Swiss science. This is a key milestone for simulation-based science in Switzerland, as it can now rely on a sustained infrastructure, as is common in experiment-driven branches of science, rather than having to reinvent itself every few years when the procurement of a new supercomputer has to be justified.

Besides the upgrade of our flagship system Monte Rosa, now equipped with about three thousand sixteen-core processors and Cray's new Gemini interconnect, CSCS introduced several new architectures in 2011. A next-generation Cray XMT system particularly well suited for graph based data analysis, as well as an SGI Ultraviolet system form the processing part of the new data analysis and storage facility EUREKA. The first two Cray XK6 cabinets, equipped with 176 hybrid nodes consisting of multi-core CPUs from AMD and Graphics Processing Units (GPU) from NVIDIA, were introduced in October 2011. Experience with the Cray XK6 and also a second hybrid-node based IBM iDataPlex cluster demonstrate that GPU-based systems could cause a real disruption within the supercomputing market. The architecture has to be seriously considered in future system developments at CSCS.

I would like to thank all CSCS staff, ETH Zurich, the university of Lugano, as well as our partners and all persons and organizations that supported us in completing another successful year in 2011. We are very much looking forward to 2012, when we will move into the new building in Lugano and begin construction of the next generation of supercomputers at CSCS.

Prof. Thomas Schulthess
Director CSCS

Content

Dear Reader,

Life science applications have become an important focus of computational science and high performance supercomputing. Fields as diverse as biology, genetics, biochemistry, pharmacy, structural and molecular biology are now major targets of computational research. In 2011 biomolecular simulations used 11% of the total CPU time available on CSCS supercomputers, and this number is set to increase in 2012. The most frequently used code is NAMD, followed by GROMACS and AMBER.

The CSCS Panel Committee consists of four members from very different disciplines. It is their duty to rate project proposals based on technical and scientific evaluations and to make final allocation recommendations. Adrian Mulholland, member of the committee, is Professor of Chemistry and directs the Computational Enzymology group at the University of Bristol, UK. He has kindly agreed to contribute a feature article on biomolecular simulation to this annual report.

Biomolecular simulation: harnessing emerging technologies and embracing new communities

By Adrian Mulholland[1], Christopher Woods[1,2] and Simon McIntosh-Smith[2] (University of Bristol - [1]Centre for Computational Chemistry, School of Chemistry, [2]Department of Computer Science,)

Nearly 50 years ago, Richard Feynman famously said that everything that living things do can be understood in terms of the "jigglings and wigglings" of atoms. Molecular dynamics simulations of proteins and other biological molecules are vital for understanding the details of this jiggling and wiggling. Modelling of protein structures and interactions is also a vital tool in drug design and the development of new catalysts. New methods and emerging computational technologies are extending biomolecular simulations to significantly greater lengths and timescales, allowing direct connection with experiments. Particular challenges include harnessing the tremendous computational power of graphics processing units (GPUs) and other emerging multicore and accelerator technologies, and making simulation methods a useful and accessible tool for experimental biologists.

Biomolecular simulation is making increasingly significant contributions to structural and systems biology. Simulations based on fundamental physics complement experiments in building a molecular level understanding of biology: they can test hypotheses and interpret and analyse experimental data, and give a uniquely detailed picture of interactions and motions at the atomic level, beyond what is possible from experiments alone. A wide variety of simulation techniques have been developed, applicable to a range of different problems in biomolecular science. Simulations have already shown their worth in helping to analyse how enzymes catalyse biochemical reactions, and how proteins fold to adopt their functional structures e.g. within cell membranes. They contribute to the design of drugs and catalysts, and to the understanding of the molecular basis of diseases. Simulations have also been central in developing the conceptual framework that is now at the heart of biomolecular science; that is, our understanding of the way that biological molecules move and flex - their dynamics which is central to their function. Developing methods from chemical physics and computational science will open exciting new opportunities in biomolecular science, including in drug design and development, biotechnology and biocatalysis.

Many cutting edge applications of biomolecular simulation require significant HPC resources: e.g. large-scale simulations of biological machines such as the ribosome, proton pumps and motors, membrane receptor complexes and even whole viruses. A particular challenge is the integration of simulations across length and timescales, as different types of simulation method are required for different types of problems. Methods such as metadynamics allow processes with large energy barriers to be studied in a reasonable amount of time. Most biomolecular simulations use simple "ball and spring" type molecular models: these "molecular mechanics" (MM) methods provide a good description of protein structure and dynamics in atomic detail. "Coarse-grained" methods treat groups of atoms together and provide simpler models that can study larger systems over longer times. There are encouraging efforts to link biomolecular simulations to larger scale mathematical and physiological models in biology and medicine. At the other extreme, methods based on quantum mechanics allow the electronic structure of biomolecules to be studied (e.g. as hybrid QM/MM methods) and modelling of chemical reactions in enzymes. Simple "docking" methods can rapidly test millions of small molecules to see whether they may fit into the binding site of a drug target (such as a virus enzyme), identifying potential leads for pharmaceutical development. More sophisticated and extensive calculations can give accurate predictions of how tightly potential drugs may bind to their target, while predictions of how drugs will be metabolized in the body assist in the later stages of drug development.

The significant HPC resources required by many state-of-the-art biomolecular simulations lead to significant challenges for software developers. As computational demands grow, and HPC architectures become more heterogeneous, so biomolecular simulation programs must become more sophisticated and flexible, and application developers become more knowledgeable. The developers of tomorrow's petascale and exascale applications will need to write code that will run efficiently over hundreds of thousands of cores, and incorporate features such as power management and fault tolerance. Equally, as the user community of biomolecular simulation software broadens beyond the traditional computational science community, it is important to make methods accessible to non-experts. Friendly and intuitive interfaces will be needed to allow new users to build, manage and navigate large HPC simulations, ideally as easily as they would use a spreadsheet or large digital photo albums.

Steps to addressing these challenges are being made on several fronts, by many groups worldwide. An example is the OpenMM toolkit being developed to provide a framework to remove the complexity of running across heterogeneous hardware platforms. OpenMM provides a single programming interface for developing of molecular simulation applications. The OpenMM developers handle the details of porting their library to new hardware, leaving the simulation developer free to concentrate on the algorithms behind their application. To improve the ease-of-use of biosimulation programs, communities such as the new CCP-BioSim project in the UK have come together to build awareness of biomolecular simulations and educate new users through workshops and online teaching materials, and are in the process of developing easy interfaces to automate common tasks. Lessons can also be learned from the Galaxy Project, which successfully broadened the audience of HPC bioinformatics applications. It provides a web-based interface to specify, submit and manage workflows of large-scale, data-intensive bioinformatics applications, without the need to learn the intricacies of each program, or have specialist knowledge of queuing systems or Unix shells.

With developments such as these, biomolecular simulations will become increasingly integral to developing molecular level understanding of biological mechanisms, and reach out to new communities of users in biomedical science.

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KEY INFORMATION

Founded in 1991, the Swiss National Supercomputing Centre, CSCS, develops and promotes technical and scientific services for the Swiss research community in the field of high-performance computing. CSCS enables world-class scientific research by pioneering, operating and supporting leading-edge supercomputing technologies.

Largest Production Machine

Monte Rosa, Cray XE6, 402 TFlops,
47 872 Cores, 46 TB Memory

Computing Time for Science

2011: 177 201 383 CPU h
2010: 168 147 399 CPU h

User Community

2011: 80 Projects, 704 Users
2010: 65 Projects, 605 Users

Employees

2011: 51
2010: 50

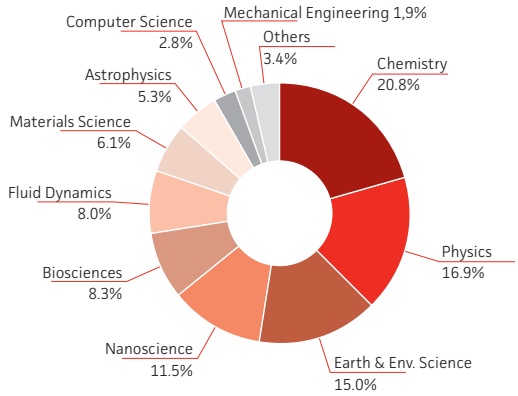
Investments

2011: 15.8 Mio CHF
2010: 8.4 Mio CHF

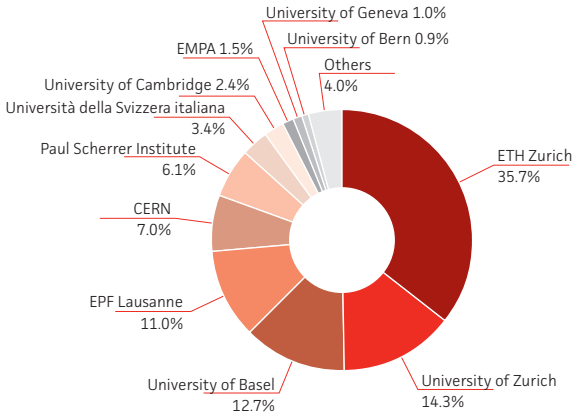
Operational Costs

2011: 11.9 Mio CHF
2010: 14.3 Mio CHF

Usage by Research Field



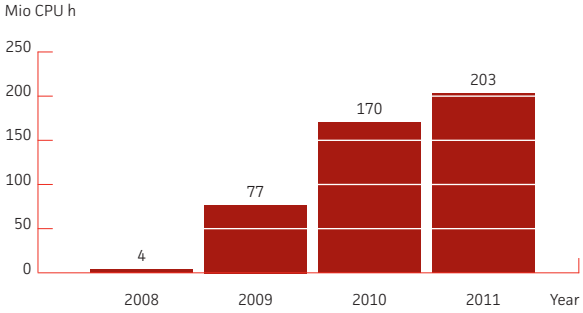
Usage by Institution



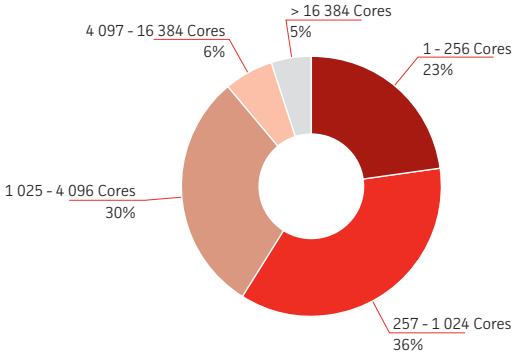
Computing Systems

Name	Supplier & Model	Installation / Upgrade	Usage / Customer	Peak Performance (TFlops)
Monte Rosa	Cray XE6	2009 / 2011	National User Lab	402.0
Tödi	Cray XK6	2010 / 2011	R&D	129.0
Piz Buin	Cray XT4	2006 / 2009	MeteoSwiss	5.0
Dole	Cray XT4	2006 / 2009	MeteoSwiss	3.3
Phoenix	Sun Cluster	2010 / 2011	CHIPP (LHC Grid)	11.8
Eiger	Dalco Cluster	2010 / 2011	R&D, Visualisation	10.2
Rigi	Sun Cluster	2007	MeteoSwiss & USI	0.5
Piz Julier	IBM/Transtec Cluster	2010 / 2011	National User Lab	3.3
Matterhorn	Cray XMT	2011	National User Lab	-
Rothorn	SGI Altix UV 1000	2011	National User Lab	2.7
Pollux / Castor	IBM iDataPlex Cluster	2011	R&D	4.1

Evolution of CPU Usage



Usage by Number of Cores per Job



January

CSCS Introduces SLURM as a New Batch Queuing System

A central element of a supercomputing centre is the batch queuing system, which allocates resources on the supercomputers and dispatches the users' jobs. CSCS moved from a proprietary solution to SLURM, an open-source resource manager designed by the Lawrence Livermore National Laboratory. CSCS will additionally invest resources in developing customized enhancements that will be shared with the growing SLURM developer community.

February

Workshop on Large-Scale Data Analysis

Scientists within Switzerland depend increasingly on large-scale data analysis - in diverse fields such as materials science, medicine, genomics, high-energy physics, climate research and astrophysics. To address this growing need, CSCS organized a workshop on large-scale data analysis. The workshop was aimed at researchers whose applications require random access to shared memory and typically do not run well on conventional systems. More than 50 researchers from Swiss universities attended the event, alongside invited international HPC vendors. Invited speakers at the workshop covered scientific case studies, specific hardware and software solutions, and the process for gaining access to the systems. During the workshop, CSCS announced having awarded a contract to Cray Inc. to acquire a next-generation Cray XMT supercomputer. The Cray XMT supercomputer features a massive, multi-threaded processing architecture designed for large data-driven problems on diverse data sets. Each processor in the Cray XMT system can handle up to 128 concurrent threads.

March

GPU Programming Workshop

CSCS hosted a two and a half day intensive course focused on GPU programming. Senior members of the PGI compiler development team, Michael Wolfe and Dave Norton (The Portland Group, Inc.), conducted two full days of instruction and hands-on training. They covered material on GPU hardware architecture, the CUDA programming model, directive-based GPU programming, performance analysis and optimization. The final half-day consisted of hands-on sessions on accelerating classical molecular dynamics simulations using GPUs, presented by CSCS staff.

HPC Advisory Council Switzerland Workshop

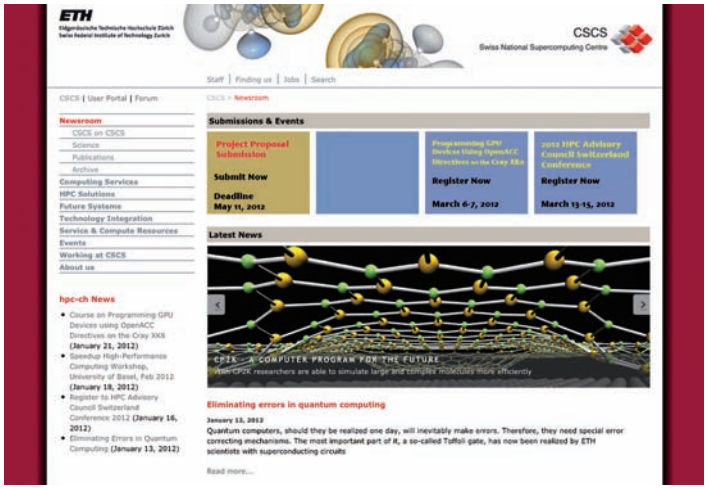
Hussein Harake, systems engineer in the Technology Integration Unit at CSCS, co-chaired this year's HPC Advisory Council Switzerland Workshop, held in the Lugano Convention Center. The well-attended workshop focused on several important areas in HPC, including high-speed networking, high-speed storage, Message Passing Interface (MPI) performance and future directions (such as GPU computing). During the two-day meeting, CSCS presented several talks, highlighting its experience with HPC storage and GPU computing.

SOS 15: Exascale in Engelberg

SOS (Sandia, Oak Ridge, Switzerland) is a series of highly interactive Workshops on Distributed Supercomputing, sponsored jointly by the Sandia National Labs, the Oak Ridge National Lab, and the Swiss Institutes of Technology (ETH Zurich and EPF Lausanne).

CSCS hosted this year's SOS meeting in Engelberg on co-design approaches for exascale computing and related legal and organizational issues. Opening the meeting, CSCS director Thomas Schulthess welcomed important stakeholders in the HPC field, including representatives from major European and American HPC centres, HPC vendors, and universities. The goal of the meeting was to bring together many of the players in HPC in order to discuss how co-design of application codes for classes of simulation problems can open up the way to develop future efficient exascale systems.

Participants at the SOS 15 workshop in Engelberg.



The redesigned CSCS home page.

April

Redesigned CSCS Website

The CSCS website was redesigned to introduce a more up-to-date, dynamic layout. The goal of the redesign was to create a platform that better informs the public as well as the users about what is happening at CSCS, especially in terms of scientific and high performance computing. This update featured three new features: a new main website, a user portal and a forum. The new main website offers insight about the ongoing research performed on CSCS supercomputers and the latest developments at the centre.

The new user portal features a blog and twitter posts about CSCS-related updates; it also offers the possibility for users to check their account and allocation status. The visitors can now also see real-time updates on the status of CSCS' systems. The forum encourages community interaction among users - enabling them to share expertise and to quickly find answers to problems.

First Annual Call for Proposals

CSCS first call for proposals starts on April 1st. In this round, CSCS allocated approximately 140 million CPU hours to 55 new proposals, 3 revised proposals, and 17 proposal renewals.

May

Cray XMT Programming Workshop for Data-Intensive Applications

CSCS hosted a two-day workshop on data-intensive programming for the next-generation Cray XMT architecture. Since this system was the first of its kind, the goal of the course was to familiarise researchers with the new architecture and enable them to program it for maximum performance. Lectures covered the following topics: hardware architecture, programming environment, performance analysis, tuning, input/output programming, and potential application areas. Since the system installation date wasn't until July, the many hands-on sessions used an internal Cray system.

June

Booth at ISC11 in Hamburg

Members from the Swiss HPC Service Provider Community (www.hpc-ch.org) organized a booth at their first international event - the International Supercomputing Conference (ISC) in Hamburg. The goal of hpc-ch's presence was to promote Switzerland as a top international player in HPC. Scientific and technical staff from CSCS, ETH Zurich, EPF Lausanne, University of Zurich, and Università della Svizzera italiana were present at the booth to introduce the visitors to the HPC activities in Switzerland. The booth itself consisted of panels, posters and videos that covered Switzerland's high-performance computing and networking (HPCN) strategy, activities at CSCS, various Swiss research projects, and hpc-ch efforts. The visitors were welcomed at the booth with Swiss chocolate and coffee.

Great success for the Swiss booth at the ISC11 in Hamburg.

The new IBM Tape library TS3500 with its 5000 tapes.

July

Deployment of an Integrated Data Storage and Analysis Facility

CSCS deployed a new integrated data storage and analysis facility. This new technical solution (codenamed EUREKA) combines three key elements: a low latency, large capacity parallel file system based on GPFS with 2.7 petabytes of storage capacity; two large shared-memory systems: An SGI Altix UV1000 and a massively multithreaded data analysis system (Cray XMT). Scientific disciplines with very high data requirements like climatology and biology are the target for these systems - data analysis and data mining applications are particularly suitable. EUREKA allows users to explore more efficient data analysis techniques that often involve irregular data (based on strings, trees, graphs and networks) without the high degree of spatial and temporal locality found in traditional HPC codes.

August

CSCS Summer School on Parallel Computing

CSCS hosted and taught a three-day "summer school" on parallel computing, aimed at graduate students who are new to the world of high performance computing and who wish to learn the basic skills needed to develop, optimize, and maintain parallel scientific computing applications.

Over the three-day course, instructors from CSCS covered topics such as parallelism and computer architecture, distributed memory programming with MPI, shared memory programming with OpenMP, parallel input/output strategies to improve productivity and performance, and tools for debugging and performance analysis. Along with lectures, students participated in several "hands-on laboratories" on CSCS systems designed to reinforce concepts taught in class.

September

CSCS User Community Meets in Lucerne

The annual User Day in Lucerne was attended by approximately 60 of the user community. The day was a chance for users and CSCS staff to meet and exchange information about each others activities via talks, poster sessions and a common lunch. Highlights of the meeting were the three keynote lectures. Jeroen Tromp of Princeton University presented novel numerical methods implemented on supercomputers which allow realistic simulations of seismic events. Such simulations can be used to determine various properties inside of the Earth, and they can be thought of as working like tomography scans of the human body. Lucio Mayer, University of Zurich, reported on pioneering simulations of the genesis of the Milky Way galaxy. Rustam Khaliullin, also University of Zurich, presented novel simulations of the complex behaviour found in the phase diagrams of elemental carbon and sodium. At the end of the meeting, doctoral student Samuel Hertig (group of Prof. Viola Vogel, ETH Zurich) received the best poster award for his presentation on how tensile forces in tissues act on bacteria.

Maria Grazia Giuffreda presents Samuel Hertig with the best poster award during the User Day 2011 in Lucerne.

October

World's First Installation of a Cray XK6

The Swiss computational science community has shown significant interest in large-scale GPU computing; therefore, CSCS has greatly increased its GPU computing capability by acquiring a first-of-its-kind Cray XK6 system. Tödi, a two-cabinet Cray XK6, was successfully installed in October. The XK6 system is based on NVIDIA Fermi GPUs, AMD Interlagos multi-core processors, and a high-performance Gemini interconnect. Additionally, a unified CPU/GPU programming environment aims to ease the challenging task of programming heterogeneous systems.

Additional 27 Million CPU Hours Allocated to Research Projects

For the second allocation period on CSCS supercomputers, 26 new project proposals were submitted along with 5 revised proposals from the previous submission. In total an additional 27 million CPU hours were granted on our production systems.

November

SC11 Booth Represents Swiss Supercomputing Efforts

After the successful hpc-ch booth at ISC, a follow-on booth was organized at the Supercomputing Conference (SC11) in Seattle. Members from CSCS together with their colleagues from Swiss universities attended the booth to promote Switzerland's strong role in scientific computing. Additionally, hpc-ch interviewed many of the conference's top researchers on topics such as the role of Swiss HPC in the international context and novel HPC developments. All of hpc-ch's interviews are available to the public via YouTube.

Introduction of a Hierarchical Storage Management Solution

In late autumn, a new Hierarchical Storage Management (HSM) solution provided by IBM was installed at CSCS. This system is currently composed of 2.2 petabytes of online storage and a highly scalable, automated tape library (IBM TS3500) capable of storing 8.6 petabytes of uncompressed data. HSM automatically moves data that has not been accessed for a long time to tape, reducing the overall costs for storage. The tape library is also used as a disaster-recovery solution for the central file system.

Monte Rosa Upgrade

In November, the Cray XT5, Monte Rosa, was taken offline for approximately two weeks in order to upgrade the system to a Cray XE6 with 47 872 cores, roughly twice the number of cores of the previous system. Each of the compute nodes now consists of two 16-core AMD Opteron (Interlagos) chips running at 2.1 GHz, for a total of 32 cores per node accessing 32 GB of memory. The new Rosa system yields a peak performance of about 400 TFlops, placing it 34th on the international Top500 list of supercomputers. A key feature of the new machine is the new high-speed network, named Gemini, which is able to provide 5 GB/s of injection bandwidth in each direction per node. It is also capable of handling direct memory access references, which, if taken advantage of by the programmer, should dramatically increase the speed at which external messages are passed between processes.

December

HP2C Project Review

In order to perform an independent evaluation of the High Performance and High Productivity Computing (HP2C) initiative, representatives of the different projects, CSCS and USI presented their results and future plans to an international review panel. The panel consisted of distinguished parallel computing experts from Iowa State University, Jülich Supercomputing Centre, King Abdullah University of Science and Technology, and University of Zurich. Although the report from the review panel is confidential, excellent progress towards new science was reported by the HP2C teams.

HP2C review at USI in Lugano and the international review panel.

IV SCIENTIFIC REPORT

An Eventful Year

The year 2011 was an eventful one for CSCS, not least because of its preparations to relocate to the new home base in Lugano-Cornaredo. Beyond this CSCS witnessed a major expansion in term of computational infrastructure to meet various types of supercomputing needs: Matterhorn, a shared-memory and massively multi-threaded next-generation Cray XMT platform has been acquired with large-scale data analysis, data mining, and data structuring projects in mind, such as those used in pharmaceutical and genetic research. Tödi, a 176-node Cray XK6, is the world's first GPU/CPU hybrid system ever delivered by Cray; it strives for high scalability of computationally intensive data-parallel applications. Castor is a 16-node GPU system based on the IBM iDataPlex platform, acquired primarily for GPU code development, tuning, and performance optimization. Finally, the flagship supercomputer Monte Rosa went through a major upgrade which more than doubled its compute capacity to 47 872 cores and about 46 TB of memory.

GPUs promise enormous potential for high computational performance at reasonable cost, but they require that portions of compute-intensive code be re-written and adapted to the massively parallel data models of modern graphics cards. In order to motivate researchers to adapt their codes or develop new codes for GPU architectures and thus harvest their potential, CSCS has introduced an additional type of project proposal dedicated to development. A number of groups have taken advantage of this already, and GPU-codes are currently being developed within the HP2C initiative in a number of disciplines, including materials science, earth and environmental science, life science, and plasma physics. A number of small development projects have also been established for conventional (CPU) code and algorithm development, targeting massively parallel CPU-computing on Monte Rosa.

Allocated Resources per Scientific Field and Discipline

Notwithstanding the recent foray into new and promising types of compute architectures, Monte Rosa is the centrepiece of CSCS and will likely remain so for the foreseeable future. Its 47 872 cores are currently shared by 605 users working on 80 different production projects, of which 17 are renewals from 2010. Compute allocations are distributed fairly evenly over a number of disciplines including climate science (15%), chemical (14%), physical (13%), and biological (11%) sciences, geoscience (10%), fluid dynamics (12%) and astrophysics (9%). a total of 16% was further allocated to various projects in nanoscience and materials science. ETH Zurich takes the lead, contributing 20 out of 63 new projects started in 2011, followed by EPF Lausanne, the Universities of Zurich and Lugano (8), and the Universities of Basel (6), Geneva (3), Bern (1), as well as several research institutes, CERN (1), EMPA (2), PSI (3) and foreign universities with collaborations in Switzerland (3). The number of projects submitted in the areas of astrophysics, fluid dynamics, and geoscience has doubled with respect to 2010, certainly testifying to the inherently high degree of parallelism of many of the computational problems tackled in these disciplines, which make massively parallel architectures such as the Cray XE6 Monte Rosa ideal research platforms.

First Year of the Reviewing Process

Almost all Monte Rosa computational resources are distributed to researchers who have successfully applied for them with regular production project proposals. In summer 2010 CSCS established an improved review process that entails the solicitation of two independent expert reviews per proposal, two in-house technical reviews, and a final evaluation by a panel review committee.

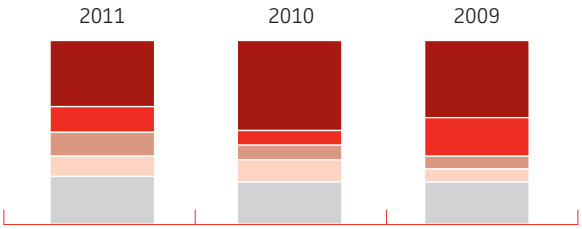
As the new review process has gone into its 2nd year, it seems timely to comment on some of the experiences made so far. Reviewers have been drawn almost exclusively from academic institutions abroad, with European and US institutions contributing 45% and 42% to the reviewer base in 2011, respectively. A smaller number of reviewers (13%) have been recruited from Australia, Japan, and Canada. A fairly large reviewer base is needed since it is CSCS policy to assign different proposals from the same scientist to different reviewers in order to minimize the possible risk of undue personal conflict. The overwhelming number of proposals (92% in 2011) received marks from both reviewers that differed by no more than one unit on the scale 5 "outstanding", 4 "excellent", 3 "good", 2 "fair", 1 "poor". Only in 8% of the cases the two reviewers disagreed substantially in their final verdict, requiring the opinion of a third reviewer.

The overall quality of the proposals was very encouraging: Almost half of the 74 new production project proposals submitted in 2011 were considered to be "outstanding" or "excellent", and thus received a strong recommendation for acceptance (46%). 39% were judged slightly less favourably with final verdicts between "excellent" and "good". Only 11% of

Usage Statistics

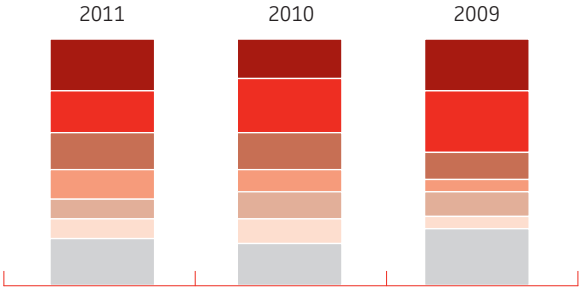
Usage by Institution (%)

Institution	2011	2010	2009
ETH Zurich	36	49	42
University of Zurich	14	8	21
University of Basel	13	8	7
EPF Lausanne	11	12	7
Others	26	23	23
Total Usage	**100**	**100**	**100**



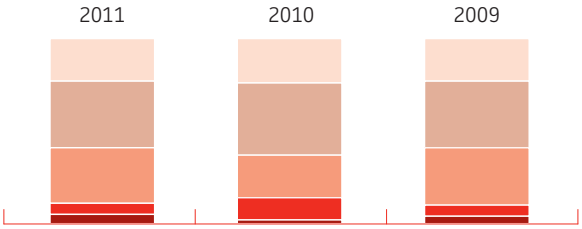
Usage by Research Field (%)

Research Field	2011	2010	2009
Chemistry	21	16	21
Physics	17	22	25
Earth & Env. Science	15	15	11
Nanoscience	12	9	5
Biosciences	8	11	10
Fluid Dynamics	8	10	5
Others	19	17	23
Total Usage	**100**	**100**	**100**



Usage by Number of Cores per Job (%)

Cores	2011	2010	2009
1 - 256	23	24	23
257 - 1 024	36	39	36
1 025 - 4 096	30	23	31
4 097 - 16 384	6	12	6
> 16 384	5	2	4
Total Usage	**100**	**100**	**100**



the proposals were rejected because of unfavourable reviews and another 4% were reassigned to preparatory project status because they were not considered mature enough for large-scale computation. Only 6% of the accepted proposals were granted for a shorter period of time (typically half a year), as the panel review committee recognized their overall scientific value but still criticized certain aspects and demanded improvement and clarification in re-submissions.

The reviews bear testimony to the high quality of research carried out on CSCS computational resources. Maintaining these standards is an important goal considering the significant expenditure in hardware, infrastructure, and personnel. The 2012 move to the new building in Lugano prepares CSCS and the Swiss computational science community for the challenges of the future. The new site will provide sufficient reserves in both space and electrical power to accommodate future generations of supercomputers.

Abstracts of the 10 Largest Projects

Noise emission and vortex breakdown in round subsonic jets

Leonhard Kleiser, ETH Zurich (Fluid Dynamics, 8.4 Mio CPU h) - In this three-year project, three specific aspects of compressible jet flows will be studied: the generation of jet noise for single and for coaxial configurations, and the vortex breakdown in swirling jets. These flow problems find their application, for instance, in aircraft jet noise reduction and mixing in combustion chambers. The project comprises several highly resolved, high fidelity simulations of compressible jet flows which are mostly turbulent. Accuracy and efficiency requirements for such investigations are far above what is offered by widespread commercial CFD codes. Therefore, in our research code PARACONCYL we apply high-order numerical methods (e.g. compact finite-differences and spectral schemes) and use parallel algorithms which are able to run very efficiently on massively parallel supercomputing facilities.

Regional climate modelling on European to Alpine scales

Christoph Schär, ETH Zurich (Climate, 8.4 Mio CPU h) - In recent years, a horizontal resolution of 20 to 50 km has emerged as a standard for long-term regional climate change experiments. This scale is sufficiently detailed to represent major regional forcing mechanisms (e.g., those triggered by regional topography and coastlines) and, at the same time, allows long-term simulations. Besides performing hydrostatic-scale regional climate simulations, this project also intends to make use of high-resolution cloud-resolving (about 2 km grid spacing) simulations integrated over the large Alpine region to increase the knowledge about small-scale processes and physical feedback mechanisms that shape the European and Alpine climate.

Numerical lattice gauge theory with a symmetry constrained Monte Carlo II

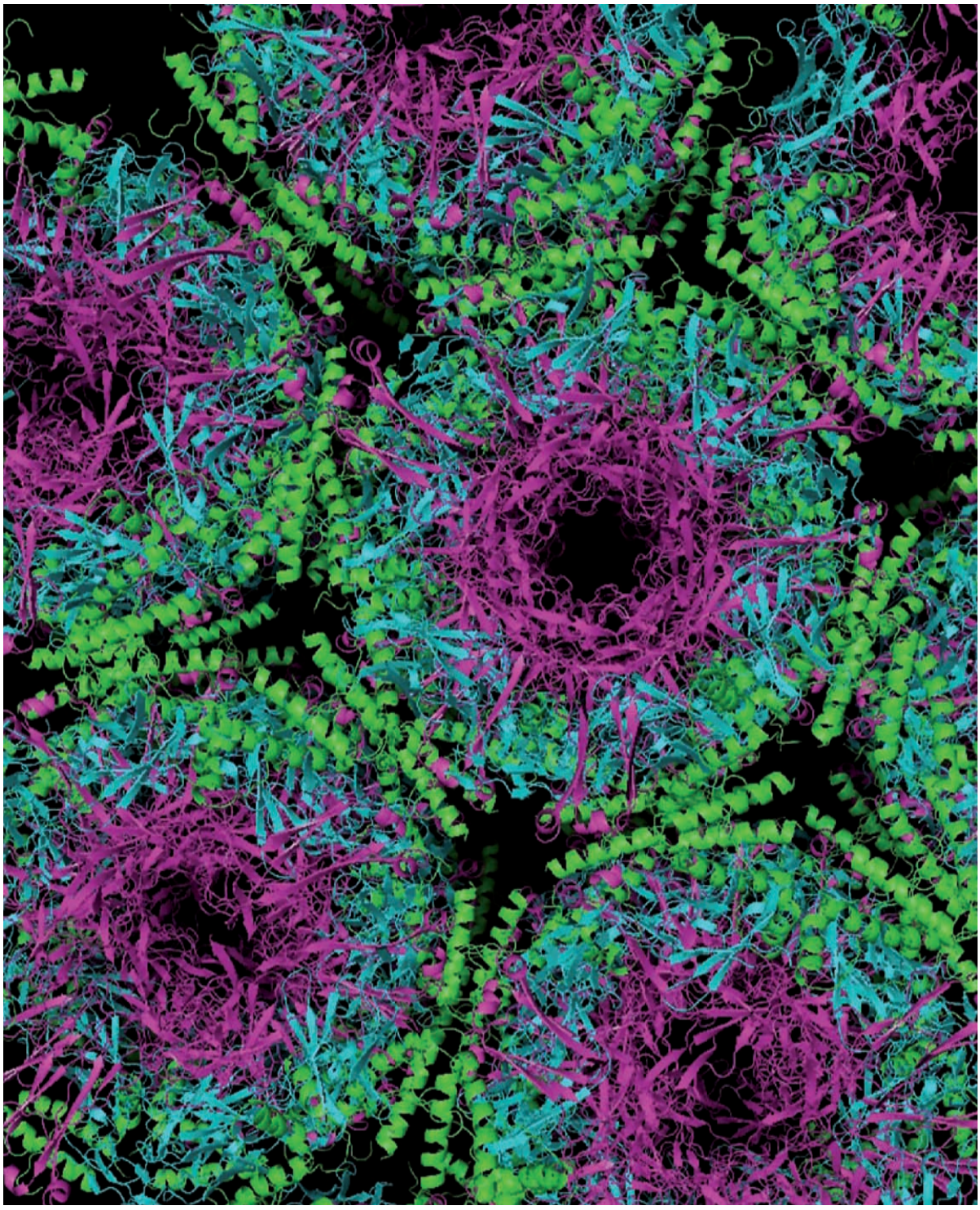
Leonardo Giusti, CERN (Lattice Gauge Theory, 6.0 Mio CPU h) - Recent progress in lattice field theory has made it possible to define and compute by Monte Carlo simulations the relative contribution to the partition function due to states carrying a given set of quantum numbers associated with the exact symmetries of a theory. This opens the possibility to compute fundamental dynamical properties of Yang–Mills theories that are hardly or not accessible to other methods. The long term goals of this project are: (a) to provide a theoretically solid determination of the mass and multiplicity of the lightest glueballs in the various symmetry sectors of the SU(3) gauge theory, and (b) to compute its thermal properties, such as entropy and pressure (full and partial pressure from the different sectors), at (high) temperatures that have not been accessible so far.

Boron nitride nanomesh for guided self-assembly of molecular arrays in solution

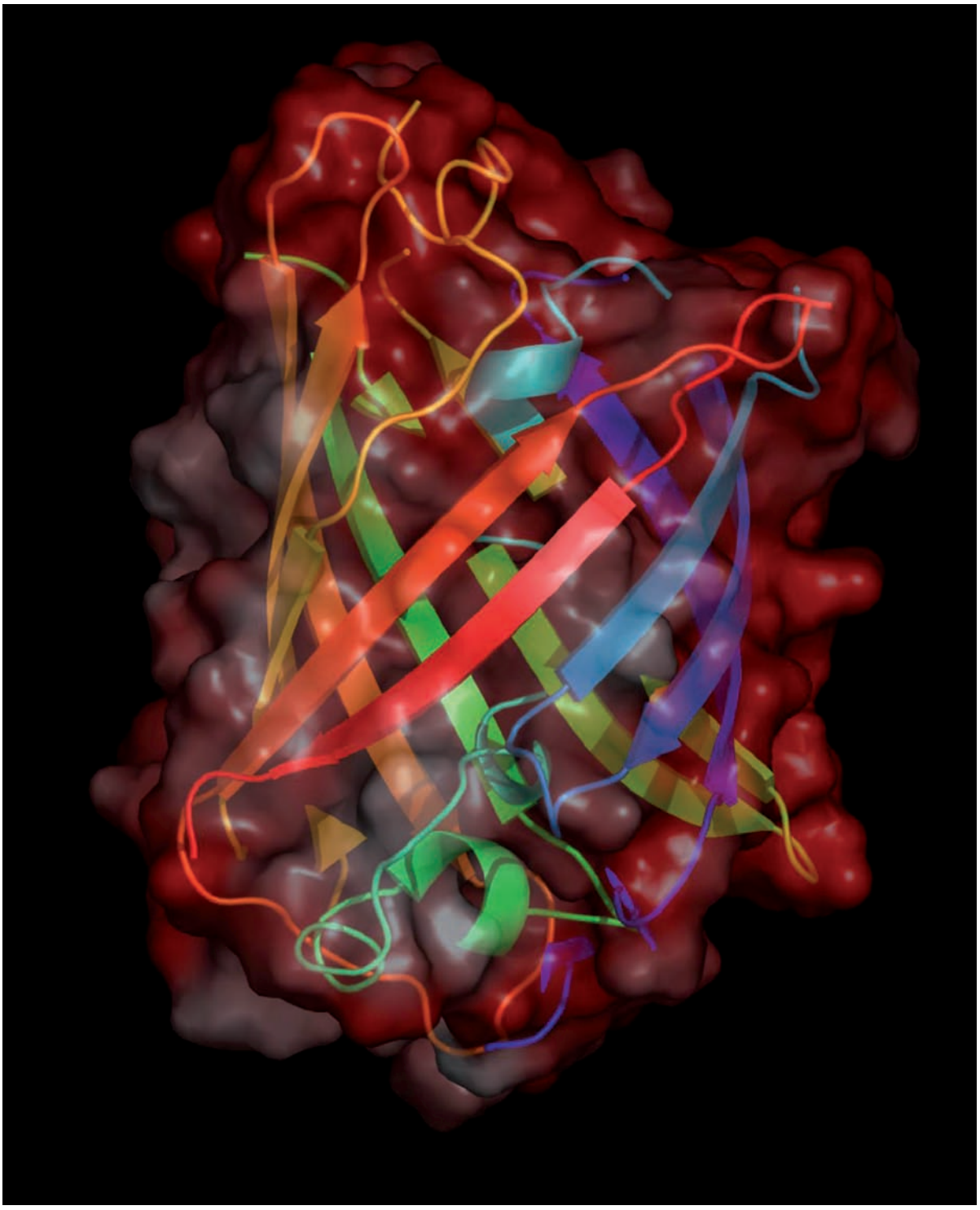
Jürg Hutter, University of Zurich (Chemistry, 6 Mio CPU h) - The template, h-BN/Rh(111) nanomesh, is a superstructure based on 12x12 Rh unit cells on top of which 13x13 BN unit cells coincide. It is a corrugated single layer of sp2 hybridized hexagonal boron nitride with a super-lattice constant of 3.2 nm. If the nitrogen atom sits close to an on top position of a substrate Rh atom, h-BN is tightly bound and forms the so-called “holes” or “pores” with a diameter of about 2 nm. The loosely bound regions form a connected network and are called “wires”. This peculiar morphology implies a functionality which can be used for trapping single molecules. The trapping mechanism was found to be related to the presence of large lateral electric fields in the surface, where the rims of the holes act like dipole rings, that lower the electrostatic potential in the holes. In order to assist experiments and to add to the basic understanding of the nanomesh superstructure we propose to perform density functional electronic structure calculations.

Optimization of shape and motion patterns of single and multiple aquatic swimmers

Petros Koumoutsakos, ETH Zurich (Fluid Dynamics, 6.0 Mio CPU h) - The understanding and quantification of biolocomotion in fluids can provide us with inspiration for engineering applications, ranging from robotics to energy harnessing devices. Simulations can greatly assist in characterizing aquatic propulsion, and help unveil how fish swim individually and in schools. The simulation of swimmers presents significant challenges due to the unsteady, complex geometries involved and the coupling of the flow with the body deformations. We follow a reverse engineering approach to identify swimming patterns for individuals and school of fish. We specify objectives such as efficiency, speed, acceleration and swimming configurations, to identify the corresponding optimal body motions. We implement a remeshed Vortex Method to study fluid structure interactions, and a Covariance Matrix Adaptation Evolutionary Strategy tailored to optimize nonlinear, multimodal problems with expensive cost functions, such as those encountered in the present problem. These algorithms have been implemented for massively parallel and heterogeneous computer architectures and have demonstrated excellent scaling abilities, allowing for large problems, necessary for the study of multiple swimmers.



Biomolecular simulation: Study of how the structure of prion proteins degenerates in the mad cow disease.



Biomolecular simulation: Understanding the behaviour of a green fluorescent protein used in several molecular dynamics studies.

Applications of novel AIMD methods

Joost VandeVondele, University of Zurich (Chemistry, 5.0 Mio CPU h) - In ten years of active development, the group has contributed significantly to make the CP2K program unique in its capabilities. The program has become a leading tool to perform large scale density functional theory simulations. Among the recent breakthroughs are the implementation of massively parallel Hartree-Fock exchange for the condensed phase, long time scale molecular dynamics, Ehrenfest electronic dynamics, and linear scaling SCF. With this proposal, we will establish these methods with pioneering applications to challenging systems, and at the same time obtain the necessary feedback to further improve the robustness and scalability of CP2K. With four sub-projects, we will highlight each of these methods convincingly, and increase the range of AIMD in the respective fields. The first is related to the electronic dynamics and structure in dye sensitized solar cells (DSSC), and aims at understanding the level structure of the dye binding to an oxide in the presence of an electrolyte (solvent) for various geometries and protonation states. The second focuses on vibrational spectroscopy, demonstrating the quality of hybrid functionals for solvated anions. The third aims at understanding chemical reaction dynamics directly from AIMD.

ORB5 – Turbulance

Laurent Villard, EPF Lausanne (Plasma Physics and Fusion Energy, 5.0 Mio CPU h) - This project aims at first-principles based direct numerical simulations of turbulence in magnetically confined plasmas. More specifically, the effects of finite system size and of finite collisionality on the development and saturation of turbulence are sought over long timescales relevant for transport studies. The numerical tool used is the ORB5 code, a well-tested, highly scalable application code using numerical particles developed by the CRPP with major contributions from the Max-Planck Institute for Plasma Physics (IPP) in Garching, Germany.

Low viscosity rotating flows and magnetic field generation in Earth's core

Andrew Jackson, ETH Zurich (Earth and Environmental Science, 4.8 Mio CPU h) – This project describes a program of computations aimed at elucidating the physics of rapidly rotating flows with low viscosity in a spherical shell geometry, including the processes of convection and magnetic field generation in Earth's core. Spectral methods are used to evolve the underlying fluid dynamical (Navier-Stokes, heat, electrodynamic) equations in time. The focus is to investigate the physics that occur when rotation and magnetic effects dominate the force balance and viscosity plays only a minor role.

Coupled atmosphere-ocean carbon cycle simulation from 850 to 2100 A.D. A Swiss PMIP III contribution

Christoph C. Raible, University of Bern (Climate, 4.7 Mio CPU h) - The overall aim of this project is to deepen our understanding of the climate-biogeochemical system and its variability during the last millennium to improve climate projections. The plan is to carry out a continuous simulation over the last 1150 years, followed by climate projections for the next century with a state-of-the-art Earth System Model. The Community Earth System Model of the National Center for Atmospheric Research (USA) is applied in high resolution (1°×1°), with an interactive carbon cycle and driven by natural (solar, volcanic) and anthropogenic forcings. The model output will be exploited by the applicants and their teams to address a broad array of research questions related to climate-forcing response relationships, carbon cycles, extreme events, and adaption to regional climate change. Particular emphasis will be on the dynamics and decadal-to-century scale variability of extreme events, such as storms, heavy precipitation, and droughts, with large-socio-economic impacts. We expect important lessons to be learned for adaptation to regional climate change.

Uncovering the nature of chemical reactivity of gold and platinum nano-sized particles

Gianluca Santarossa, ETH Zurich (Nanoscience, 4.5 Mio CPU h) - The project focuses on the theoretical investigation of the physical properties and reactivity of metal nanoparticle surfaces. The dynamic and electronic properties relevant for the chemical reactivity of metallic (gold and platinum) nanoparticles will be elucidated by means of ab initio molecular dynamics and metadynamics simulations. The metal particles will be simulated as small clusters, surrounded by reactive molecules. Relevant examples in nanocatalysis will be investigated: the hydrogenation reaction of a model aldehyde on Pt nanoparticles in the absence and presence of tertiary amines, and the oxidation of carbon monoxide on Au nanoparticles. The combination of ab initio MD and of metadynamics simulations represents an innovative method to study reactivity at the surface of metal nanoparticles and is expected to add considerable complementary information to the present understanding of the mechanism of heterogeneous hydrogenation and oxidation reactions.

List of Projects by Institution

CERN

Numerical lattice gauge theory with a symmetry constrained Monte Carlo II, Leonardo Giusti (Lattice Gauge Theory, 6.0 Mio CPU h)

EMPA

Regional scale impacts of changing anthropogenic emissions on aerosols and climate, Dominik Brunner (Climate, 0.8 Mio CPU h)

Active molecules at substrates: bottom-up design of graphene-like nanostructures and novel catalysts, Daniele Passerone (Nanoscience, 2.6 Mio CPU h)

EPF Lausanne

Large-scale simulations of carbon nanotubes for NANOTERA device applications, Wanda Andreoni (Nanoscience, 4.4 Mio CPU h)

Oxidation reactions by triplet state transients in aquatic environments, Samuel Arey (Chemistry, 2.0 Mio CPU h)

Energetic particle physics in magnetically confined configurations, Anthony W. Cooper (Plasma Physics and Fusion Energy, 1.1 Mio CPU h)

Mechanistic studies of metal-dependent DNA-processing enzymes of pharmaceutical relevance, Matteo Dal Peraro (Biological Sciences, 1.1 Mio CPU h)

Molecular dynamics simulations of DNA minicircles, John Maddocks (Multiscale Mathematical Modelling, 1.9 Mio CPU h)

Study of land-atmosphere interaction over complex terrain by large eddy simulation, Marc Parlange (Geoscience, 2.4 Mio CPU h)

Atomic-scale modelling at semiconductor-oxide interfaces, Alfredo Pasquarello (Condensed Matter Physics, 2.5 Mio CPU h)

Application of large eddy simulation to atmospheric boundary layer flows, Fernando Porte-Agel (Geoscience, 1.0 Mio CPU h)

Cardiovascular simulations: sensitivity to modelling, discretization parameters, and patient specific geometries, Alfio Quarteroni (Fluid Dynamics, 0.4 Mio CPU h)

Cell cultures in orbitally shaken reactors, Alfio Quarteroni (Fluid Dynamics, 0.2 Mio CPU h)

Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Studies of biological systems, Ursula Röthlisberger (Chemistry, 1.8 Mio CPU h)

Large eddy simulation of topographically forced flow, Craig Smith (Fluid Dynamics, 1.5 Mio CPU h)

ORB5-Turbulence, Laurent Villard (Plasma Physics and Fusion Energy, 5.0 Mio CPU h)

ETH Zurich

Large scale micro-finite element analysis for bone structure analysis and remodelling, Peter Arbenz (Materials Science, 0.2 Mio CPU h)

Gradient-based iterative waveform inversion of seismic ambient noise, Piero Basini (Geoscience, 2.0 Mio CPU h)

Chemistry-climate interactions since the pre-industrial time, Isabelle Bey (Climate, 0.6 Mio CPU h)

Development of dynamic rupture models to study the physics of earthquakes and near-source ground motion, Luis Dalguer (Geoscience, 2.5 Mio CPU h)

Computational science and engineering in nanoelectronics, Wolfgang Fichtner (Nanoscience, 2.0 Mio CPU h)

Direct numerical simulations of heat transfer and catalytic combustion in three-dimensional channels, Christos Frouzakis (Combustion, 1.5 Mio CPU h)

Direct numerical simulation of flow, heat transfer, and auto-ignition in engine-like geometries, Christos Frouzakis (Combustion, 2.0 Mio CPU h)

Atomistic study on thermal transport in thermoelectric nanowires: Application to energy conversion, Ming Hu (Nanoscience, 0.6 Mio CPU h)

Low viscosity rotating flows and magnetic field generation in Earth's core, Andrew Jackson (Geoscience, 4.8 Mio CPU h)

Numerical modelling of lithospheric deformation on geological timescales, Boris Kaus (Geoscience, 1.5 Mio CPU h)

Noise emission and vortex breakdown in round subsonic jets, Leonhard Kleiser (Fluid Dynamics, 8.4 Mio CPU h)

Direct and large eddy simulation of particle transport processes in estuarine and oceanic environments, Leonhard Kleiser (Fluid Dynamics, 1.0 Mio CPU h)

Nanoparticle-lipid bilayer interactions, Petros Koumoutsakos (Nanoscience, 2.0 Mio CPU h)

Vortex collision at high reynolds numbers using remeshed vortex methods, Petros Koumoutsakos (Fluid Dynamics, 2.0 Mio CPU h)

Optimization of shape and motion patterns of single and multiple aquatic swimmers, Petros Koumoutsakos (Fluid Dynamics, 6.0 Mio CPU h)

Role of anthropogenic versus natural forcing on decadal scales in global climate models, Ulrike Lohmann (Climate, 4.4 Mio CPU h)

Seismic-wave propagation and inversion at the global scale, Tarje Nissen-Meyer (Geoscience, 0.5 Mio CPU h)

Past and future solar influence on climate (FUPSOL), Thomas Peter (Climate, 0.6 Mio CPU h)

Source, path and site effects during large earthquakes analysed from forward and adjoint simulations, Daniel Roten (Geoscience, 0.1 Mio CPU h)

Uncovering the nature of chemical reactivity of gold and platinum nano-sized particles, Gianluca Santarossa (Nanoscience, 4.5 Mio CPU h)

Regional climate modelling on European and Alpine scale, Christoph Schär (Climate, 8.4 Mio CPU h)

Land-climate interactions: modelling and analysis, Sonia Seneviratne (Climate, 0.7 Mio CPU h)

Theoretical design of novel multifunctional materials, Nicola Spaldin (Materials Science, 0.8 Mio CPU h)

3D spherical simulations of mantle convection and plate tectonics: Influence of a free surface and buoyant continents, Paul Tackley (Geoscience, 1.5 Mio CPU h)

Simulating fractional quantum hall devices, Matthias Troyer (Condensed Matter Physics, 2.0 Mio CPU h)

Image-based analyses of bone competence and bone remodelling for optimizing fracture prevention and improving implant longevity, Harry van Lenthe (Biomedical Engineering, 1.0 Mio CPU h)

Simulating integrin junctions under tension: From the extracellular matrix to the cytoskeleton, Viola Vogel (Biological Sciences, 4.0 Mio CPU h)

Paul Scherrer Institute

Large eddy simulation of particle dynamics inside a differentially heated cavity, Abdel Dehbi (Fluid Dynamics, 0.6 Mio CPU h)

Simulation of actinide materials, Matthias Krack (Materials Science, 1.3 Mio CPU h)

Nano-optics for advanced photocathodes, Benedikt Oswald (Accelerator Physics, 0.5 Mio CPU h)

The atomistic modelling of size effects in nanocrystalline metals, Helena van Swygenhoven (Materials Science, 0.5 Mio CPU h)

SUPSI

Molecular dynamics study of the wetting properties of graphitic surfaces by complex fluids, Giulio Scocchi (Materials Science, 0.3 Mio CPU h)

Trinity College Dublin

Computational approaches toward energy conversion, Clotilde Cucinotta (Chemistry, 1.0 Mio CPU h)

University of Geneva

Photophysics and photochemistry of transition metal compounds: Theoretical approaches, Andreas Hauser (Chemistry, 1.0 Mio CPU h)

Accurate spin-state energetics of transition metal complexes, Max Lawson Daku (Chemistry, 2.0 Mio CPU h)

Molecular modelling of functional anion-π complexes, Jiri Mareda (Chemistry, 0.4 Mio CPU h)

University of Basel

Structure, dynamics, and function of membrane transport proteins, Simon Bernèche (Biological Sciences, 2.4 Mio CPU h)

The aftermath of neutron star mergers and the neutrino driven wind, Ruben Cabezon (Astrophysics, 0.8 Mio CPU h)

Structure prediction of clusters, solids and surfaces, Stefan Goedecker (Nanoscience, 2.0 Mio CPU h)

Sensitivity of multi-dimensional supernova models with respect to nuclear input physics, Matthias Liebendörfer (Astrophysics, 1.8 Mio CPU h)

The role of dimerization in protein activation and signalling, Markus Meuwly (Chemistry, 0.2 Mio CPU h)

Maximum likelihood-based classification reconstruction in three dimensional cryo-electron microscopy, Henning Stahlberg (Biological Sciences, 2.5 Mio CPU h)

3D models for supernovae dynamics and stellar jet formation, Nicolas Vasset (Astrophysics, 1.0 Mio CPU h)

University of Bern

Chemical climate change during the past 400 years (ccc400), Stefan Brönnimann (Climate, 1.0 Mio CPU h)

CARBOFEED (Modelling CARBOn Cycle Climate FEEDbacks), Fortunat Joos (Climate, 0.4 Mio CPU h)

Achievements of MONALISA III, Christoph Raible (Climate, 1.2 Mio CPU h)

Coupled atmosphere-ocean carbon cycle simulation from 850 to 2100 A.D. - A Swiss PMIP III contribution, Christoph Raible (Climate, 4.7 Mio CPU h)

University of Cambridge

Full CI quantum Monte Carlo studies of molecular dissociation energies, Ali Alavi (Chemistry, 2.0 Mio CPU h)

University of Zurich

Numerical simulation of nonoptimal dynamic equilibrium models, Zhigang Feng (Economics, 0.1 Mio CPU h)

Boron nitride nanomesh for guided self-assembly of molecular arrays in solution, Jürg Hutter (Chemistry, 6.0 Mio CPU h)

CP2K program development, Jürg Hutter (Chemistry, 0.6 Mio CPU h)

Connecting mergers of supermassive black holes and their formation in hierarchical galaxy assembly - II: Cosmological simulations with realistic host galaxies, Lucio Mayer (Astrophysics, 2.2 Mio CPU h)

BATS: The first simulation of all luminous structures in the universe, Darren Reed (Astrophysics, 2.5 Mio CPU h)

The Hecto Lactea simulation: 100 high-resolution Milky Way analog halos, Darren Reed (Astrophysics, 2.0 Mio CPU h)

Galaxy formation and fault tolerant computing, Romain Teyssier (Astrophysics, 4.2 Mio CPU h)

Applications of novel AIMD methods, Joost VandeVondele (Chemistry, 5.0 Mio CPU h)

Predicting accurate energies beyond DFT: From molecular nanojunctions to OLEDs applications, Laura Zoppi (Materials Science, 0.7 Mio CPU h)

Università della Svizzera italiana

Metadynamics study of the conformational behaviour of NK1 fragment of the hepatocyte growth factor, Alessandro Barducci (Biological Sciences, 0.5 Mio CPU h)

Neural Network interatomic potentials for phase change materials, Sebastiano Caravati (Materials Science, 2.4 Mio CPU h)

Elucidating mechanisms of DNA repair using well-tempered metadynamics, Ali Hassanali (Biological Sciences, 1.0 Mio CPU h)

Simulation of the docking/undocking process of a series of inhibitors in the two isoforms of COX enzyme, Vittorio Limongelli (Biological Sciences, 0.6 Mio CPU h)

Sensitivity analysis of electrocardiograms simulated with a realistic large-scale heart model, Rolf Krause (Numerical Simulations in Medicine, 0.8 Mio CPU h)

Conformational study of p38 alpha MAP kinase in free and ligand bound forms, Michele Parrinello (Biological Sciences, 1.0 Mio CPU h)

First principles study of the structural phase transition and the high temperature phase of lithium imide, Michele Parrinello (Materials Science, 1.0 Mio CPU h)

Mechanical sensing of red blood cells by the human spleen: Parallel simulations, Igor Pivkin (Computational Biomechanics, 0.9 Mio CPU h)

Three dimensional reconstruction of the M83 spiral galaxy obtained using a technique developed in a collaboration between CSCS, MPI Munich and ATNF Sydney, and visually rendered using the Splotch software.

CP2K – a computer program for the future

On the research work of Jürg Hutter and Joost VandeVondele at the Institute of Physical Chemistry, University of Zurich.

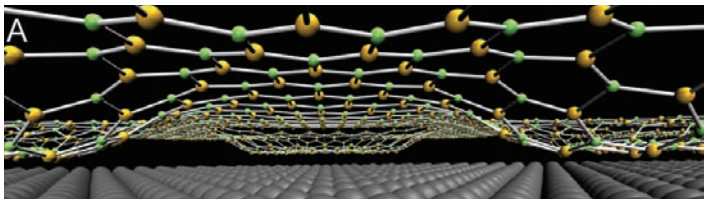
Finding and accessing alternative energy sources is the goal of many scientists worldwide. Simulations on high-performance computers such as the CSCS supercomputer Monte Rosa have an important role to play. One of the essential programs for this type of simulation is CP2K.

The growing demand for energy from the world's population represents a continuing challenge for researchers and engineers and alternative energy sources are being called for more than ever. Finding them, storing their energy and using it efficiently will require technical advances and scientific breakthroughs.

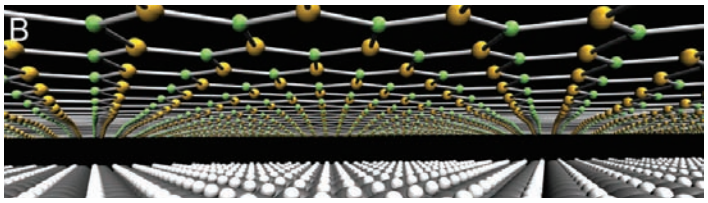
Using computers to explore new energy sources

An important contribution to exploring alternative energy sources – such as innovative fuels or solar cells – can be made by supercomputers such as those made available to Swiss scientists at CSCS. With the help of the Monte Rosa supercomputer, scientists can simulate new materials and their molecular properties. While quantum mechanics can deliver the theory about the chemical, electrical and physical properties of a material, only digital simulations can show the potential benefits of new chemical compounds. By means of these simulations, researchers can investigate how physical conditions such as temperature and pressure can break down chemical compounds or create new ones.

One of the most important codes for this type of simulation is CP2K (Car-Parrinello 2000 project), which is developed in an international collaboration. The molecular scientist Jürg Hutter began developing CP2K about ten years ago in collaboration with the research group led by Michele Parrinello, Professor of Computational Science at ETH Zurich and the Università della Svizzera italiana.



Structured two-dimensional surface. These so-called nanomeshes can be used as a type of template for developing new materials. The picture shows the structure of boron nitride on rhodium.



Boron nitride on rhodium with intercalated hydrogen.

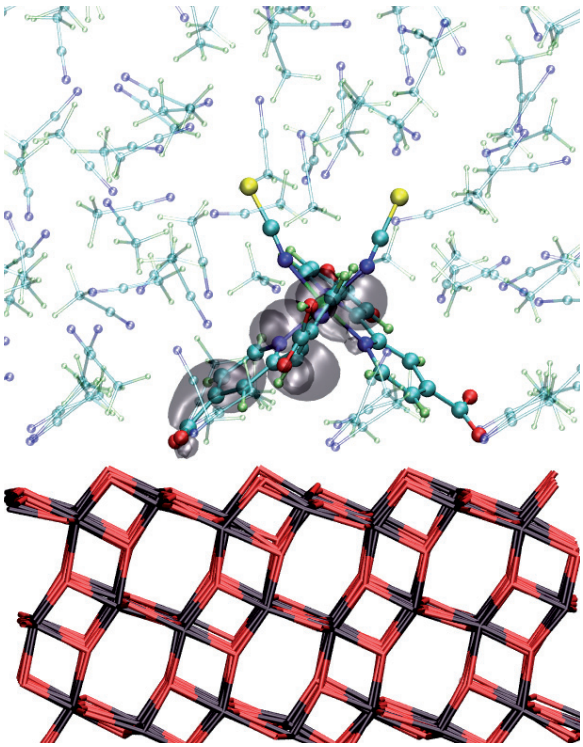
Fifteen years ago, Michele Parrinello and Roberto Car developed the *Car-Parrinello method*. The Car-Parrinello Molecular Dynamics method and its implementation in the CPMD program meant a breakthrough in the digital simulation of molecular processes: For the first time it was possible to calculate both the dynamics of a molecule and its electronic structure simultaneously and relatively quickly on a computer. However, ten years ago Hutter and Parrinello realized that new algorithms would be required in order to be able to compute even bigger systems. Thus CP2K was born.

Material transitions with a lot going for them

CP2K can be used to simulate large and complex chemical systems, such as the interfaces between materials or between different phases. With simulations based on CP2K it is possible to investigate what happens when different materials come together in specific conditions, how their structure changes and how this affects the dynamics of the molecules at their surface.

Looking for new materials, simulations with CP2K can often complement experimental work . As a molecular scientist, Hutter researches interfaces such as a single layer of boron nitride on the metal rhodium. These so-called "nanomeshes" create structured two-dimensional surfaces. The idea is that such a nanomesh can be a template to influence, through its chemical structure or morphology, the shape of a new material that researchers want to create.

Hutter is currently working with scientists from the Swiss Federal Institute for Materials Testing and Research (EMPA) on the catalysed conversion of CO_2 in methanol. They are investigating how CO_2 reacts with nickel on cerium dioxide, one of the main catalysts in the conversion of CO_2 in fuel.



An atomistic model of the active interface in a prototype Grätzel cell shows the dye, the solvent and the oxide. The grey contour plot represents the electron prior to injection into the oxide.

Joost VandeVondele, former senior research assistant in Hutter's team and now professor at the ETH Zurich, is using CP2K to study special solar cells known as Grätzel cells. Grätzel cells function on a similar principle to photosynthesis and are a typical example of an interface: a solid body on one side and a solvent on the other, with a dye in between. How this electrochemical dye-sensitised solar cell – which is currently achieving levels of efficiency of 12.3% in the laboratory – works in detail is not entirely understood. In order to be able to build cells that are more efficient, the process of how the dyes and solvents interact with the surface and with light, and thus generate electricity, needs to be clarified. VandeVondele is studying this using computer simulation.

Multiple applications

The CP2K program is flexible and can be used not only in materials research but in many different fields of physics, chemistry, biology and pharmacy. The program now consists of nearly a million lines of code and is continuously being developed by international teams. It uses many different algorithms and complex numerical structures. It is hard to target these to current computer architectures, so in the last two years Hutter and his team have been focusing on optimizing the program for use on new computer architectures that are based on multicore processors, where there are several processors on one chip, or graphic processors (GPUs).

When the program is fully implemented on the new architectures, it will enable more extensive simulations to be carried out. It will use massive parallel computer resources more efficiently and work better on the ever-increasing number of processors. CP2K is an important simulation tool, which enables scientists to use the latest generation of computers at CSCS to make an important contribution to current research, and not only in the energy sector.

CH2011 – climate development in Switzerland

It is getting warmer in Switzerland and dryer in summer, and climate change will also affect the frequency and character of extreme events. The current climate scenarios in Switzerland were presented in September 2011 with the publication of the "CH2011" report. The scenarios are based on a comprehensive assessment conducted by Swiss scientists. ETH climate scientist Christoph Schär provides information on the results of the study.

Professor Christoph Schär, ETH Zurich.

Mr. Schär, as Chairman of the C2SM Competence Centre (Center for Climate Systems Modeling) you were significantly involved in creating the report "Swiss Climate Change Scenarios" (CH2011). Did this cooperation make the CH2011 report possible?

C2SM certainly played a decisive role and brought together researchers from ETH Zurich and MeteoSwiss. However, one should also mention other institutions including the National Centre of Competence in Climate Research (NCCR Climate).

C2SM's key task is to develop and use climate models. Climate models are becoming ever more complex. Developing them further, maintaining them and using them in an optimal way on supercomputers is beyond the resources of a single research group. That's why there is a need for cooperations like C2SM that bring together the entire know-how from all the relevant areas.

What was the aim of the study?

Our aim was to analyse the latest climate simulations and present the results in a suitable form. In this respect, we had two target groups in mind. Firstly, the wide-ranging scientific community that deals with the consequences of climate change and is very interested in scenario data. For example, this involves effects on agriculture, hydrology, hydroelectric power, permafrost or glaciers. Secondly, administrations, politicians and economies can use the report as a basis for planning.

As a result of CH2011, do you know more about the future of Switzerland's climate than you did when a previous report was published four years ago?

In particular we were able to estimate and quantify the uncertainties more accurately by using new climate simulations and new statistical methods. Better models with improved modelling components and finer computational resolution were available to us for this report compared to the OcCC Report published in 2007. We also used more than twenty new climate simulations for the scenarios. The input into the 2007 report consisted of models with a resolution of 50 to 100 kilometres, whereas in CH2011 we took into account data from models with a grid spacing of only 25 kilometres. In the current report, we also distinguish between different emission scenarios, including an intervention scenario which specifies a halving of global greenhouse gas emissions. This scenario is new and was not considered in the 2007 IPCC report. We can use it to visualise the effects of a global climate policy on Switzerland's climate. We had been unable to make any specific statements about this until now.

The Report says it will become warmer and dryer and we must expect more extreme events and heat waves. Exactly which scenarios do the models depict?

In the report, we assessed the resulting changes in relation to extreme events mainly based on the available literature. The clearest signal emerges with regard to heat waves. Within Switzerland, the effects of heat waves and droughts are greatest in Ticino, but not as strong as expected for parts of the Mediterranean region and the Po Valley. The picture there will change: the summery "dolce vita" will probably need to move out of the street cafés and into air-conditioned rooms.

The scenarios also show that there will be significant changes in precipitation as well, especially an increase in rain at the expense of snowfall. That will affect the runoff of many rivers and streams. However, this change in precipitation will not take place continuously. Natural variability is a decisive factor until approximately the middle of the century. That is, natural fluctuations may hide or intensify man-made signals.

In the second half of the century, however, the climate change will become clearly noticeable in even more climate variables. Even if by 2050 we succeed in halving global greenhouse gas emissions compared to 2000, the Swiss climate will by then become warmer by 1.2 to 1.8 degrees Celsius compared to the period between 1980 and 2009.

Are there serious differences between the OcCC Report in 2007 and the new CH2011 Report?
The current research results contain three major advances. Firstly, it was possible to estimate the uncertainties more objectively. Secondly, we can now submit detailed scenario data, for example artificial climate series for the present and the future which are available for the study of climate impacts. Thirdly, we have now taken different greenhouse gas scenarios into account. In addition to a scenario that assumes regionally-oriented industrial development and a scenario based on the balanced use of fossil and non-fossil fuels, we took what is known as an intervention scenario into account.

In the new report, you included models with twice the resolution. Why are models with increasingly resolution important?
In summer, for example, a large part of the precipitation is of a thundery nature. A thunderstorm has a horizontal scale of a few kilometres and thus falls through the computational mesh of the current models, which use a grid spacing of 25 km. As the next step, in a globally coordinated project, we will carry out calculations using 10 km and the associated simulations will start soon. We are also already working on the next-but-one step and then we want to model the climate at a resolution of two kilometres. Only then can we take the physical processes in thunderclouds explicitly into account, thus eliminating key uncertainties in our models.

Higher resolution means more computing time. How has the demand for computing time developed in the past four years?
Doubling the resolution results in an eight-fold increase in computing time. That's why high-resolution simulations are very expensive and laborious. However, an almost even greater problem than the increasing computing time is the amount of data generated during the process. Our own climate simulation took 20 weeks on CSCS computer, at that time the fastest in Switzerland, and produced 9.5 terabytes of data. We need to keep this data available for at least five years because it is used and needed by various different groups. Data storage has become an enormous cost driver and is a big burden on these projects' budgets.

C2SM has a project at the Swiss Platform for High Performance and High Productivity Computing (HP2C). The aim is to optimise the existing computer codes for future computer architectures. That means, among other things, adapting the codes and algorithms. Did the CH2011 models already include the initial results?
No, because we had already started four years ago with the model runs for the scenarios that are now available. However, with the new supercomputers, for example with graphical processor units (GPU), we are confronted with fundamental changes. We need to make our models run on these new architectures. That's why we are extremely pleased about the collaboration with the CSCS in the HP2C project. Thanks to this collaboration, we are among the first climate groups internationally to adapt their codes and algorithms to these new architectures. More specifically, we want to rewrite the core of our regional weather and climate code accordingly and adapt them to the new GPUs.

Does that mean that close collaboration between specialists in high performance computing, hardware and software developers and climate scientists will become increasingly important?
Undoubtedly. The collaboration with CSCS is a stroke of luck for us and it has all developed very well. However, it will take time before the new models are reflected in better climate scenarios.

CH2011 ***(www.ch2011.ch)***
In a project lasting several years, the *Center for Climate Systems Modeling (C2SM)*, MeteoSwiss, ETH Zurich, *NCCR Climate (the National Centre of Competence in Research – Climate)* and *OcCC (the Advisory Body on Climate Change)* have worked out scenarios for the future development of temperature and precipitation in Switzerland. The climate scenarios are based on refined climate simulations and new statistical methods. Detailed scenario data in digital form is also available for the first time. This data should provide impetus for research into the consequences of climate change, and should enable political and industrial decision-makers to have access to comprehensive information about the development of the climate in Switzerland in the 21st century.

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New building for CSCS in Lugano

The office block with its distinctive double layered glass facade.

In 2011 the creation of the new CSCS building was in its final stage. The defining features of the building are innovation, flexibility and ecological sustainability.

The new CSCS building is part of the national High-Performance Computing and Networking Strategy (HPCN) that was passed by the Swiss Federal Council and Parliament in 2009. The overall aim of the HPCN strategy is to ensure that high-performance computing, an increasingly important technology for many scientific fields, is made available to all Swiss researchers. The new building will ensure that even the supercomputers of the future can be operated to full capacity and in an energy-efficient manner at the Swiss National Supercomputing Centre.

The design specification set by the ETH Zurich Executive Board stated that the new computer centre should be able to accommodate the supercomputing infrastructure for Swiss science for the next 40 years.

An intelligent and innovative building design

Work on the new computer centre in Lugano-Cornaredo began in January 2010. Two separate buildings were erected, one for the offices and one for the supercomputers. The five-storey office block has been built to meet the Minergie standard and offers a total surface area of 2600 square metres. Special care was taken during construction to use environmentally friendly materials.

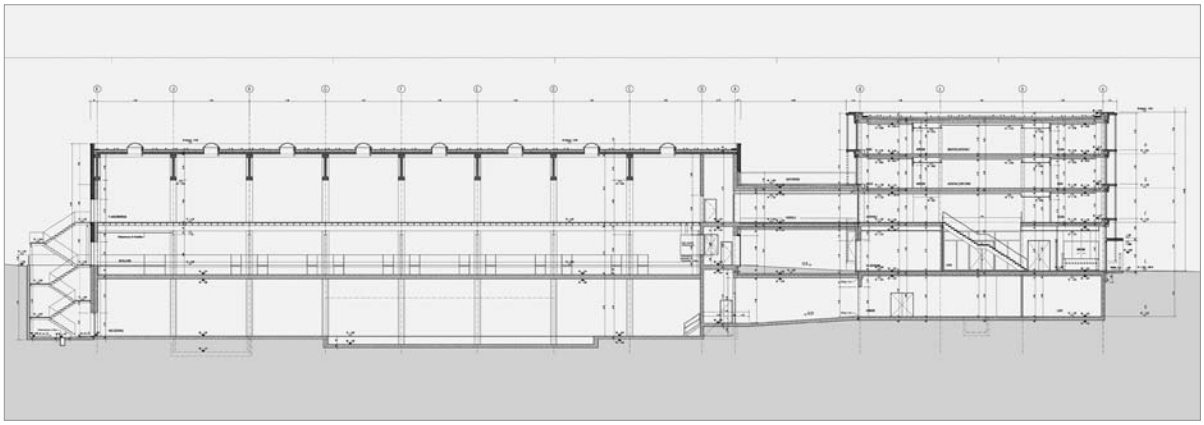
The spacious halls and landings will provide meeting areas for the employees and encourage communication, while the white decoration and large windows in the offices will provide light-flooded work spaces.

An underground corridor and a footbridge on the first floor lead from the office block into the heart of the new site, the computer building. The inconspicuous, windowless three-storey concrete cube of the computer building is an unadorned structure, but one which, technically and logistically, has been carefully thought through down to the last detail.

The construction of the computer room, which measures 2000 square metres, was designed to provide no restrictions to the installation and operation of supercomputers in the future. In order to maximise flexibility of future system acquisitions, the computer room has no supporting pillars or partitioning.

The new building design also solves some of the typical limitations in terms of the layout of cabling and power distribution units (PDUs). In a conventional computer centre, the machine room uses a raised floor measuring 40 to 60 cm in height through which kilometres of cable are fed; further limiting the flexibility, the conventional computer centre typically locates the cabinets for the PDUs in the computer room. However, in the new CSCS building, the raised floor has been replaced by a five-metre high storey which houses the entire technical infrastructure - thus greatly enhancing the flexibility and practicality of the computer centre.

South-West view of the computer and office buildings.



Cross-section of the three-storey computer building (left) and the five-storey office block.

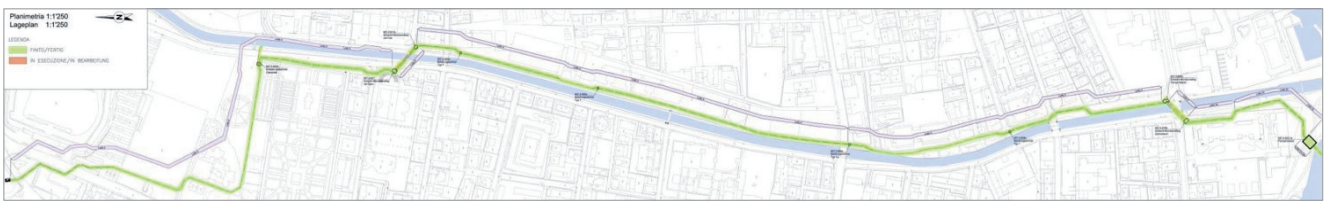
CSCS sets new standards

Today the new CSCS building is one of the most energy-efficient and ecologically sustainable supercomputer centres in the world. This is the result, among other things, of the use of water from Lake Lugano to cool the supercomputers as well as the building itself in summer. By using the 6 degree cold water from the lake to cool the computers it was possible to forego the installation of conventional power-hungry cooling systems, which would otherwise have accounted for about a third of the total electricity consumption. To operate the cooling system, a pumping station has been built on the lake shore in Parco Ciani, in the centre of Lugano. On its way to CSCS, the water will climb 30 metres and cover a distance of 2.8 kilometres.

The whole building has been planned to be modular in structure, allowing as much flexibility as possible in developing it and adapting it for subsequent technologies. A hoisting crane (with a weight-bearing capacity of up to 10 tonnes and the ability to reach all storeys of the computer building from the delivery area) ensures that any later modifications to the building can be made without difficulty.

In the labyrinth of the pumping station: five metres beneath the lawns of Parco Ciani, over 700 litres of water per second are pumped out of Lake Lugano.

Only a trapdoor indicates the existence of the pumping station below the surface of Parco Ciani to visitors.



The water pipe (green) stretches 2.8 km accross the city to connect the lake (right) with the computing centre. On its way it crosses under the Casserate river twice.

Facts on the building

The parameter by which the energy efficiency of a supercomputer centre is measured is the PUE rating (power usage effectiveness). The target PUE for the new CSCS building is below 1.25. At the time of planning, this rating was extremely ambitious for a supercomputing centre. For this reason, CSCS is today one of the most energy-efficient and ecologically sustainable supercomputer centres in the world.

In order to achieve the low PUE rating, CSCS cools its supercomputers with lake water. Energy savings were also made with the battery-supported emergency power supply (UPS) - only those parts of the computer centre's infrastructure that cannot tolerate any power interruption are connected. This affects infrastructure such as data storage, networks and the MeteoSwiss computer. UPS systems can suffer losses of up to 30% in the conversion from direct current to alternating current.

The existing power supply allows the centre to operate computers with a load of about 11 megawatts, and it could even be extended to operate up to 25 megawatts. The power enters CSCS with a medium voltage of 16 000 volts. Braided copper cables distribute it to the twelve currently installed transformers where it is converted to 400 volts. From the transformers, it is taken via power rails to the "installation deck" and finally to the supercomputers.

Facts on the lake water cooling system

The pumping station in Parco Ciani is connected by a pipe to 13-tonne, 6-metre high suction baskets that have been immersed at a water depth of over forty metres. Through this pipe, three pumps in the pumping station will pump up to 760 litres of water per second. 460 litres will go to CSCS for cooling purposes, while up to 300 litres will be available to AIL (Aziende Industriali Lugano) for its water reservoir, which has yet to be built.

The lake water pipe, measuring 80 cm in diameter, enters the building. A pipe of the same size leads back to the lake. Between the incoming and outgoing pipes, there is a sophisticated cooling system in operation: the lake water and the internal cooling water circuit meet in heat exchangers which are as tall as a person. There the low temperature of the lake water is transferred to the internal cooling circuit. In the first cooling circuit, water is delivered at about 8 or at most 9 degrees to the supercomputers to cool them. By the time the water has passed through this first cooling circuit, it is eight degrees warmer. However, this water is still cold enough to cool the air in the housings of lower-density computers and hard discs. To this end, it is sent through another heat exchanger that is connected to a second, medium-temperature cooling circuit. This allows one pumping operation to supply two cooling circuits in order to cool several types of systems. Even the mechanism for cooling was designed with energy efficiency in mind.

Rendering of the machine room with supercomputers in the foreground and cooling islands for additional hardware in the background.

Finances

Expenditures

	CHF
Investments	**12 186 451.93**
Material/Goods/Services	**9 703.80**
Personnel	**6 379 975.76**
Payroll	5 005 690.35
Employer's contributions	815 793.45
Further education, travel, recruitment	558 491.96
Other Material Expenses	**5 671 634.43**
Maintenance Building	317 503.59
Energy & Media	2 228 062.97
Administrative expenses	55 430.03
Hardware, software, services	2 859 862.76
Services & Remunerations	208 396.84
Other	2 378.24
Extraordinary Income/Expenditures	**-112 927.63**
Membership fees / Overhead	82 233.30
Third party funds transfers	-195 160.93
Expenses Total	**24 134 838.29**

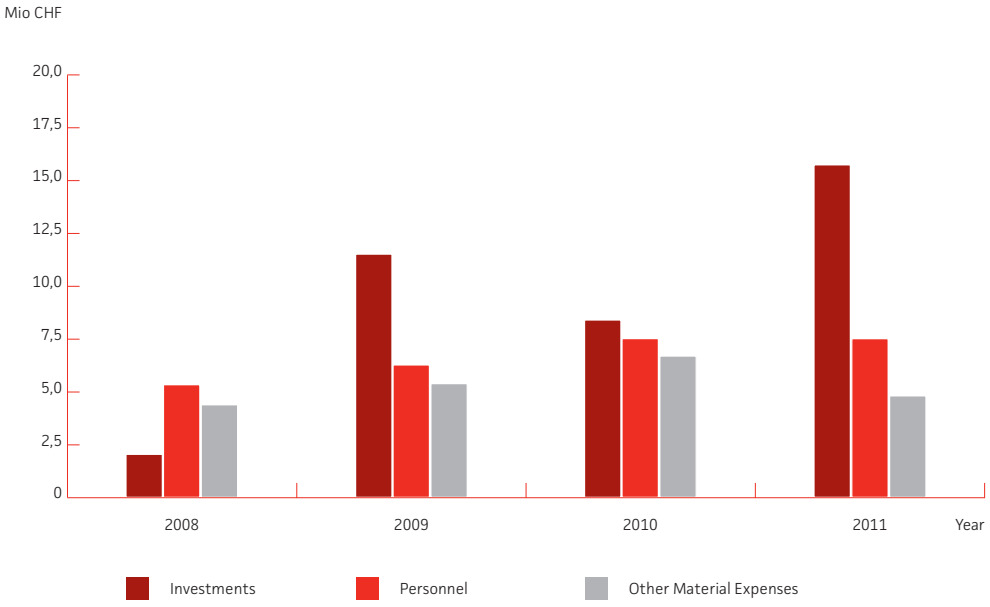
Income

	CHF
Basic Budget	**18 943 376.94**
Contribution ETH Zurich	18 848 567.92
Other Income	
Training, courses, sponsorship	94 809.02
Rollover 2010	**5 324 007.50**
Income Total with Rollover 2010	**24 267 384.44**
Balance	**132 546.15**

Third party contributions	
ETH Council Contributions	**3 571 000.00**
Project Eureka	3 000 000.00
HP2C Project	571 000.00
Contributions of third parties	2 165 866.46
European Projects (PRACE, Next Muse, LinkSCEEM)	857 106.06
MeteoSwiss	731 250.00
HP2C Project (CRUS Contribution)	452 828.90
Università della Svizzera italiana	88 200.00
Others	36 481.50

Development of Overall Expenses

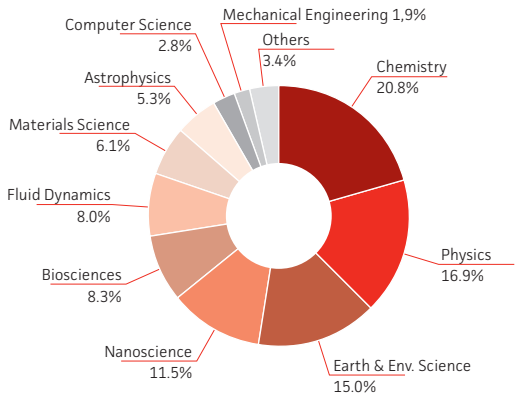
	2008	2009	2010	2011
Investments	2 044 641	11 540 846	8 417 349	15 777 324
Personnel	5 347 691	6 284 972	7 534 853	7 530 745
Other Material Expenses	4 395 150	5 399 155	6 706 740	4 818 411



Usage statistics

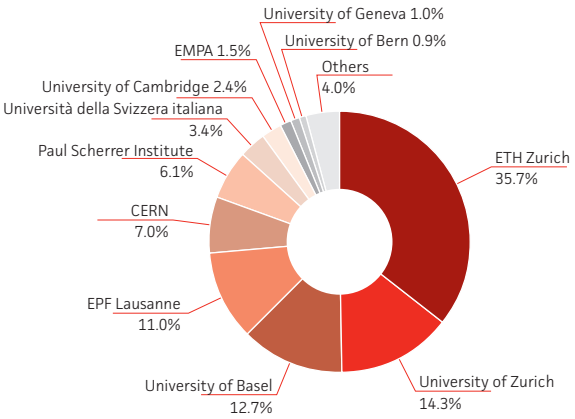
Usage by Research Field

Research Field	CPU h	%
Chemistry	42 058 323	20.8
Physics	34 136 408	16.9
Earth & Environmental Science	30 463 417	15.0
Nanoscience	23 329 382	11.5
Biosciences	16 898 385	8.3
Fluid Dynamics	16 182 061	8.0
Materials Science	12 440 734	6.1
Astrophysics	10 738 957	5.3
Computer Science	5 714 434	2.8
Mechanical Engineering	3 765 872	1.9
Others	6 797 286	3.4
Total Usage	**202 525 259**	**100.0**

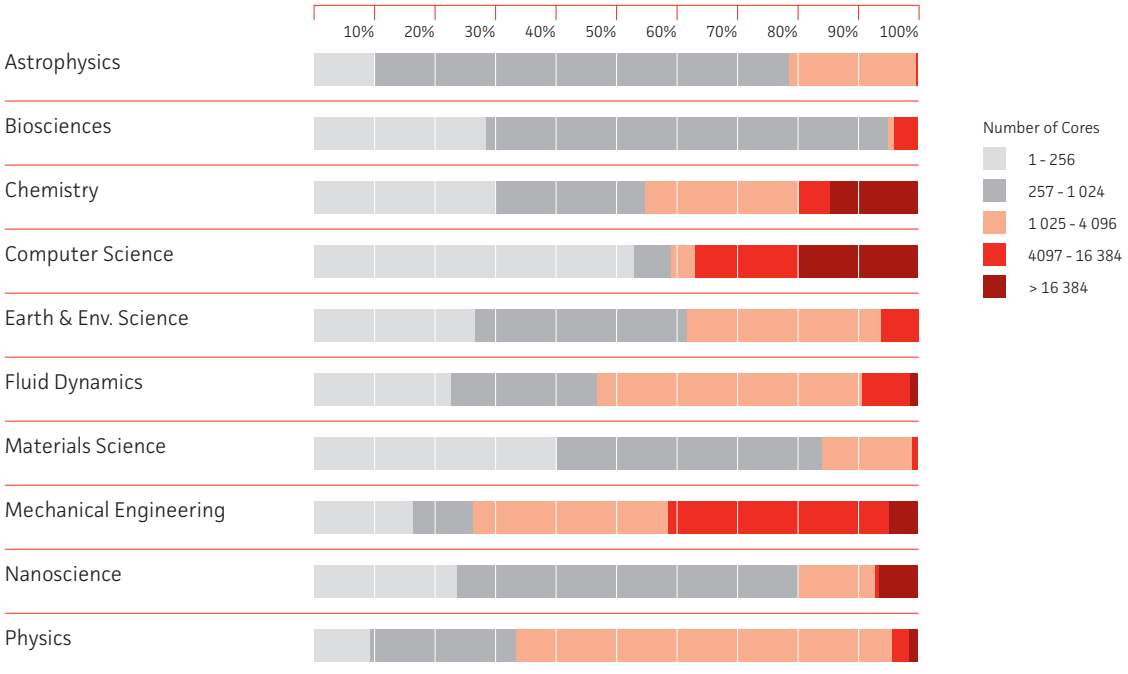


Usage by Institution

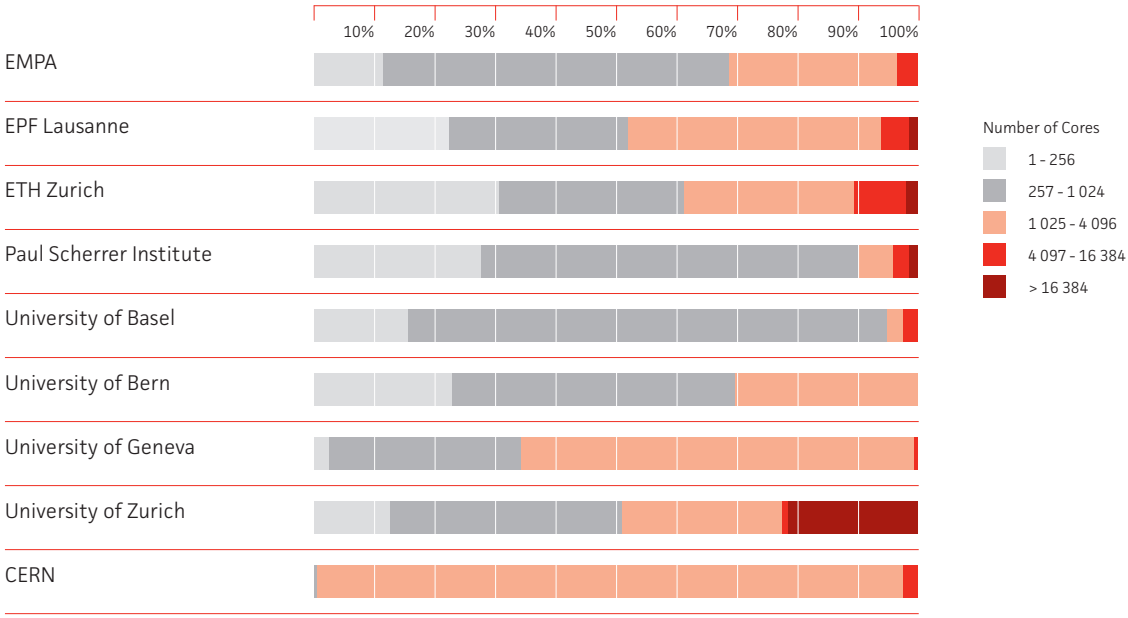
Institution	CPU h	%
ETH Zurich	72 527 834	35.8
University of Zurich	28 885 082	14.3
University of Basel	25 788 857	12.7
EPF Lausanne	22 182 224	11.0
CERN	14 237 813	7.0
Paul Scherrer Institute	12 258 017	6.1
Università delle Svizzera italiana	6 823 691	3.4
University of Cambridge	4 861 927	2.4
EMPA	3 031 165	1.5
University of Geneva	2 101 250	1.0
University of Bern	1 811 430	0.9
Others	8 015 969	4.0
Total Usage	**202 525 259**	**100.0**



Job Size by Research Field (in Cores)



Job Size by Research Institution (in Cores)



Compute Infrastructure

HPC Systems

Name	Supplier & Model	Installation / Upgrade	Usage / Customer	(h) CPU Capacity	(h) CPU Produced	Availability (%)
Monte Rosa	Cray XE6	2009 / 2011 [1]	National User Lab	212 634 400	182 216 774	76.6 [2]
Tödi	Cray XK6	2010 / 2011 [3]	R&D	4 122 624	819 125	[4]
Piz Palü	Cray XE6	2010	R&D	30 818 304	18 738 563	[4]
Piz Buin	Cray XT4	2006 / 2009	MeteoSwiss	9 250 560	3 635 311	99.8
Dole	Cray XT4	2006 / 2009	MeteoSwiss	5 606 400	2 293 450	99.7
Phoenix	Sun Cluster	2010 / 2011	CHIPP (LHC Grid)	11 675 000	9 633 539	95.7 [5]
Eiger	Dalco Cluster	2010 / 2011	R&D, Visualisation	2 628 000	184 713 [6]	99.3
Rigi	Sun Cluster	2007	MeteoSwiss & USI	911 040	359 117	99.2
Piz Julier	IBM/Transtec Cluster	2010 / 2011	National User Lab	981 120	184 713	[4]
Matterhorn	Cray XMT	2011	National User Lab	[4]	[4]	[4]
Rothorn	SGI Altix UV 1000	2011	National User Lab	[4]	[4]	[4]
Pollux / Castor	IBM iDataPlex Cluster	2011	R&D	[4]	[4]	[4]

Name	CPU Type	No. of Cores	Interconnect Type	(TFlops) Peak Performance	(GB/s) Injection Bandwidth
Monte Rosa	AMD Opteron 16 core 2.1 GHz	47 872	Cray Gemini	402.0	9.4
Tödi	AMD Opteron 16 Core 2.1 GHz + Nvidia X2090	2 816 + 176 GPUs	Cray Gemini	129.0	9.4
Piz Palü	AMD Opteron 12 core 2.1 GHz	4 224	Cray Gemini	35.1	9.4
Piz Buin	AMD Opteron 4 Core 2.3 GHz	1 040	Cray SeaStar	5.0	7.6
Dole	AMD Opteron 4 Core 2.3 GHz	688	Cray SeaStar	3.3	7.6
Phoenix	AMD Opteron 12 Core 2.1 GHz + Intel 4 Core 3.0 GHz	1 472	Infiniband QDR PCI Gen2	11.8	4.0
Eiger	AMD Opteron 6+12 Core 2.2 GHz + Fermi & Tesla Nvidia GPU	276 + 20 GPUs	Infiniband QDR PCI Gen2	10.2	4.0
Rigi	AMD Opteron Dual Core 2.6 GHz	104	Infiniband DDR PCI Gen1	0.5	2.0
Piz Julier	Intel Xeon E7540 + Intel Xeon X5649 2.53 GHz	312	Infiniband QDR PCI Gen2	3.3	4.0
Matterhorn	Cray Threadstorm Processor	64	Cray SeaStar	-	-
Rothorn	Intel Xeon E7-8837 2.67 GHz	256	SGI NUMAlink5	2.7	9.0
Pollux / Castor	Intel Xeon X5650 2.66 GHz + Nvidia M2090	384 + 64 GPUs	Infiniband QDR PCI Gen2	4.1	4.0

[1] Upgrade from Cray XT5 to Cray XE6 on November 2011 - number of cores before upgrade 22 128 (212.4 TFlops)

[2] Long down time due to upgrade and problems with end-of-life infrastructure in Manno

[3] Upgrade of Piz Palü to Tödi at the end of October 2011

[4] No statistical data available

[5] Availability of Phoenix also depends on external grid factors

[6] The average utilisation is low because of its interactive usage pattern

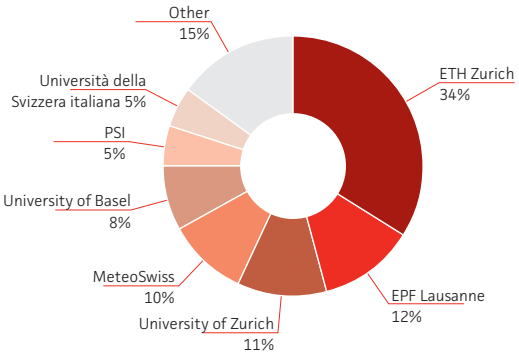
Monte Rosa, the flagship supercomputer of CSCS, was upgraded to a Cray XE6 in November.

Customer Satisfaction

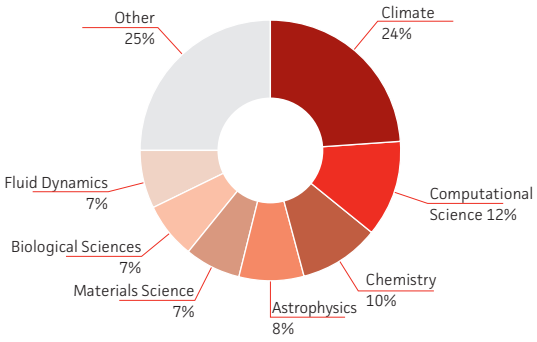
A customer satisfaction survey was submitted to 704 users in January 2012. The response rate was of 25% (173 answers).

User Profile

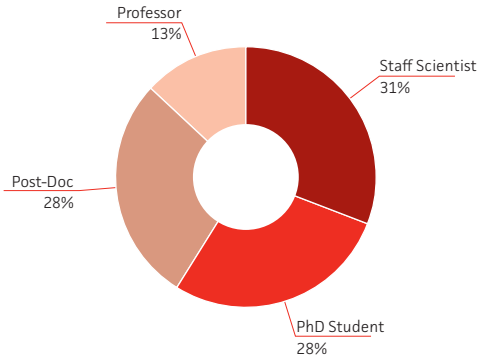
Your institution



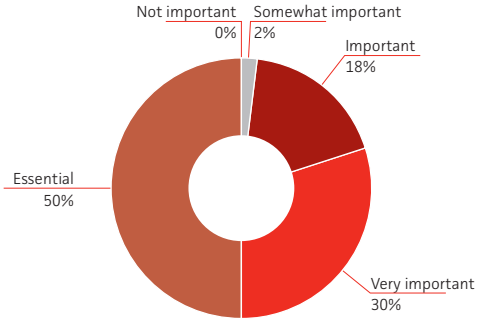
Your scientific field



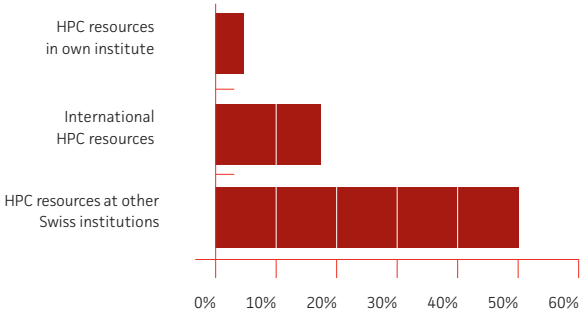
Your position



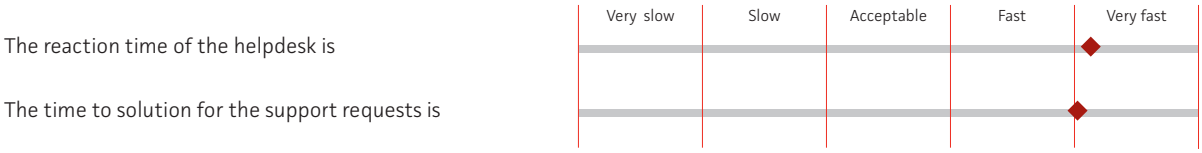
For my research, CSCS resources are



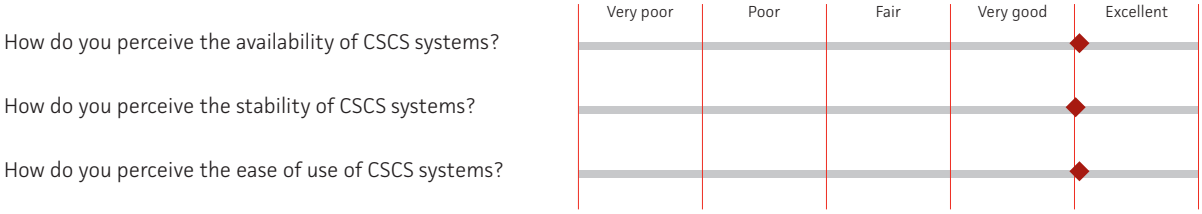
Which additional HPC resources are you using?



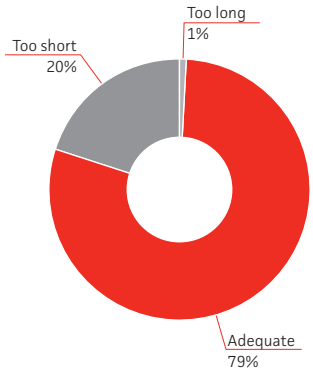
User Support



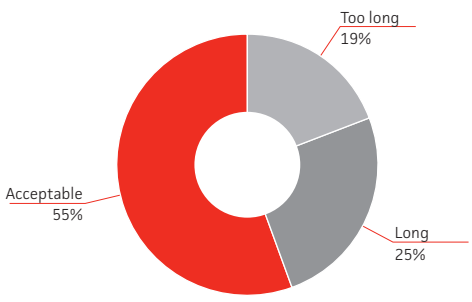
System Availability, Stability and Usability



The run time limits for batch jobs are:

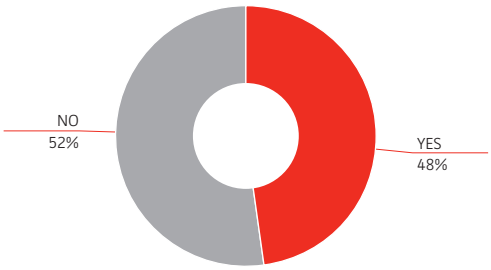


The job waiting time in the queue is:

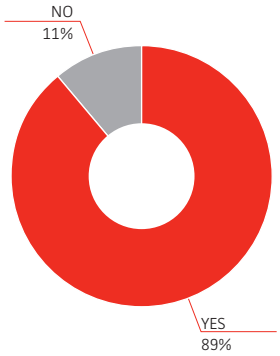


Project Proposal Process

Do you submit project proposals to CSCS (as PI or supporting the PI)?

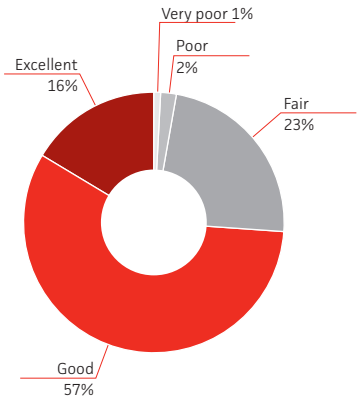


Is the review process transparent?

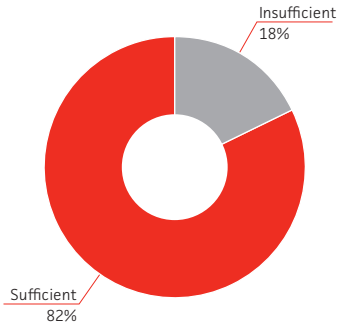


Adequacy of Allocated Resources

The resources assigned to my project are:

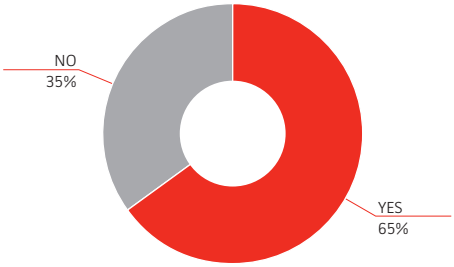


My storage allocation on /project is:

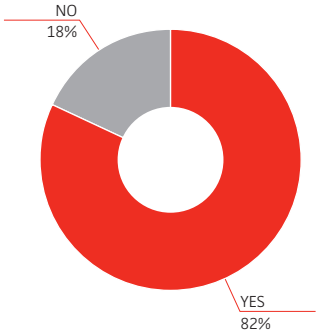


Application Development

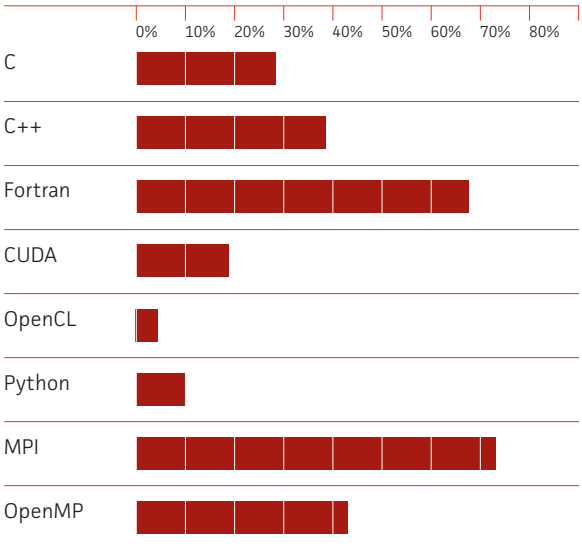
Do you develop and maintain application codes?



Do you measure the performance of your application code?

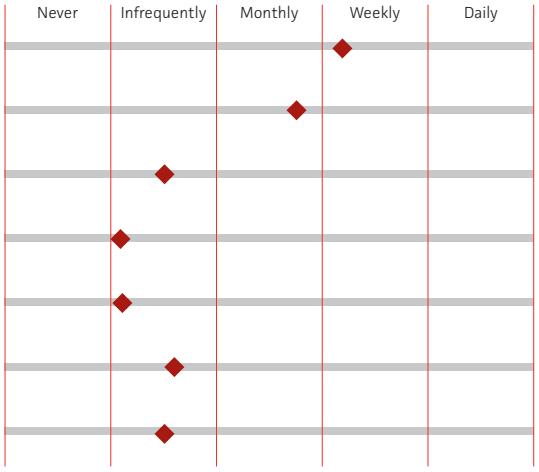


What programming languages and parallelisation paradigms are you using?



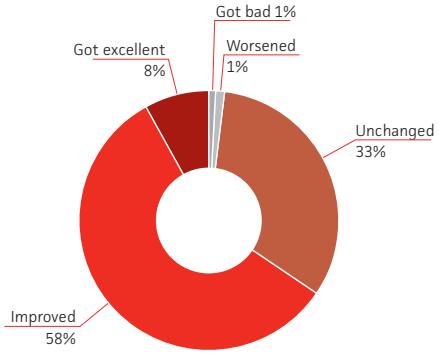
Information & Communication

How often do you access the following communication channels?

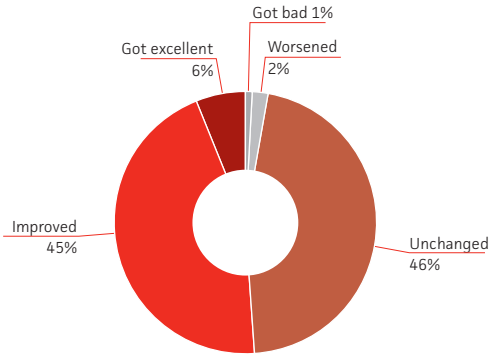


Perception of CSCS

My general view in the last year is that the services provided by CSCS are:



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



The machine room in the new building is ready for the move of the supercomputers from Manno.

Impressum

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