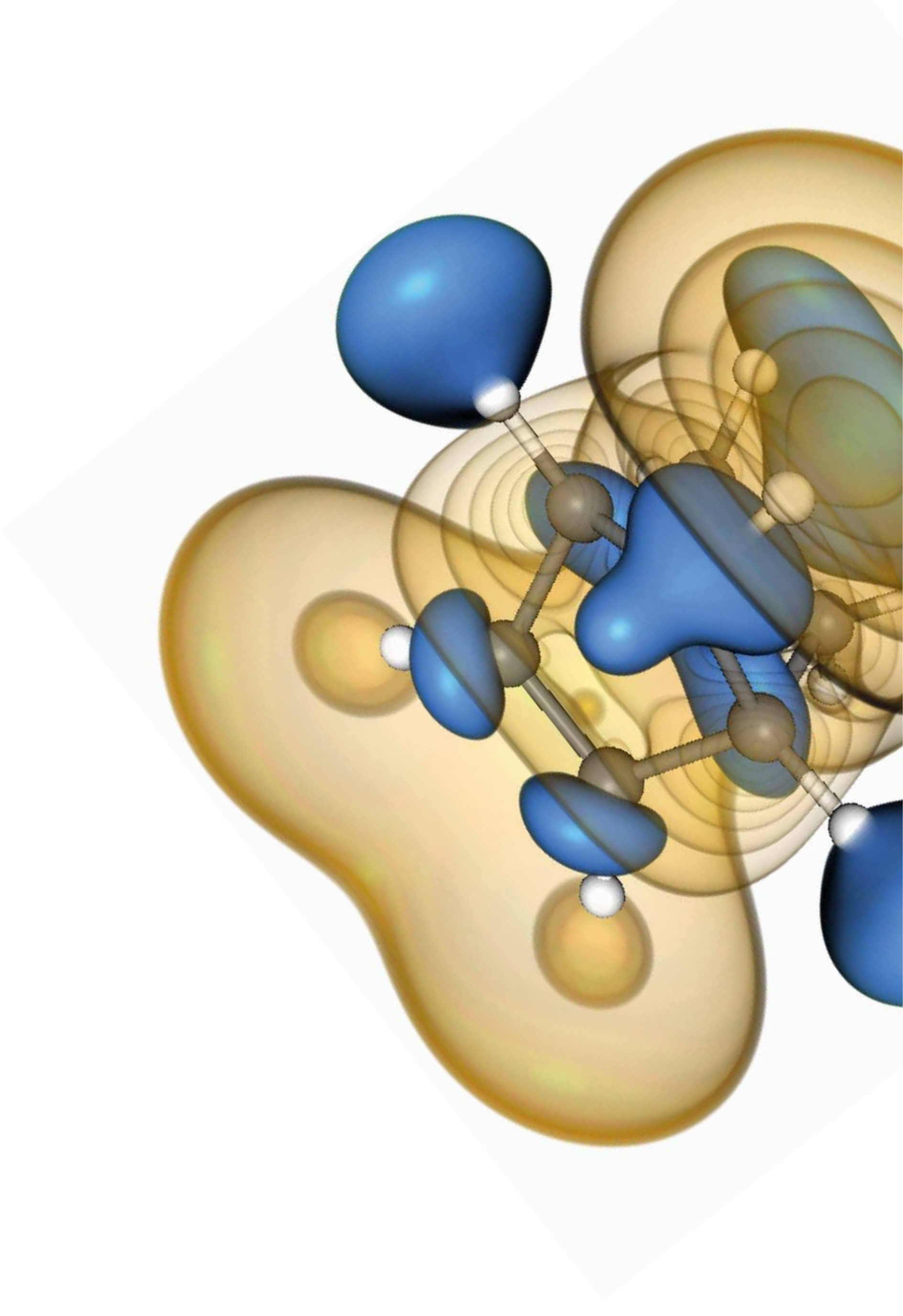
CSCS

Swiss National Supercomputing Centre

Annual Report 2010



ETH

Eidgenössische Technische Hochschule Zürich

Swiss Federal Institute of Technology Zurich

CSCS
Swiss National Supercomputing Centre

Annual Report 2010

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Welcome from the Director

Thomas Schulthess, Director of CSCS

Welcome to CSCS in 2010!
I would like to invite you to revisit CSCS's most important activities and achievements of last year.

Following a disruptive year in 2009, with a tenfold increase in supercomputer performance, the reorganisation of the centre, and the launch of the High Performance and High Productivity Computing (HP2C) platform, the year 2010 has been a year of refinement and tuning, but with continued steady innovation. This is exemplified by the new layout of this report - its improved layout enables simpler navigation, giving you a quick grasp of our activities and relevant information on operations and research at CSCS.

In the 'Activity Report' section we present how new, innovative systems, such as a GPU cluster or the first Cray XE6 system worldwide, replaced older HPC systems that were decommissioned to free up space and infrastructure. We discuss the special effort in our education and outreach activities, which received an award from the HPC Advisory Council at the International Supercomputing Conference (ISC'10). The construction of our new building in Lugano has continued to run on time, and within scope. This was celebrated symbolically during the ceremony for the laying of the foundation stone.

The 'Scientific Report' section highlights some of the results of user projects in several articles. During the last year CSCS distributed a total of 168 Mio hours to Swiss scientists from different domains in a transparent resource allocation process, in which international peers assess proposed projects and an external panel of experts makes allocation recommendations. An impressive list of publications by users reflects the quality of research performed with our supercomputing resources.

In a section dedicated to 'HP2C' the results of the platform's first year are summarised and an insight is provided into how the vision is being implemented and how state-of-the-art applications are being mapped to newly emerging computer architectures.

Finally, the 'Facts & Figures' section, provides a detailed insight in the area of finances and usage statistics, as well as a description of the supercomputer infrastructure.

The annual report closes with the results of a customer satisfaction survey, where our users attest to the positive development of our services. This was also recognised by a peer review of external experts who reported to the executive board of ETH Zurich.

I would like to thank all CSCS employees, ETH Zurich, as well as all persons and organisations supporting us for their contribution to a successful 2010. We all look forward to a challenging 2011.

Prof. Thomas Schulthess

Letter from the President of ETH Zurich

Ralph Eichler, President of ETH Zurich

Dear Reader

Scientific research can reveal a fascinating virtual world: Sophisticated models show specific material properties, demonstrate climate change, or surprise us with complex socio-economic behaviour. Computer-based simulations for processes or problems in nature and society on different scales have become the third pillar of science, alongside theory and experiment. Hence, supercomputers are a key technology for cutting-edge research and strengthen a nation's competitiveness. For this reason, ETH Zurich is strongly committed to operate and further develop the Swiss National Supercomputing Centre for the academic community.

Today, modelling is the keyword in computer science and engineering. Many fields in natural science, technology, and social sciences will profit from the increased computing power available for simulations and modelling. In this context, not only the computing capabilities are important but also the capacity as far as data storage, data collection, and data mining are concerned. Data handling is crucial; therefore, more attention should be given to it, which is also recommended in the CSCS peer review. In addition energy consumption is increasingly becoming the financial bottle neck. It scales with the processor speed but data access consumes even more energy than bare arithmetic operations. This is a second reason for giving data handling a higher priority.

CSCS has to fulfill a user laboratory function. It has to operate an efficient, cost and energy effective infrastructure for a reliable computing service. Specific tasks are the development of fast algorithms together with hardware vendors, consulting customers, and preparing the evaluation of the next generation computing hardware to be installed for users from 2015. The CSCS peer review in May 2010 concluded, that by establishing the High Performance Computing and Network (HPCN) strategy, Swiss computational science will be in a leading position.

A success story is the Swiss Platform for High-Performance and High-Productivity Computing (HP2C), a program aimed at establishing a network of experts in high performance computing in the Swiss university landscape. Topics range from weather forecast and earthquake safety to high temperature superconductivity. Recognising the need for build a computational science collaboration, HP2C was created as an important element of the HPCN – and is the proper innovative initiative to prepare Swiss computational scientists for competition at the highest level.

Focusing on computational science is a shift in the right direction. Investments are at the proper level and very competitive. Affirming

Lugano as the permanent location and building a collaboration with the University of Lugano (USI) have contributed to the stability of CSCS and form a good foundation for the development of the HPCN. The appointment of Prof. Schulthess as director with management expertise, outstanding computational as well as computer science credentials, and capability to integrate the science community, has significantly enhanced the recognition of CSCS in the Swiss research environment.

The peers found that CSCS had made outstanding progress in all areas and had established itself firmly as a national centre that Switzerland can be proud of, providing leading technology and services, at an internationally competitive level.
I sincerely subscribe to this view.

We are happy to soon completing a new building in Lugano Cornaredo within walking distance of USI, allowing CSCS to strip off its image as an intellectual desert in Manno. The scientific environment is important. The building is first of its kind with high efficiency and environmentally compatible cooling financed with money from the Swiss government economic program (Konjunkturprogramm), ETH Zurich, and a donation from the Canton of Ticino. Operation is planned to start in 2012.

Because of the vast amount of data generated by and used for simulations, it is essential to establish a fast and redundant network between CSCS and its customers, integrating the different computational resources in Switzerland. HP2C has namely shown, that depending on the algorithms for specific scientific or technical problems, different computing architectures are optimal.

I would like to thank all CSCS staff for their constant and reliable effort to provide a well maintained computing infrastructure for the benefit of scientists and engineers from Swiss universities and research institutes. Sincere thanks are also given to the Canton of Ticino and the city of Lugano for the warm welcome and financial support.

Prof. Ralph Eichler

Key Information

Founded in 1991, CSCS, the Swiss National Supercomputing Centre, 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 XT5, 212 TFlops,
22 128 cores, 29 TB memory

Computing Time for Science

2010: 168 147 399 CPU h
2009: 85 596 470 CPU h

Employees

2010: 50
2009: 46

User Community

65 Projects, 605 Users

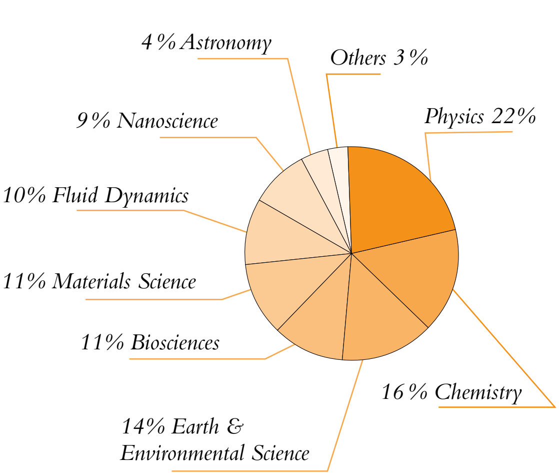
Investments

2010: 8.4 Mio CHF
2009: 11.5 Mio CHF

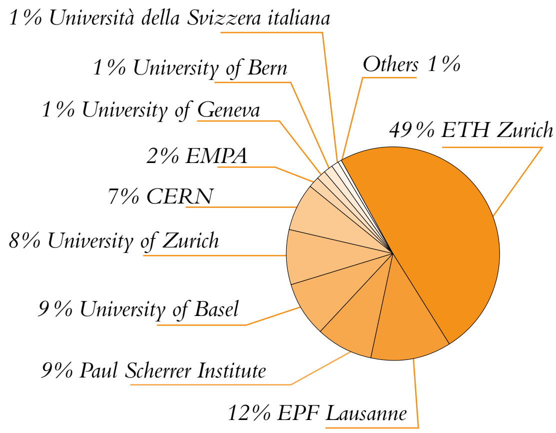
Operational Costs

2010: 14.3 Mio CHF
2009: 11.7 Mio CHF

Usage by Research Field



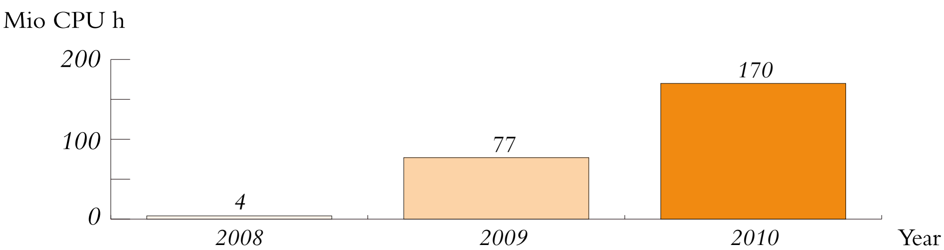
Usage by Institution



Computing Systems

Name	Supplier & Model	Installation/ Upgrade	Usage / Customer	Peak Performance (TFlops)
Monte Rosa	Cray XT5	2009	National HPC Service	212.4
Piz Palü	Cray XE6	2010	R&D	35.1
Phoenix	Sun Cluster	2010	CHIPP (LHC Grid)	11.2
Eiger	Dalco Cluster	2010	R&D, Visualisation	10.2
Piz Buin	Cray XT4	2006/2009	MeteoSwiss (Production)	5.0
Dole	Cray XT4	2006/2009	MeteoSwiss (Failover, R&D)	3.3
Fuji	Transtec Cluster	2010	R&D	0.7
Rigi	Sun Cluster	2007	MeteoSwiss & USI	0.5
Piz Julier	IBM x3850	2010	National HPC Service, R&D	0.4

Evolution of CPU Usage



Activity Report

January

Decommission of the Cray XT3 'Piz Palü'

The Cray XT3 'Piz Palü' named after the mountain in the Bernina range in Grisons reached its end of life and was decommissioned. Its last configuration was 6 cabinets with 137 compute blades comprising 548 dual core nodes (1096 compute cores).

The Cray XT3 was an important milestone in the history of CSCS as it was CSCS' first massively parallel supercomputer and the very first Cray XT machine to set foot in Europe.

Piz Palü had started its life as a production system on January 2006 and was used by researchers of Swiss universities as well as by MeteoSwiss for weather forecasts.

Veteran Supercomputers Donated to ENTER-Museum

Three of the six racks of the dismantled Piz Palü supercomputer and a discharged SGI Origin 9500 have been donated to the ENTER-Museum.

This is the only Swiss museum dedicated to all kinds of computers, computer peripherals, and computer technology. The museum close to Solothurn displays an amazing array of 400 fully-functional computer systems, 100 pocket calculators, 50 mechanical calculators, telecommunication equipment, and more.

The recent donation from CSCS furthers the scope of the exhibition to cover computing technology of the early 21st century.

Dismantling of the Cray XT3 Piz Palü.

Decommission of the IBM P5 'Mont Blanc'

The IBM P5 'Mont Blanc', another milestone in the development of CSCS, was decommissioned. This computer had been named after Mont Blanc, a mountain in the French-Italian Alps. Its last configuration was 48 nodes with 16 IBM Power5 processors each, 1780 GB DDR2 memory and a 10 Gbit Infiniband interconnect.

Mont Blanc had started its life as a production system in January 2007. It was the first Power5-based supercomputer worldwide running Linux with an Infiniband as a high-speed interconnect.

Mont Blanc had been used mainly for high-memory jobs and for problems involving algorithms with only limited scalability.

February

New Computing Systems for MeteoSwiss

Since 2007 MeteoSwiss has produced the national daily weather forecasts on the Cray XT4 'Piz Buin' named after another Swiss mountain in Grisons, using the Cray XT3 Piz Palü as a backup system.

After Piz Palü was decommissioned, the fail-over functionality was re-established by splitting Piz Buin into two distinct systems (three and two racks) and upgrading all processors from dual-core to quad-core. The second half of the system is now called 'Dole', after a mountain of the same name in the Jura range in Vaud. This mountain happens to be one of the three sites where MeteoSwiss maintains meteorological radars.

Agreement Between ETH Zurich and USI

ETH Zurich and the Università della Svizzera italiana (USI) agreed to offer joint professorships enabling synergies in computational science, engineering and economics in collaboration with CSCS.

In addition, the presidents of both universities Ralph Eichler (ETH Zurich) and Piero Martinoli (USI) signed an agreement to introduce a support framework for dual professorships.

According to Ralph Eichler these agreements will further boost the intellectual exchange with USI once CSCS moves to Lugano in 2012.

First HPC Advisory Council Infiniband Workshop

Dominik Ulmer, General Manager of CSCS, opened the HPC Advisory Council Switzerland Workshop 2010 in Lugano. With more than 110 registrations this was the largest conference ever dedicated to HPC technologies in Switzerland. As sponsor and co-organiser CSCS presented its broad spectrum of HPC activities with a particular focus on Infiniband technologies.

Upgrade of the MeteoSwiss computing systems from Cray XT3 to XT4.

March

The New CSCS Building

The construction of the new supercomputer centre began with the demolition of a disused bus terminal and subsequent excavation work. The new building in Lugano is planned to be ready by the end of 2011 and relocation from Manno to Lugano is expected to take place during the first half of 2012.

April

140 Million Hours Allocated to New Research Projects

On 1st April 2010 a total of 140 Mio CPU hours was allocated to 56 new research projects starting production on the Cray XT5 'Monte Rosa', the largest supercomputer at CSCS. The resource allocation was based on technical and scientific review, assessing both the fitness of each research proposal for the supercomputer architecture at CSCS and the scientific merit.

The largest allocations (each 16% of the total available resources) went to projects in the biological, chemical, and materials science; smaller allocations of 13, 9, and 7% respectively were granted to projects in climatology, physics, and nanoscience. ETH Zurich held the largest share of all institutions (46%), followed by EPF Lausanne (16%) and the University of Zurich (11%).

Upgrade of 'Phoenix'

Phoenix is the HPC system dedicated to researchers of the Swiss Institute of Particle Physics (CHIPP) who analyse data from the Large Hadron Collider (LHC) experiment at CERN. The 'Phase C' upgrade was delivered and installed by Sun Microsystems (now Oracle) thus by doubling the computing and storage capacity of the previous system.

The new cluster has 96 Sun X6275 compute nodes with a total of 768 cores and 7.6 TFlops of peak performance. The interconnect is based on Infiniband QDR. The available storage for experimental data amounts to 1152 TB.

The project team for the new Sun cluster Phoenix. The cluster analyses data from the LHC experiment at CERN.

New Visualisation Cluster 'Eiger'

'Eiger' is a new cluster installed for visualisation, research, and development. It features a hybrid multi-core and multi-GPU computing environment for visualisation, data analysis, and general-purpose pre- and post-processing activities. Specifically, it comprises 19 nodes of dual-socket hexacore AMD Opteron processors, and 24 GB of main system memory per node, i.e. a total of 228 CPU cores and 456 GB aggregate memory. Each node is equipped with a GPU.

May

Peer Review of CSCS

From May 17th to 19th, a group of external experts scrutinised CSCS in a peer review. Chaired by Horst Simon (Associated Director of

Lawrence Berkeley National Laboratory), the panel visited the centre as well as ETH Zurich and interviewed the CSCS staff, users, and stakeholders.

In his cover letter of the report, which summarises the observations and recommendations, Simon writes: 'The reviewers considered developments in the years 2007-2010. During this time period significant changes occurred in high performance computing in Switzerland that had a very strong positive impact about the state of the art in computational science in the country. The peers found that CSCS has made outstanding progress in all areas and has established itself firmly as a national centre that Switzerland can be proud of, providing leading technology and services, at an internationally competitive level.'

The expert panel of the peer review (from left to right): Thomas Lippert (Forschungszentrum Jülich), Giovanni Ciccotti (Università di Roma 'La Sapienza'), Horst Simon (Lawrence Berkeley National Laboratory and UC Berkeley), Anwar Osseyran (SARA Amsterdam).

June

Monte Rosa: One Year Later

One year has passed since the inauguration of Monte Rosa in June 2009. The massively parallel usage pattern is impressive: 57% of all jobs used more than 512 cores each, and 33% used more than 2048. Roughly a quarter (24%) of the users were from fluid dynamics, 23% from physics, followed by nanoscience (12%), earth & environmental science (11%) and chemistry (8%).

In the TOP500 list, Monte Rosa started at rank 23 (June 2009), moved to position 21 (November 2009) after an upgrade to hexacore processors and positioned itself 27th in June 2010.

Introduction to the Physics and Experiments at the LHC

The Swiss Institute of Particle Physics (CHIPP) organised a one-day workshop for CSCS staff to present one of the most challenging experiments ever done on earth: The Large Hadron Collider experiment at CERN.

Christoph Grab (ETH Zurich) introduced the world of particle physics and explained the importance of the Higgs particle to modern physics. Szymon Gadomski (University of Geneva) gave an overview of the LHC experiments and Michele Weber (University of Bern) explained what accelerators are and how they work. An additional presentation was dedicated to every single experiment using the compute infrastructure at CSCS, namely CMS, ATLAS and LHCb.

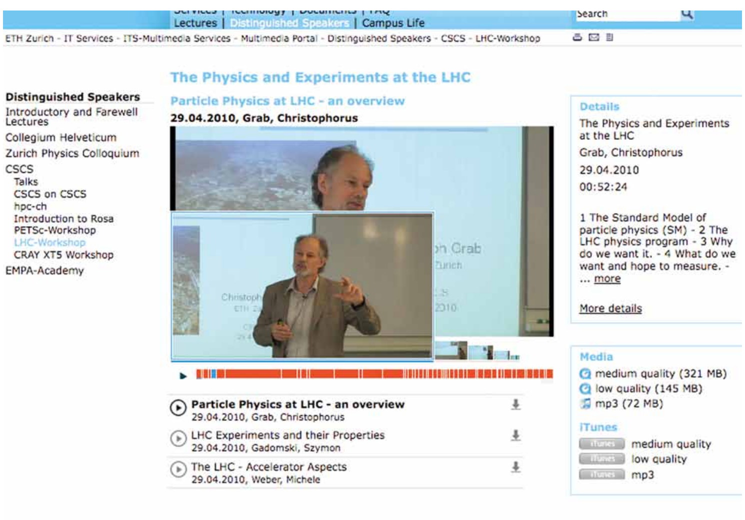
Education and Outreach Award by HPC Advisory Council

During the closing session of the ISC'10 conference in Hamburg, the HPC Advisory Council named CSCS as the recipient of the Education and Outreach Award in recognition of its excellent HPC outreach and education activities. The prize was received by Hussein Harake of CSCS, the initiator of the Infiniband Workshop 2010 conference in Lugano.

The HPC Advisory Council is a leading worldwide organisation for high-performance computing research, development, outreach and education.

Supercomputing Experts in the Swiss Capital

The President of ETH Zurich, Ralph Eichler, invited members of the Swiss parliament to a lunch-time presentation of ETH Zurich activities in high performance computing. Thomas Schulthess introduced CSCS and the Swiss National Supercomputing strategy (HPCN) to the politicians, Peter Binder from MeteoSwiss outlined why supercomputers are essential for meteorology, while Alessandro Curioni from IBM Rüschlikon explained how fast the field of HPC is developing and why regular HPC investments are so important.



Talks and courses can be accessed over the new video portal.

ETH Board Appoints New Professor to Strengthen the Collaboration with CSCS

The ETH Board announced the appointment of Markus Püschel, previously Professor in the Department of Electrical and Computer Engineering at Carnegie Mellon University in Pittsburgh, USA, as full Professor of Informatics at ETH Zurich. Püschel's research interests combine techniques in mathematics, computer science, and engineering. His interdisciplinary research will strengthen the cooperation between the Department of Informatics and CSCS.

July

Easier Access to CSCS Video Productions

The recordings of talks and courses produced by CSCS were finally published on the multimedia portal of ETH Zurich (www.multimedia.ethz.ch) allowing easy access to all recordings. Users can browse through the videos and search for relevant content. Videos can be downloaded in different file formats and file sizes.

Phase-out of Old Phoenix

After the successful implementation of Phase C to upgrade the Phoenix cluster, the old hardware (Phase B) was switched off, decommissioned, and transferred to the universities of Bern and Geneva where they were re-deployed as part of the local grid infrastructure.

August

HPC Advisory Council Appoints CSCS as Centre of Excellence

The HPC Advisory Council announced the formation of regional Centres of Excellence, broadening the scope and mission of the Council's programs throughout the world. These centres provide local support for the HPC Advisory Council's programs, organise local workshops and conferences, and host local computing centres that can be used to extend such activities. CSCS was appointed as the first Centre of Excellence in Europe.

Worldwide First Installation of a Cray XE6

CSCS announced the successful installation of an early-release version of the new Cray XE6 supercomputing architecture. The new system, called again Piz Palü, emerged from of a collaboration with Cray. The user community now has the chance to test Cray's next generation hardware and software technology.

Piz Palü is the first Cray XE6 installed worldwide.

Piz Palü features Gemini, Cray's new interconnect network with increased performance and fault tolerance. Compared to current SeaStar networks, Gemini improves support for Partitioned Global Address Space (PGAS) languages such as Co-array Fortran (CAF) and Unified Parallel C (UPC). At the Supercomputing Conference in New Orleans (November 2010), the new Gemini interconnect used for Piz Palü was named Best HPC Interconnect Product or Technology by the editors of HPCwire. This recognition was part of the

2010 Readers' and Editors' Choice Awards.

September

'Technology Integration' to Support the Development of New HPC Systems

A new unit 'Technology Integration' was created to support the development of HPC prototypes and to transfer these technologies to operational systems.

This additional unit emphasises the life-cycle orientation of the centre and aims to rapidly make new technologies and programming paradigms available to Swiss scientists.

Università della Svizzera Italiana Co-invests at CSCS

A second cabinet of the Cray XE6 Piz Palü financed by the Università della Svizzera italiana (USI) was installed. The computing power will be used mainly by researchers of the Institute of Computational Science at USI.

Record CPU Time on Phoenix

In September after upgrading to Phase C and having made several improvements, Phoenix surpassed all production records running around 200 000 jobs and computing more than 850 000 CPU h – doubling the average numbers since 2009.

October

23 Mio CPU Hours Allocated to New Research Projects

The second allocation period on Monte Rosa started on 1st October 2010. A total of 120 Mio CPU hours were reserved for the continuation of running projects, and another 23 Mio of CPU hours were allocated to 21 revised and 3 new research proposals.

Raffaele Balmelli, Head of Implenia Ticino, Thomas Schulthess, Director of CSCS, and Roman Boutellier, Vice President Personal and Resources of ETH Zurich, during the foundation stone ceremony on the construction site.

Foundation Stone for the New Building

The representatives of ETH Zurich, Canton of Ticino, City of Lugano and the construction company Implenia together with CSCS celebrated the laying of the foundation stone for the new building.

The building will cost around 80 Mio CHF and is built with energy efficiency in mind. The offices are designed according to Swiss minimal-energy standards and the supercomputer will be cooled with lake water. Finally, excess heat will be made available to the city of Lugano.

November

New Video Channel

A new video channel named 'CSCS on CSCS' informs about the activities of the supercomputing centre. Two of the first videos show how scientists use supercomputers in astrophysics and drug design. In three additional videos CSCS employees illustrate different aspects of their work. Finally the assembly of Monte Rosa is shown as a time-lapse movie (www.multimedia.ethz.ch/speakers/cscs/cscsonscscs).

CSCS at the International Supercomputing Conference SC'10

Sadaf R. Alam served at the International Supercomputing Conference SC'10 in New Orleans as member of the Technical Paper Program Committee and of the Performance Committee. She further chaired the Doctoral Research Showcase, presented a technical paper as co-author on 'Optimal Utilization of Heterogeneous Resources for Biomolecular Simulations', and presented a poster at the PGAS booth. William Sawyer was chair of the technological thrust area 'Addressing Climate Change Uncertainties'. John Biddiscombe moderated the panel discussion 'Parallel I/O: Libraries and Applications, Making the Most of Resources'.

Gordon Bell 2010 Prize: Honorable Mention to Thomas Schulthess and Co-Workers

Thomas Schulthess, Anton Kozhevnikov (ETH Zurich) and Adolfo G. Eguiluz (University of Tennessee, Knoxville) received the Gordon Bell honourable mention for special achievements in scalability for their project 'Toward First Principles Electronic Structure Simulations of Excited States and Strong Correlations in Nano- and Materials Science'. To perform their work Schulthess and his team used the Cray XT5 at Oak Ridge National Laboratory's Leadership Computing Facility.

December

Shell of New Building Almost Complete

In December 2010, the shell of the new CSCS building in Lugano was almost complete. Just before the New Year break, the roof of the new data centre was assembled using the strongest mobile crane on the market, featuring a telescoping beam that extends from 20 to 100 meters and lifts weights of up to 1 200 tons. Each of the eight beams weighs 50 tons and is 35 meters long. The new data centre covers an area of 2 000 square meters and is free of pillars, allowing more freedom in placing future supercomputers.

The new building in Lugano with on the left side the administrative building and on the right the machine room.

Scientific Report

Improved Project Review Procedure

Since 2009 CSCS has undertaken several measures to improve the quality of the project review, to make it fully transparent to the applicant, and rigorously based on external review in order to ensure the high scientific standards that are required to justify the substantial expenditures of acquiring and maintaining the centre's supercomputer infrastructure.

As of 2010 each production project proposal is first reviewed by two CSCS analysts to assess its technical feasibility and readiness. The proposal and the internal technical review are then submitted to two independent (typically foreign) experts for scientific evaluation. Reviewers are asked to assess the soundness of the computational approach, the validity of the tools and codes, and the quality of the proposed simulations and resource request. The opinion of a third expert may be requested if the two scientific reviews come to substantially different conclusions. Based on the technical and scientific reviews, an external panel finally makes a proposal to the director for computing time and storage allocations.

The applicant is not only informed of the final decision but he or she is also provided with all technical and scientific reviews and the reasoning of the panel committee. Hence the review process is entirely transparent to the applicant, and the material provided should help him or her to further improve the quality of future project proposals.

Increased Allocated Resources

A total of 61 project proposals were submitted in 2010, requesting a total of 191 Mio CPU hours, thus oversubscribing available resources (140 Mio CPU hours) by more than one third.

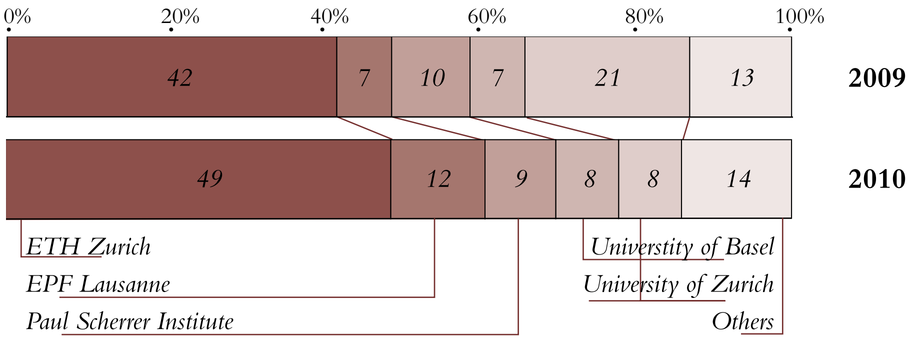
The three graphs on next page illustrate usage of the Cray XT5 Monte Rosa, CSCS' flagship supercomputer.

ETH Zurich remains the largest user of CSCS resources, but some changes in ranking are seen for the remaining institutions. Whilst the University of Zurich and PSI followed up in 2009, it was EPF Lausanne and PSI that did so in 2010.

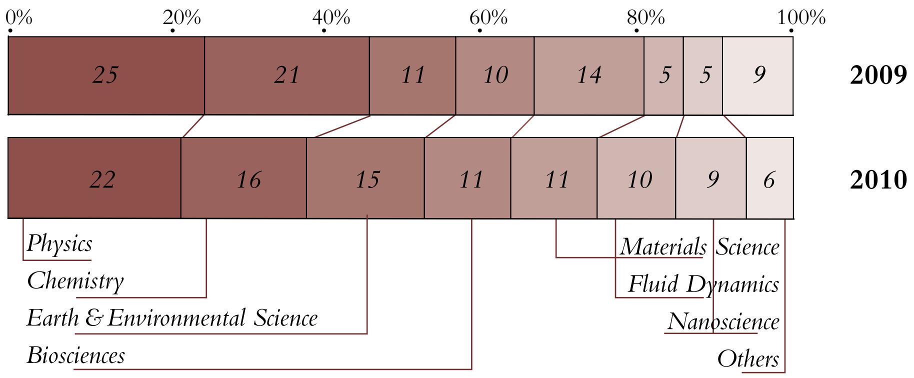
The usage by scientific field has largely remained unchanged in 2010, with most of the CPU hours consumed by projects in the domains of physics, chemistry, earth and environmental sciences.

From 2009 to 2010 there has been a reduction of large jobs (>8192 cores). The statistical data for 2009 is based on the first 6 months of operation where a special call for 'New High-Impact and Early User Projects' has been issued. Statistical data for 2010 corresponds to the normal usage pattern. The job size in cores is computed on the total of CPU hours per job size.

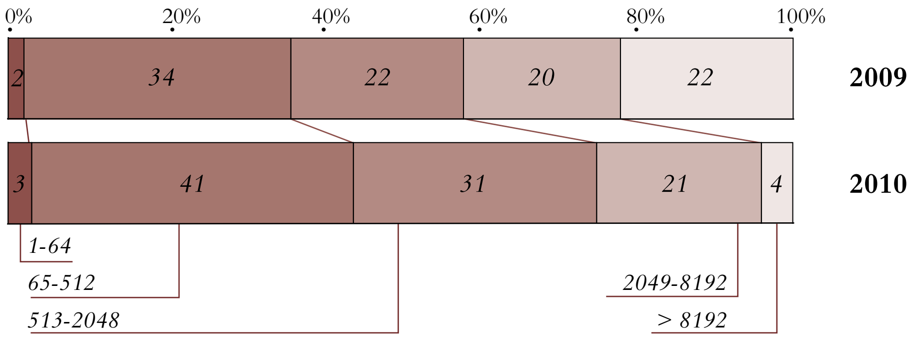
Usage by Institution



Usage by Research Field



Job Size in Cores



Abstracts of the 10 Largest Projects

Regional Climate Modelling on European to Alpine Scales

Christoph Schär, ETH Zurich (Earth & Environmental Science, 14.0 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 of small-scale processes and physical feedback mechanisms that shape the European and Alpine climate.

Numerical Lattice Gauge Theory with a Symmetry Constrained Monte Carlo

Leonardo Giusti, CERN (Physics, 9.0 Mio CPU h) - The self-coupling of the gauge field in Yang–Mills theories suggests the existence of glueballs, bound states of gluons. The long term goal of this project is to provide theoretically solid evidence of their existence in the SU(3) theory, and a precise determination of the mass and multiplicity of the lightest ones which are odd under parity and/or charge-conjugation. The value of the mass of the lightest parity-odd glueball is also of absolute phenomenological interest given the disagreement among the various experimental and theoretical findings.

Low Viscosity Rotating Flows and Magnetic Field Generation in Earth's Core

Andrew Jackson, ETH Zurich (Earth & Environmental Science, 8.7 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 occurs when rotation and magnetic effects dominate and the force balance and viscosity play only a minor role.

Numerical Simulation of Transitional, Turbulent and Multiphase Flow

Leonhard Kleiser, ETH Zurich (Fluid Dynamics, 8.0 Mio CPU h) - Transitional, turbulent and multiphase flows are of interest to a large number of technical applications, from biomedical research, to geophysical research and many other fields of science. High-fidelity simulations of such flows require sophisticated numerical methods, efficient algorithms and high-performance computing platforms. We develop such simulation codes and apply them to a variety of flow problems. The objective is to gain new insight into the physics of these flows.

Atomistic Simulations of Nanostructures

Stefan Goedecker, University of Basel (Nanoscience, 6.0 Mio CPU h) - The field of nanosciences still has many unanswered basic questions. In many cases these questions are related to uncertainties about the structure of the nano-systems. New insights into nano-systems can also lead to new technological breakthroughs in fields such as catalysis, energy storage, information storage and medicine. New theoretical tools for the structure determination of nano-systems have been developed that can help to answer both fundamental and applied questions. The BigDFT density functional code is a highly optimised parallel code, stable and accurate, aimed at the treatment of nano-systems.

Study of Land-Atmosphere Intercation over Complex Terrain by Large Eddy Simulation

Marc Parlange, EPF Lausanne (Earth & Environmental Science, 5.0 Mio CPU h) – This proposal will enable to continue and expand our existing and successful work in the large eddy simulation (LES) of atmospheric boundary layer (ABL). LES has become an important tool for investigating micro-scale turbulent transport phenomena in ABL since 1990. A development of the existing computer code (EPFL-LES) will allow the simulations of larger scale problems with higher resolution, to incorporate a wider range of subgrid scale models and scalar transport equations, and to improve the implementation of immersed boundary method.

ORB5-Turbulence

Laurent Villard, EPF Lausanne (Physics, 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.

The Old Stellar Population in Clusters of Galaxies: from Globular Clusters to Red Ellipticals

George Lake, University of Zurich (Astronomy, 5.0 Mio CPU h) – The objective of this project is to run a series of high-resolution N-body and hydrodynamical simulations of large clusters, to produce a representative statistical sample of these extreme objects. The stellar population contained in the giant elliptical galaxies and hundreds of satellites will be followed in the simulations. The modelling is based on the standard physics of galaxy formation (cooling, star formation, radiative and thermal stellar feedback), but new physical processes that control star formation in massive elliptical galaxies will also be explored. All simulations will be run using the RAMSES code.

Role of Anthropologic Versus Natural Forcing on Decadal Scales in Global Climate Models

Ulrike Lohmann, ETH Zurich (Earth & Environmental Science, 4.9 Mio CPU h) – The overarching objectives of this global climate modelling work are: to increase the understanding of anthropogenic versus natural forcings on global dimming and brightening using transient simulations; to further improve the representation of aerosol-cloud interactions in the ECHAM5 GCM; and to investigate if aerosols have an influence on the strength of hurricanes. The most powerful tools to investigate the potential impact of human activities on the Earth's climate are three-dimensional numerical models of the global climate system. The emphasis is on the simulation of past and future climate changes using ECHAM5-HAM.

Applications of Hybrid Functionals

Joost VandeVondele, University of Zurich (Chemistry, 4.5 Mio CPU h) – A recent breakthrough in the development of the CP2K program is the implementation of massively parallel Hartree-Fock exchange for the condensed phase. Therefore, extensive molecular dynamics simulations based on hybrid density functionals have become possible. This new technique will be applied to two challenging problems that are beyond the reach of standard local density functionals (GGAs). The first is related to the electronic structure of dye sensitised solar cells (DSSC). The second is related to the aqueous chemistry of radicals, and in particular the hydroxyl radical.

List of Projects by Institution

CERN

Numerical lattice gauge theory with a symmetry constrained Monte Carlo, Leonardo Giusti (Physics, 9.0 Mio CPU h)

EMPA

Regional scale impacts of changing anthropogenic emissions on aerosols and climate, Dominik Brunner (Earth & Environmental Science, 0.4 Mio CPU h)

Bottom-up design of graphene-like nanostructures at surfaces using ab initio simulations, Daniele Passerone (Nanoscience, 2.6 Mio CPU h)

EPF Lausanne

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

Quantum chemical study of contaminant oxidation reactions in acquatic systems, Samuel Arey (Chemistry, 1.6 Mio CPU h)

Integrated modelling of ion cyclotron heated plasmas, Anthony Cooper (Physics, 2.6 Mio CPU h)

Cardiovascular simulations: sensitivity to meddling, discretisation parameters, and patient specific geometries, Simone Deparis (Mathematics, 0.3 Mio CPU h)

Molecular dynamics simulations of DNA minicircles, John Maddocks (Biosciences, 2.0 Mio CPU h)

Study of land-atmosphere interaction over complex terrain by large eddy simulation, Marc Parlange (Earth & Environmental Science, 5.0 Mio CPU h)

Atomic scale modelling at semiconductor-oxide interfaces, Alfredo Pasquarello (Materials Science, 2.5 Mio CPU h)

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

ORB5-Turbulence, Laurent Villard (Physics, 5.0 Mio CPU h)

ETH Zurich

Multi-level micro-finite element analysis for human bone structures, Peter Arbenz (Computer Sciences, 0.6 Mio CPU h)

Uncovering the nature of chemical reactivity of nano-sized materials and environmental catalysts, Alfons Baiker (Materials Science, 1.2 Mio CPU h)

Metadynamics study of protein-protein binding mechanisms, Alessandro Barducci (Biosciences, 1.5 Mio CPU h)

Chemistry-Climate interactions since the pre-industrial time, Isabelle Bey (Earth & Environmental Science, 1.2 Mio CPU h)

Development of dynamic rupture models to study the physics of earthquakes and near-source ground motion, Luis Dalguer (Earth & Environmental Science, 3.2 Mio CPU h)

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

Direct numerical simulations of reactive flows, Christos Frouzakis (Mechanical Engineering, 4.5 Mio CPU h)

Heat transfer in nanochannel flow: a molecular dynamics study, Ming Hu (Nanoscience, 3.0 Mio CPU h)

Low viscosity rotating flows and magnetic field generation in earth's core, Andrew Jackson (Earth & Environmental Science, 8.7 Mio CPU h)

Microscopic origins of complex behaviour in carbon and sodium, Rustam Khaliullin (Materials Science, 2.7 Mio CPU h)

Numerical simulation of transitional, turbulent and multiphase flow, Leonhard Kleiser (Fluid Dynamics, 8.0 Mio CPU h)

Multiphysics simulations using multiscale particle methods: I. particle methods and parallel computing. II. biology, nanotechnology, fluids and their interfaces, Petros Koumoutsakos (Earth & Environmental Science, 3.8 Mio CPU h)

Aircraft wake evolutionary optimization, Petros Koumoutsakos (Fluid Dynamics, 1.5 Mio CPU h)

Investigation of the binding mode of novel adenosine deaminase inhibitors and development of new methodologies for the calculation of the ligand binding free energy, Vittorio Limongelli (Biosciences, 1.5 Mio CPU h)

Role of anthropologic versus natural forcing on decadal scales in global climate models, Ulrike Lohmann (Earth & Environmental Science, 4.9 Mio CPU h)

Ab-initio study of the decomposition mechanism of complex hybrides for hydrogen storage, Michele Parrinello (Materials Science, 1.0 Mio CPU h)

Conformational dynamics of the RET kinase domain by means of metadynamics simulation, Michele Parrinello (Biosciences, 1.5 Mio CPU h)

Ab-initio study of amorphization and crystallization processes in phase change materials, Sebastiano Caravati (Materials Science, 0.8 Mio CPU h)

Computational materials science for energy conversion, Clotilde Cucinotta (Materials Science, 2.4 Mio CPU h)

Ab-initio investigation of nucleation, crystallisation and aggregation of flame-made materials, Gianluca Santarossa (Nanoscience, 0.5 Mio CPU h)

Regional climate modelling on European to Alpine scales, Christoph Schär (Earth & Environmental Science, 14.0 Mio CPU h)

Land-climate interactions: modelling and analysis, Sonia Seneviratne (Earth & Environmental Science, 1.3 Mio CPU h)

Understanding local fluctuations of proteins: comparison to hydrogen-deuterium exchange experiments, Pär Söderhjelm (Chemistry, 1.7 Mio CPU h)

Simulating fractional quantum Hall devices, Matthias Troyer (Physics, 2.0 Mio CPU h)

Multi-level analyses of age-related bone loss, and its consequences for bone strenght and implant stability, Harry Van Lenthe (Biomedical Engineering, 1.8 Mio CPU h)

Simulating integrin junctions under tension: from the extracellular matrix to the cyto-skeleton, Viola Vogel (Biosciences, 4.0 Mio CPU h)

Paul Scherrer Institute

Simulation of actinide materials, Matthias Krack (Materials Science, 3.4 Mio CPU h)

Nano-optics for advanced photocathodes and bean dynamics for swissFEL and PSI cyclotron, Benedikt Oswald (Physics, 0.5 Mio CPU h)

SUPSI

Multiscale computational study of linear and hyperbranched polymers for biomedical appli-cations, Andrea Danani (Chemistry, 0.5 Mio CPU h)

University of Basel

Structure, dynamics, and function of membrane transport proteins, Simon Bernèche (Biosciences, 2.0 Mio CPU h)

Atomistic simulations of nanostructures, Stefan Goedecker (Nanoscience, 6.0 Mio CPU h)

Neutrino transport in stellar astrophysics, Matthias Liebendörfer (Astronomy, 3.0 Mio CPU h)

Influence of dimerization on allostery and ligand migration in multidomain proteins, Markus Meuwly (Chemistry, 0.3 Mio CPU h)

University of Bern

Chemical climate change during the past 400 years (CCC400), Stefan Brönnimann (Earth & Environmental Science, 1.8 Mio CPU h)

Computational studies on laccase from trametes versicolor: redox properties and interactions with surfaces, Michele Cascella (Biosciences, 1.0 Mio CPU h)

CARBOFEED: modelling CARBOn cycle climate FEEDbacks, Fortunat Joos (Earth & Environmental Science, 0.7 Mio CPU h)

Modelling and reconstruction of North Atlantic climate system variability (MONALISA III), Christoph Raible (Earth & Environmental Science, 1.2 Mio CPU h)

University of Geneva

Photophysics and photochemistry of transition metal compounds: theoretical approaches, Andreas Hauser (Chemistry, 3.0 Mio CPU h)

Molecular modelling of multifunctional supramolecular assemblies, Jiri Mareda (Chemistry, 0.1 Mio CPU h)

University of Zurich

Boron nitride nanomesh for guided self-assembly of molecular arrays in solution, Jürg Hutter (Chemistry, 4.0 Mio CPU h)

CP2k program development, Jürg Hutter (Chemistry, 1.0 Mio CPU h)

The old stellar population in clusters of galaxies: From globular clusters to red ellipticals, George Lake (Astronomy, 5.0 Mio CPU h)

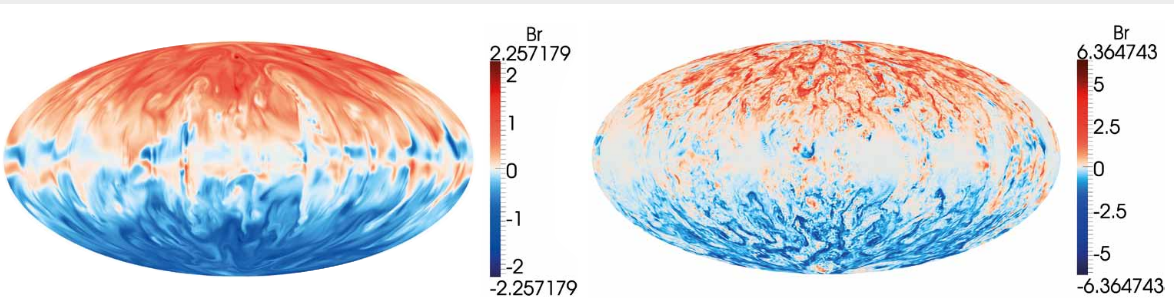
Connecting mergers of supermassive black holes and their formation during hierarchical galaxy assembly, Lucio Mayer (Astronomy, 1.6 Mio CPU h)

Applications of hybrid functionals, Joost VandeVondele (Chemistry, 4.5 Mio CPU h)

Improving molecular functionalities for opto-electronics, Laura Zoppi (Materials Science, 0.6 Mio CPU h)

Scientific Visualisation Gallery

Magnetic field (radial component) at the core-mantle boundary of a high resolution simulation of the earth dynamo. Heat transport and the magnetohydrodynamics equations are solved in a spherical shell geometry using a pseudo-spectral method (spherical harmonics to degree 256 and finite difference in radius with 512 grid points); courtesy of Andrey Sheyko, ETH Zurich.



Supercomputers Demonstrate How Bacteria Infect Wounds

On the research work of Viola Vogel, professor in the Department of Materials, ETH Zurich

Bacteria with 'Force Sensors'

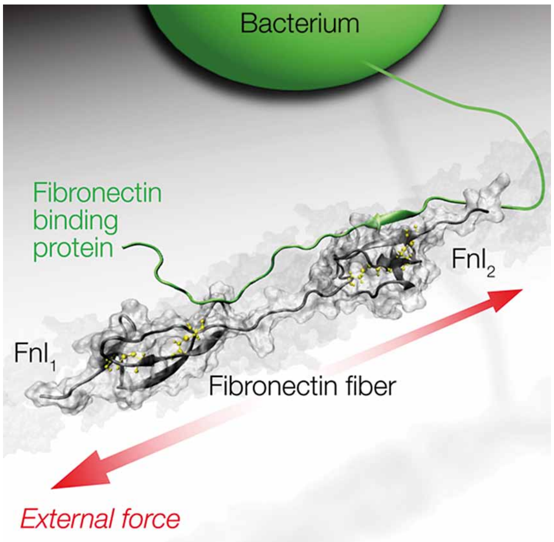
Computer simulations enable scientists to show the operation mode of connective tissue fibres. If the fibres are severed and slackened by a cut, the bacterial adhesion molecules recognise this and attach themselves, which enables them to cause infections.

The protein fibronectin dissolved in the blood plays an important part in wound healing. It is woven into a network of fibres by the cells and initiates the first step in repairing a wound. Cells in living organisms continuously pull on these fibers. Consequently the fibronectin in an intact connective tissue environment is frequently stretched. If one cuts oneself, or enzymatic processes in an inflammation degrade tissue, the tension on the fibronectin fibres is lost.

Binding Sites strung Together Like Pearls

Fibronectin is structured like a necklace of about 50 'pearls', and many of these 'pearls' expose a binding site for molecules that are important in connective tissues, e.g. for collagens or cells. At the end of the molecule there are five 'pearls' where bacteria can also bind to one of the 'pearls' via certain segments of the long protein threads that decorate bacterial surfaces. Bacteria such as Staphylococcus aureus, the dreaded hospital germ and the typical pathogen of abscesses and boils, can specifically recognise fibronectin and thus infect wounds.

The research group led by Viola Vogel, professor of Biologically Oriented Materials, has now studied how the tensile forces by which cells stretch connective tissue fibres affect the interaction between bacteria and fibronectin. The scientists did this by using the supercomputer Monte Rosa of CSCS to simulate how the structure of the complex between fibronectin and



Bacteria can adhere to fibronectin fibres in connective tissues by using their adhesion proteins (green) to bind to certain 'recognition sites' in the fibre (FnI1 and FnI2, grey). Computer models show how mechanical stretching of the fibronectin (red arrows) caused by cells leads to a partial detachment of the bacterial protein (illustration not to scale).

the bacterial protein molecule changes when a tensile force acts on fibronectin. Vogel's team wanted to find out whether the bacterial segments act like a kind of clamp during the docking process, thus preventing the fibronectin from stretching. However, the simulation shows an entirely different picture: although the bacterial adhesin initially binds to many sites on fibronectin, the structural match is destroyed as soon as tensile forces stretch fibronectin, and the bond is destroyed. 'The models give us a high-resolution picture of how the bond breaks. We would never see that using a microscope', says Vogel. However, they also show experimentally that bacterial adhesins bind less well to stretched fibronectin fibres. The scientists conclude from this that the bacterial adhesion molecules which bacteria use to stick to tissue fibres are able to detect the physical state of the fibronectin molecule.

Verified in the Laboratory

Vogel carries out research into the way mechanical factors modify the well-known classical equilibrium structures in biology, such as how stretching and pulling molecules changes the way they function. 'However, since there are still no experimental tools with which we can determine structures that are not in equilibrium, we need to use supercomputers to calculate this', says Vogel. Her team's latest discovery is an impressive example of the success and usefulness of computer-aided sciences. The simulation enabled the researchers to discover this phenomena, was later be verified experimentally.

They succeeded in this with the help of an optical method developed by the scientist and her team a few years ago, which makes the degree of stretching of the fibronectin visible through colour changes. However,

Viola Vogel

since it is difficult to carry out binding studies in tissues, the researchers 'built' a special experimental set-up in which they extracted fibronectin fibres and stretched them. They were able to show that the processes occurring with stretched fibronectin fibres in the presence of bacterial adhesion molecules are the same as those seen in the model.

The knowledge that the tiny bacterium can recognise the physical state of a protein and that the stretching process changes the adhesion is essential to an understanding of biochemical processes. It involves one of the many interactions that are mechano-regulated. Furthermore, only small elements of the entire adhesion region have been studied – new computing time has already been requested at CSCS.

Reference
Chabria M et al.: Stretching fibronectin fibres disrupts binding of bacterial adhesins by physically destroying an epitope, Nature Communications (2010). doi:10.1038/ncomms1135

Car-Parrinello Method Turns 25

On 25 years of scientific computing by Michele Parrinello, professor for Computational Science, ETH Zurich

'Sometimes, Ignorance is Bliss'

25 years ago two budding scientists, Roberto Car and Michele Parrinello, used their expert knowledge, coupled with enthusiasm and a healthy dose of naivety, to develop a groundbreaking method for computer simulation.

During the 1980s, the intellectual environment on the Adriatic – which included the International Centre for Theoretical Physics (ICPT) and the Scuola Internazionale Superiore di Studi Avanzati (SISSA) in Trieste, for instance – was just the place to research freely and easily. This is where the scientific curiosity of the two professors, coupled with a healthy dose of naivety, came together 25 years ago. These circumstances were major factors in the development of the Car-Parrinello method named after them. The method fundamentally changed the approach to simulations and thus supported both theory and experimentation. Whether in materials science, biology or geosciences, simulations are necessary when experiments are not feasible, either because they are too dangerous or it is impossible to recreate the necessary conditions.

Understanding Material

The two physicists combined their respective specialisations in the method. During his time at SISSA, inspired by a sojourn in the USA, Parrinello traded his paper-and-pencil studies for the computer. With its help, he wanted to describe the material that surrounds us through the movement of the atoms, using classical molecular dynamics. For this to work, however, computers using particular codes and algorithms have to relentlessly solve quantum mechanical equations of varying complexity.

In the 1980s, the dynamics of the molecules was calculated empirically, even though it was theoretically possible to calculate in an approximate manner the actual quantum mechanical molecule conditions 'ab initio', i.e. without using any concrete measurements, by applying the so-called Born-Oppenheimer approximation (BO approximation). The BO approximation method, however, was time-consuming and needed a computer capacity that was not available at the time: in the 1980s the computing power of a 'supercomputer' was a few gigaflops; nowadays, a conventional computer's processor can manage up to 25 gigaflops (25 billion computer operations per second).

Actual Image with 'Ab Initio'

However, the only correct way to model the actual forces exerted on an atom is 'ab initio'. This means that to illustrate how chemical compounds break up and new ones form, the structure of the electrons, their energy state, has to be calculated for every position of the ion with a quantum mechanical equation. Calculating the electron structure was Roberto Car's specialist field.

'Sometimes, ignorance is bliss', jokes Parrinello. Car and Parrinello saw beyond the opinions of the experts, who dismissed their idea of calculating both the molecular dynamics and the electron structure in one go as impossible. That meant combining the BO approximation with so-called quantum mechanical Density Functional Theory, which determines the structure of the electrons. 'We knew a bit about each other's field, but nowhere near enough. Otherwise we wouldn't have thought it possible to combine both in one approach', recalls Parrinello.

Tricks of the Trade

For Parrinello, the starting point was to describe the element silicon. Under certain temperature and pressure conditions, silicon displays the characteristics of both metals and non-metals, and is an important semi-conductor. As these changes brought on by chemical reactions could not be determined with the BO approximation and the computer capacities that were available at the time, the two scientists resorted to a trick: they expanded the so-called Lagrange function for describing a physical system so that not every position of the ion and the forces exerted had to be calculated one step at a time. Using the Car-Parrinello method, the forces have to be determined once at the beginning of the simulation, while later the ion propagates itself like a wave with its electrons. The electron follows the ion quasi-adiabatically, without an exchange with its environment.

And so the first quantum mechanical calculation of the molecular state – 'ab initio' – was successful. The Car-Parrinello method has been developed and honed for different applications over the years and has produced a lot of important information in various research disciplines. For instance, the method was used to show that the bottom 150 kilometres of the Earth's mantle did not – as had always been assumed – consist of the mineral perovskite, but rather a modified, layered variety. The properties of the new mineral were able to explain conclusively the seismic discontinuity of this field for the first time.

Michele Parrinello

Method with a Long-Term Effect

Over the years Car and Parrinello have won numerous prestigious awards for their development, including the Dirac Medal in 2009.

Today, with the leaps and bounds that have been made in computer technology over the last decade, the method is no longer as essential as it was 20 years ago; however, it is still effective in research. Alessandro Curioni, the head of the Computational Science Group at the IBM Research Lab in Rüschlikon, who uses the method and had a hand in developing it further together with Parrinello and other researchers, stresses the importance of the Car-Parrinello method for molecular dynamics.

An important side effect was also to see how Car and Parrinello's little 'trick' solved a large problem, shaping the scientists' mode of thinking and opening up new horizons for them. 'In the long run, the many ideas the Car-Parrinello method has generated for new quantum mechanical approaches to solving a problem will probably be even more important than the method itself', says Curioni.

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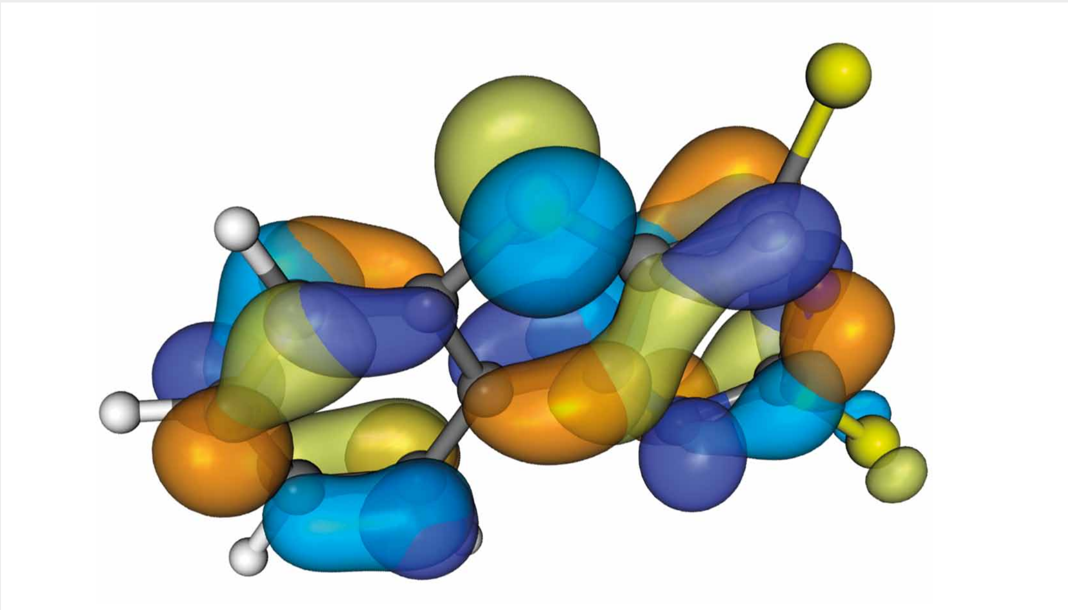
Scientific Visualisation Gallery

Visualisation of molecular orbitals..



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Andreas Adelmann, Paul Scherrer Institute

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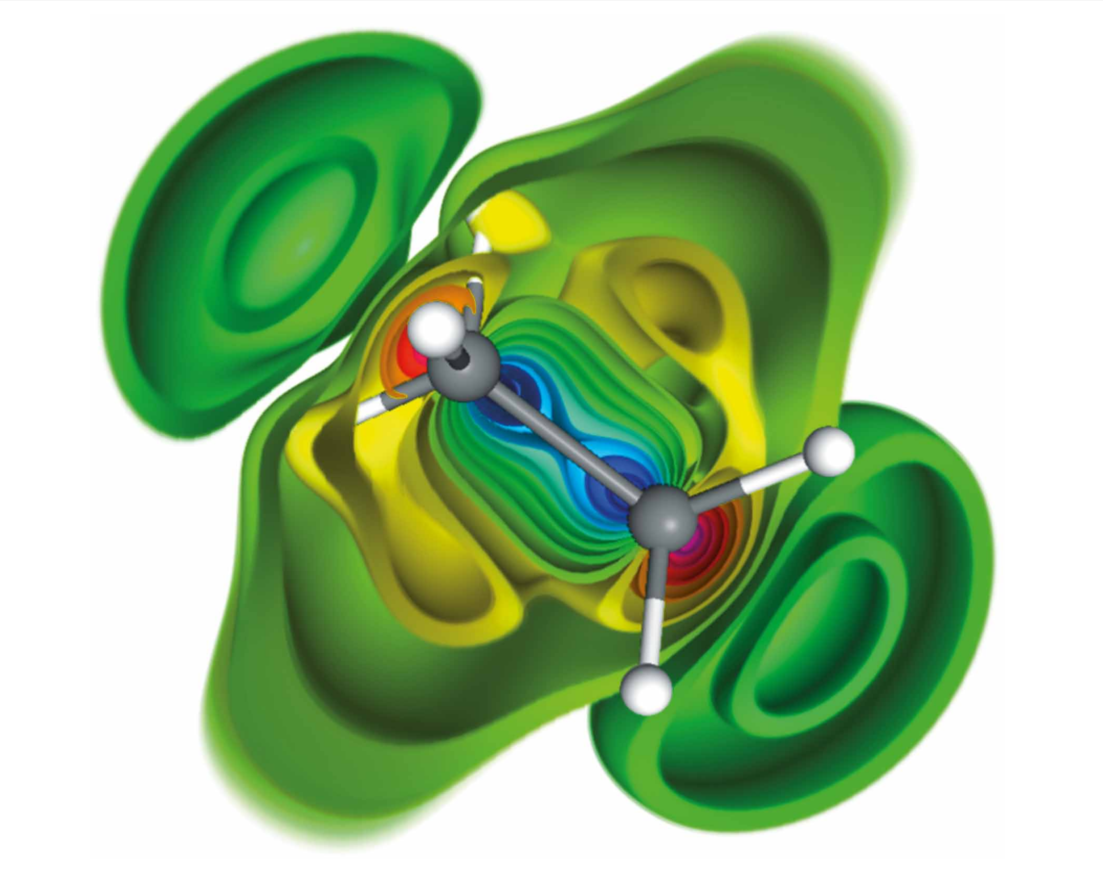
Scientific Visualisation Gallery

Visualisation of molecular orbitals.



HP2C Initiative

HP2C Completes its First Year

The High Performance and High Productivity Computing (HP2C) initiative completed its first year of funding in December 2010. The goal of the initiative is being turned into reality: a number of scientific research teams are porting state-of-the-art applications to emerging architectures, allowing them to look at much higher problem resolutions and complexities in the long term, thus enabling new science. HP2C first year objectives were exceeded remarkably.

In mid-2009 the call for proposals went out, then answered by 17 teams. They represented the gamut of science, from fluid dynamics to molecular dynamics, astronomy to seismology, evolutionary biology to meteorology. Their submissions went through a demanding review process carried out by the HP2C committee with the help of internationally recognized reviewers.

In January 2010 eight teams had just received funding. Three more projects were accepted in mid-2010 and joined the fray. They all moved quickly to populate open positions with computational scientists from around the world.

These teams are now up to speed and are taking concrete steps to enable new science. In late 2010, there was a second HP2C call for projects within the realm of 'Risk Analysis for Global Challenges'. As of December 2010, two project proposals were in the review process.

First Application Snapshots

The first eleven teams all delivered an initial 'snapshot' of their application. In some cases, this benchmark was no more than an initial implementation running on traditional platforms. However, several groups went far beyond this basic requirement. For example, one group delivered a spectral element code capable of running on GPU with excellent performance. Another group has delivered a skeleton version of a spin model, thats sparse matrix-vector multiplication already scale to thousands of cores.

HP2C advanced prototype systems have also evolved rapidly. At CSCS, the GPU-cluster Eiger was installed in early 2010, and serves simultaneously as a visualisation cluster and an experimental computational engine with NVIDIA GTX 285, Tesla C1070, C2070 and M2070 GPUs. The even more advanced 'Fuji' platform with 8 Tesla C2070 GPUs is used by the Scientific Computing Research (SCR) group of CSCS to evaluate new software.

Benefit for Swiss Science

Thomas Schulthess initiated HP2C together with Piero Martinoli, President of the Università della Svizzera italiana. They maintain that the benefits of HP2C are long-term: the emphasis is on revision and development of algorithms, not, at this point, raw computing. The success should be seen when the HP2C applications produce new science on the next round of production computers, such as the one to be installed in the new CSCS facility in Lugano in the 2012-2013 time frame. Thanks to HP2C, the Swiss academic community is well-positioned to reap the maximum benefit from the wave of new computing technologies.

Cross-Cutting Topics

While the HP2C teams are largely autonomous, they are linked together through 'cross-cutting' topics – common algorithmic motifs which recur in multiple projects. The SCR group as well as the Institute for Computational Science (ICS) at USI try to exploit such commonality by concentrating on individual motifs. For example, SCR has launched a research project to create a domain specific language for stencil-based problems which can generate code for both CPUs and GPUs. Together with ICS, they have embarked on a project to extend NVIDIA's CUDA Sparse (CUSP) library for GPUs with a new solver and preconditioner. ICS is researching parallel time integration methods, while SCR is looking into parallel I/O libraries and techniques for in-situ visualization.

Project List

Large Scale Density Functional Electronic Structure Calculations in a Systematic Wavelet Basis Set; Stefan Goedecker, University of Basel

HPC for Cardiovascular System Simulations; Alfio Quarteroni, EPF Lausanne

Regional Climate and Weather Modelling on the Next Generations High-Performance Computers: Towards Cloud-Resolving Simulations; Isabelle Bey, ETH Zurich

Computational Cosmology on the Petascale; George Lake, University of Zurich

New Frontiers in ab initio Molecular Dynamics; Jürg Hutter, University of Zurich

Numerical Modelling of the Ear: Towards the Building of New Hearing Devices; Bastien Chopard, University of Geneva

Advanced Gyrokinetic Numerical Simulations of Turbulence in Fusion Plasmas; Laurent Villard, EPF Lausanne

Modern Algorithms for Quantum Interacting Systems; Thierry Giamarchi, University of Geneva

Petaquake - Large-Scale Parallel Nonlinear Optimization for High Resolution 3D-Seismic Imaging; Olaf Schenk, University of Basel

Selectome - Looking for Darwinian Evolution in the Tree of Life; Marc Robinson-Rechavi, University of Lausanne

Productive 3D Models of Stellar Explosions; Matthias Liebendörfer, University of Basel

Large-Scale Parallel Nonlinear Optimisation for High Resolution 3D-Seismic Imaging

An HP2C project under examination 'Large-Scale Parallel Nonlinear Optimisation for High Resolution 3D-Seismic Imaging'

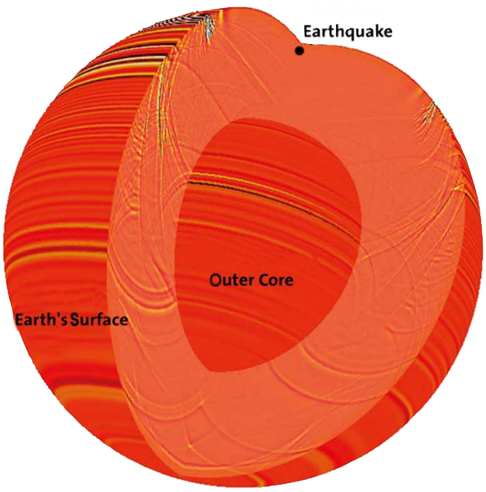
Interdisciplinary Look Inside the Earth's Interior

Swiss seismologists are developing in the HP2C platform optimised scientific simulations for high-performance computers.

What is the exact structure of the Earth's interior? What are the processes that take place there? Where and how do earthquakes originate? These are some of the central questions concerning our planet that we have not yet been able to answer with certainty. A view into the Earth's interior similar to computer tomography for a human being could provide these answers, thus helping to improve seismic risk maps. This would be an important basis for assessing the risk of the locations of nuclear power plants or hospitals in Switzerland for example.

Tomographic Recording

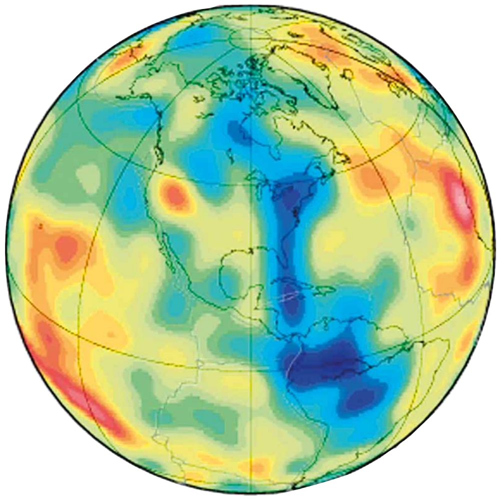
Although today's supercomputers can already perform a quadrillion calculation steps per second, the computers and programs for modelling are not sufficiently coordinated to compute high-resolution complex images of the Earth's interior in a reasonable period of time. Compared to the human body, screening the Earth is a difficult endeavour because earthquakes occur irregularly and seismographs are spread unevenly across the Earth's surface. Also, unlike the X-rays used in computed tomography, there are large portions of the Earth's interior that seismic waves do not penetrate. Someday, however, the 'Petaquake' project could provide a similar insight into the Earth as into the human body. Scientists from the Institute of Geophysics (www.geophysics.ethz.ch) at ETH Zurich under the supervision of Domenico Giardini, have joined forces with mathematicians and computer scientists from the University of Basel (www.unibas.ch) under the supervision of Helmar Burkhart, Marcus Grote and Olaf Schenk to carry out this project.



A snapshot of seismic wave propagation through the three-dimensional Earth 20 minutes after an earthquake. The hypothetical earthquake has been placed at the northpole. Such simulations are numerically possible, but for realistic 3D models and high resolution (more than 100 Mio grid points) this is only possible on supercomputers.

Images courtesy of Institute of Geophysics, ETH Zurich

Seismic tomography helps to understand the dynamics of the Earth: at a depth of about 1 300 km in the mantle, it reveals a long and narrow region (shown here in blue) where seismic waves propagate at higher speed. Geophysicists interpret this as an ancient tectonic plate, that after getting too cold and heavy has been slowly (tens of millions of years) sunk deep into the mantle.



'Petaquake' is one of the promising projects launched by the Swiss platform for High-Performance and High-Productivity Computing (HP2C – www.hp2c.ch) in 2009. The objective of the HP2C platform is to use interdisciplinary cooperation between hardware manufacturers, computer scientists, mathematicians and end users to develop special methods and algorithms for high-performance computers by 2013, which will allow complex simulations to be completed in just a few hours in future instead of months or even years.

Visualising the Earth's Interior

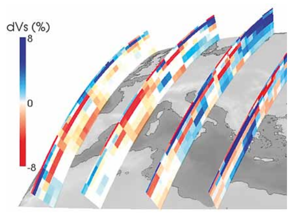
The seismic waves triggered by an earthquake travel through the Earth at different speeds depending on the material they penetrate. Our knowledge of the structure of the Earth's interior is based primarily on the modelling of these seismic waves, which is carried out based on certain assumptions about the Earth's interior. 'We made many findings from assuming that seismic waves behave in the same way as optical waves', says Lapo Boschi, a senior assistant lecturer to Giardini. However, he said, this is only an approximation of how things work in practice. The aim of Petaquake is to compute high-resolution tomographic images of processes at scales of tens of kilometres. For Boschi, the most exciting aspect of the project is obtaining such images through improved algorithms that take adequate account of factors such as wave physics.

Together with the mathematicians and computer engineers, Giardini's group – which also includes the two senior assistant lecturers Tarje Nissen-Meyer and Luis Dalguer – developed numerical methods that describe both the propagation of the seismic waves (solution to the forward problem) and new tomographic models using real seismic data (solution to the inversion problem). 'Taking into account the full wave character, resolving relevant geophysical processes with the help of supercomputers as well as the flood of high-quality new data all contribute to an exciting phase in modern seismology', says Nissen-Meyer. Among other things, he would like to use the new models to examine the dynamics of the Earth's mantle and magnetic field.

Safety of Nuclear Power Plant Locations

The new algorithms are also used for research into earthquakes, in particular for assessing risk. Luis Dalguer is using the new models to research the dynamics and the behaviour of the ruptures zones where earthquakes occur. For example, Petaquake shall facilitate a local, small-scale, three-dimensional resolution to show in detail how rupture zones develop, where they are initiated and why and when they end. The results shall contribute to develop a model for ground motion resulting from the rupture process. According to the researchers, this is relevant for assessing the safety of locations for nuclear power plants.

Since the evaluations of the PEGASOS project ('Probabilistische Erdbebengefährdungsanalyse für AKW-Standorte in der Schweiz', probabilistic seismic hazard analysis project for locations for nuclear power plants in Switzerland) were presented to the public in 2007, it has become clear that the seismic risk to nuclear power plants in Switzerland may have been underestimated. The assessment is based on extensive series of measurements carried out at locations around the world since the 1980s. These show that earthquake ground shaking could be stronger than previously assumed even in areas in which moderately large earthquakes are expected. This is why new methods for risk assessment are now focusing on the composition of the subsurface through which the seismic waves propagate: strong earthquakes near the rupture zone are simulated in order to reduce uncertainties in the assessments.



Seismologists analyse the recordings of earthquakes to determine how fast seismic waves propagate through the interior of the Earth. Similar to medical tomography, cross-sections of different parts of our planets are then visualized. Regions where waves are faster are shown here in blue, and correspond to the older, colder continental plates like the Eurasian 'shield'.

Supercomputers already opened up a whole new generation of earthquake research to seismologists around twenty years ago. 'With the 3D-models, we are even able to visualize the mechanics and physics behind the propagation of the rupture zones', says Dalguer.

Key Components for Success

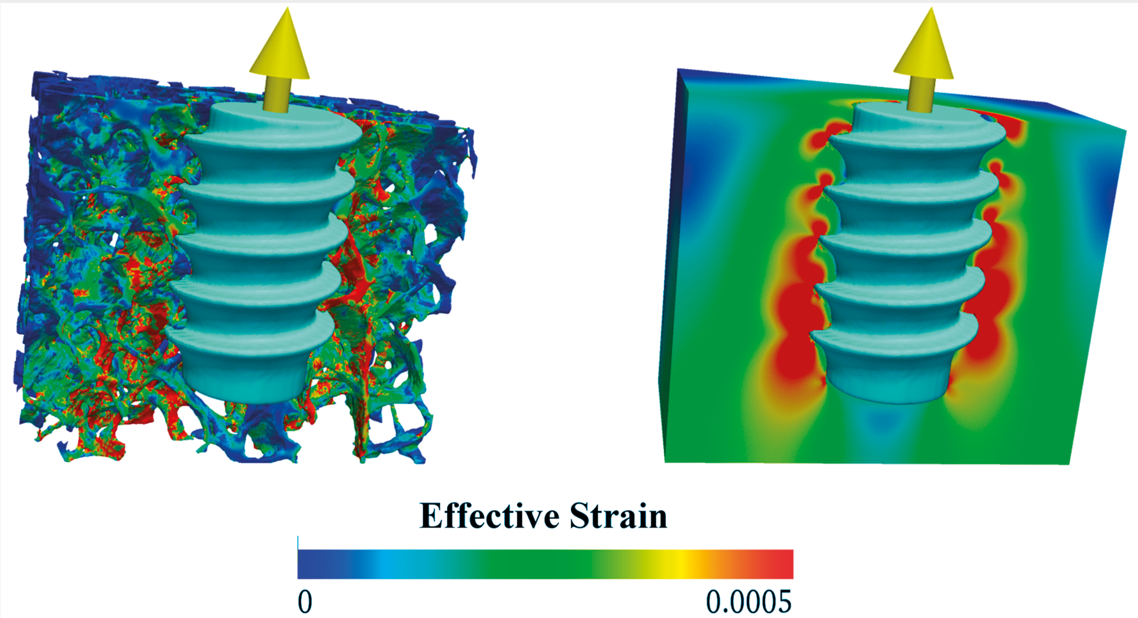
Marcus Grote and Olaf Schenk deliver the hardware-related algorithms for the project which tell the computer the program workflow for generating a simulation that is as close to reality as possible. The mathematic modelling is the 'language' used for formal communication between all those involved. This is a language that covers the entire physics of an elastic wave equation. In order to obtain a realistic image, the scientists divide up the Earth using a flexible grid. Tetrahedra of different sizes make it possible to portray the space- and time-dependent wave propagation at defined intervals. They also had to develop a procedure that makes it possible to choose different time intervals at which the waves travel through a given area in neighbouring tetrahedra of different sizes.

For Marcus Grote, both of these procedures are key to the success of the project. 'The aim is now to optimize these components in such a way that they simulate the wave within a short period of time and satisfy the seismic wave equation exactly', says Olaf Schenk. If the simulated waves and the data recorded by the seismometer match, the penetrated medium can be described and the Earth's interior can be portrayed in a new three-dimensional model.

Marcus Grote sees the project as a catalyst: 'Normally it takes up to ten years from the time a new algorithm is presented at a conference until it is published and ultimately used by seismologists.' Grote and Schenk are specialized in numerical procedures for the simulation of wave phenomena on high-performance computers. In addition to their use in seismology, these can also be used in imaging procedures in medicine for example.

Scientific Visualisation Gallery

Strain distribution around an orthopedic screw in trabecular bone as simulated by micro-finite element analysis. A discrete material model (left) with resolved microarchitectural network (6.0 Mio elements) was compared with (right) a conventional continuum representation (22.6 Mio elements) by using a dedicated parallel micro-finite element solver. Courtesy of Institute for Biomechanics, ETH Zurich.



Facts & Figures

Finances

Expenditure

	CHF
Investments	8 417 349.30
Material/Goods/Services	3 155.45
Personnel	7 534 853.39
Payroll	5 904 741.80
Employer's contributions	904 151.70
Further education, travel, recruitment	725 959.89
Other Material Expenses	6 706 740.00
Floor space	366 807.42
Maintenance	1 582 194.49
Energy & Media	1 864 184.16
Administrative expenses	36 179.04
Hardware, software, services	1 321 347.72
Services & Remunerations	1 531 276.96
Other	4 750.21
Extraordinary Income/ Expenditures	73 861.15
Membership fees/Overhead	73 861.15

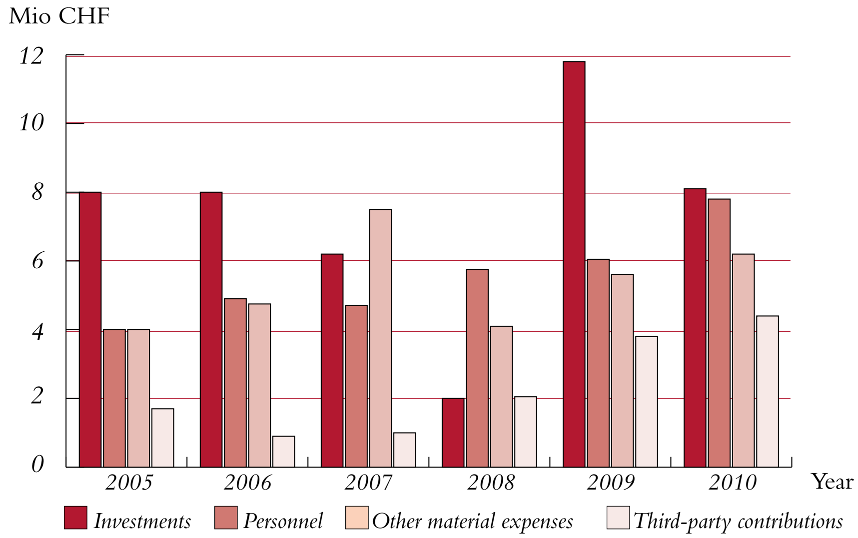
Income

	CHF
Basic Budget	14 926 000.00
Contribution ETH Zurich	14 330 000.00
Economic stabilisation measures	596 000.00
Third-party Contributions Projects	1 909 801.79
European projects	453 723.39
HP2C	1 456 078.40
Third-party Contributions Services	3 132 221.07
CHIPP	748 608.23
MeteoSwiss	1 218 750.00
PSI, Part II Upgrade Cray XT3	250 000.00
USI Upgrade Cray XE6	822 534.96
Other income	92 327.88

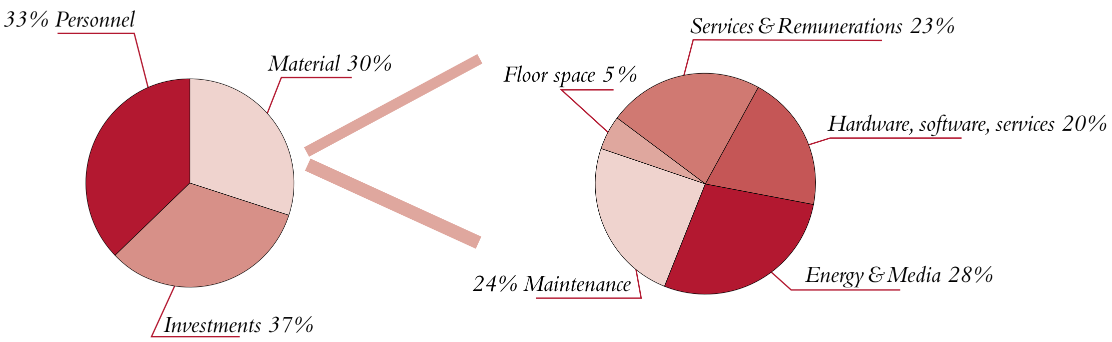
Expenses Total	**22 735 959.29**	**Income Total**	**19 968 022.86**
Balance			-2 767 936.43

The balance is rolled over to the 2011 budget.

Income and Expenditure Development



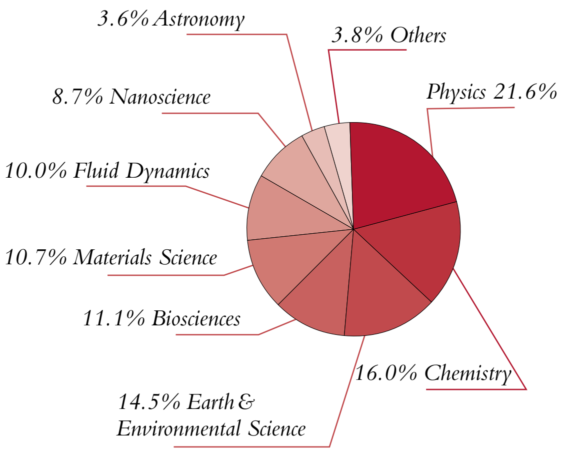
Expenditure Distribution



Usage Statistics

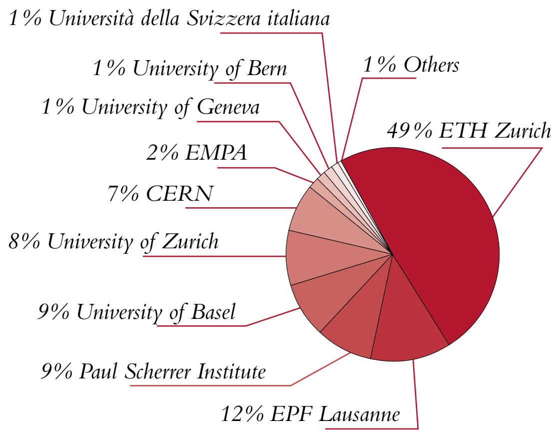
Usage by Research Field

Research Field	CPU h	%
Physics	36 385 226	21.6
Chemistry	26 965 176	16.0
Earth & Env. Science	24 413 331	14.5
Biosciences	18 589 203	11.1
Materials Science	17 913 569	10.7
Fluid Dynamics	16 859 772	10.0
Nanoscience	14 624 720	8.7
Astronomy	6 090 946	3.6
Mechanical Engineering	5 839 411	3.5
Computer Sciences	284 230	0.2
Mathematics	180 462	0.1
Economics	28 353	0.0
Total Usage	**168 174 399**	**100**

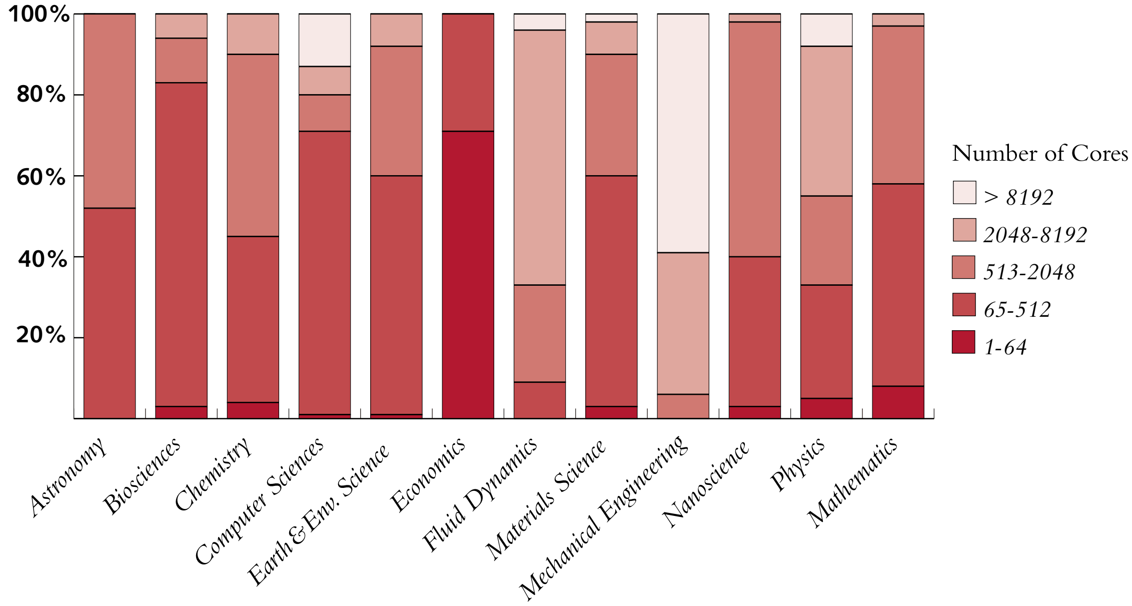


Usage by Institution

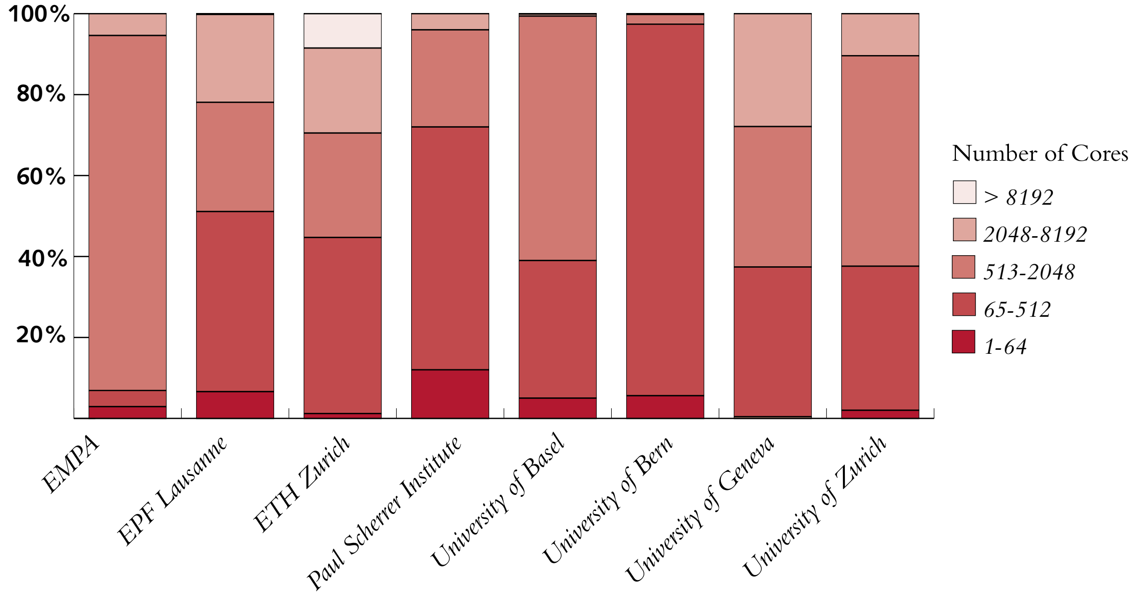
Institution	CPU h	%
ETH Zurich	82 765 628	49.2
EPF Lausanne	20 641 756	12.3
Paul Scherrer Institute	14 472 852	8.6
University of Basel	14 352 391	8.5
University of Zurich	13 861 571	8.2
CERN	11 868 282	7.1
EMPA	3 003 507	1.8
University of Geneva	2 598 801	1.5
University of Bern	2 102 468	1.3
Università della Svizzera italiana	767 682	0.5
Others	1 739 461	1.0
Total Usage	**168 174 399**	**100**



Job Size by Research Field



Job Size by Institution



Compute Infrastructure

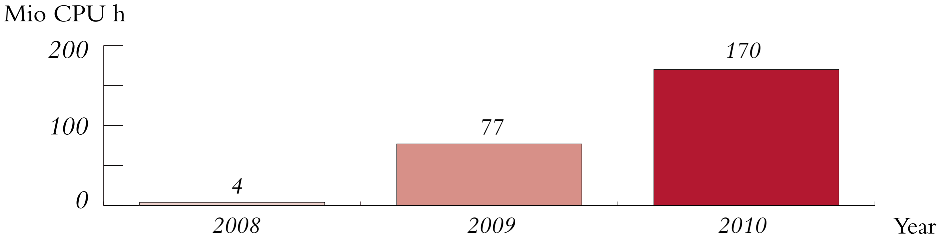
HPC Systems

Name	Supplier & Model	Installation / Upgrade	Usage / Customer	Capacitiy (h)	CPU Produced (h)	Availability (%)
Monte Rosa	Cray XT5	2009	National HPC Service	193 841 280	169 599 457	[2] 99.1
Piz Palü	Cray XE6	2010	R&D	37 002 240	[1]	[1]
Phoenix	Sun Cluster	2010	CHIPP (LHC Grid)	8 847 360	7 056 908	[3] 92.7
Eiger	Dalco Cluster	2010	R&D, visualisation	1 192 320	57 246	98.5
Piz Buin	Cray XT4	2006/2009	MeteoSwiss (Production)	9 110 400	3 635 311	98.5
Dole	Cray XT4	2006/2009	MeteoSwiss (Failover, R&D)	6 026 880	967 204	99.1
Fuji	Transtec Clu.	2010	R&D	[1]	[1]	[1]
Rigi	Sun Cluster	2007	MeteoSwiss & USI	911 040	553 349	99.4
Piz Julier	IBM x3850	2010	National HPC Service, R&D	[1]	[1]	[1]

Name	CPU Type	No. of Cores	Interconnect Type	Peak Performance (TFlops)	Interconnect Bandwidth (GB/s)
Monte Rosa	AMD Opteron 6 Cores 2.4 GHz	22 128	Cray Seastar2+	212.4	9.6
Piz Palü	AMD Opteron 12 Cores 2.1 GHz	4 224	Gemini	35.1	10.4
Phoenix	AMD Opteron 12 Cores 2.1 GHz + Intel 4 Cores 3.0 GHz	1 392	Infiniband 4x QDR	11.2	4.0
Eiger	AMD Opteron 6+12 Cores 2.2 GHz + Fermi & Tesla Nvidia GPU	276	Infiniband 4x QDR	10.2	4.0
Piz Buin	AMD Opteron 4 Cores 2.3 GHz	1 040	Cray Seastar	5.0	7.6
Dole	AMD Opteron 4 Cores 2.3 GHz	688	Cray Seastar	3.3	7.6
Fuji	Intel Xeon X5670 2.93 GHz + 4 Nvidia C2050 cards	60	Infiniband 4x DDR	0.7	4.0
Rigi	AMD Opteron 2 Cores 2.6 GHz	104	InfiniBand 4x QDR	0.5	1.6
Piz Julier	Intel Xeon E7540 2 GHz	48	Infiniband 4x DDR	0.4	1.6

[1] No statistical data available.
[2] The utilisation average of Monte Rosa was 87.5%.
[3] Availability of Phoenix also depends on external grid factors.

Evolution of CPU Usage



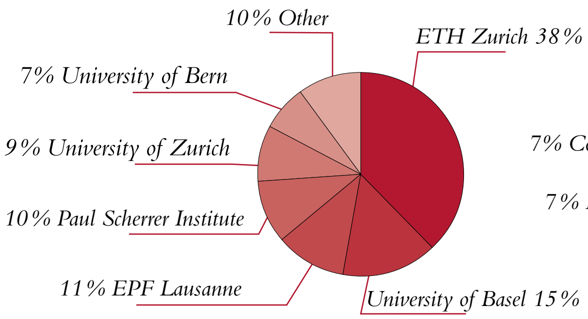
The Cray XT5 Monte Rosa.

Customer Satisfaction

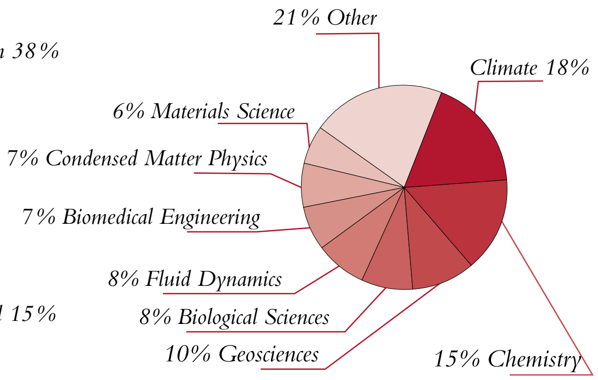
A customer satisfaction survey was submitted to 570 users in February 2011.
The response rate was of 30% (170 answers).

User Profile

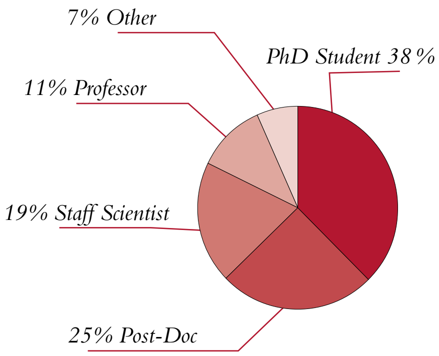
Institution



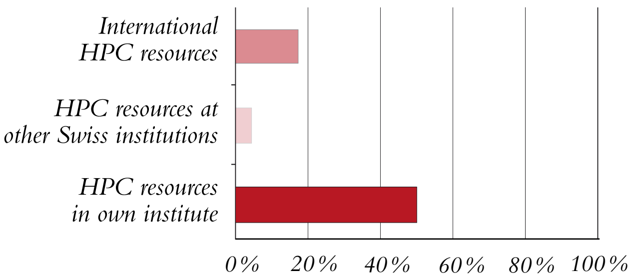
Scientific Field



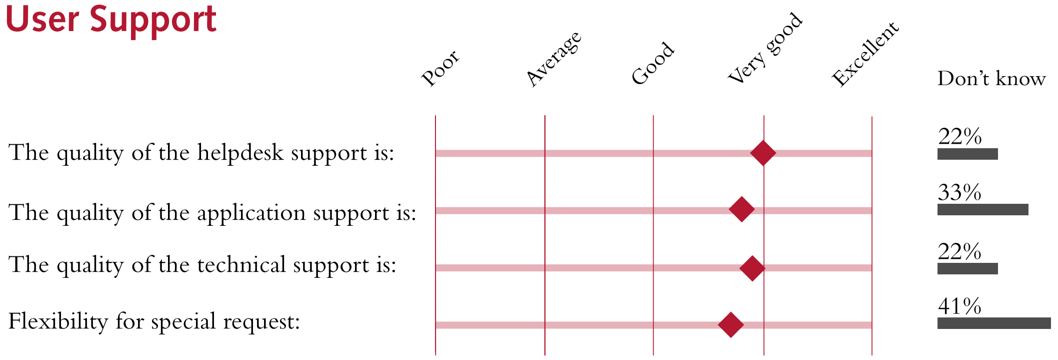
Position

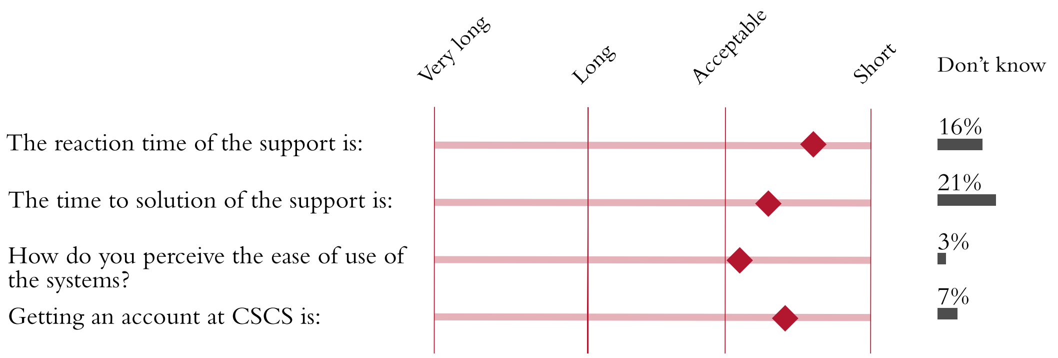


Additionally Used HPC Resources

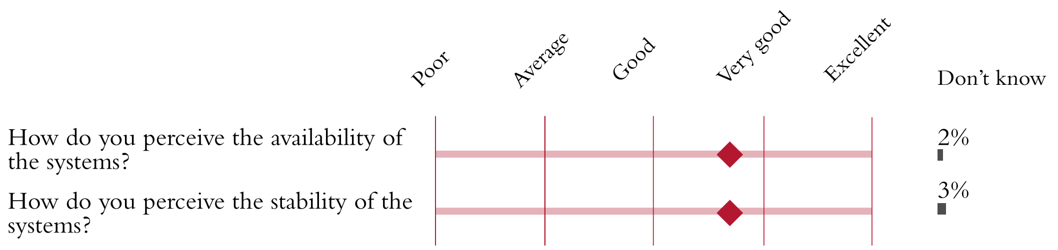


User Support

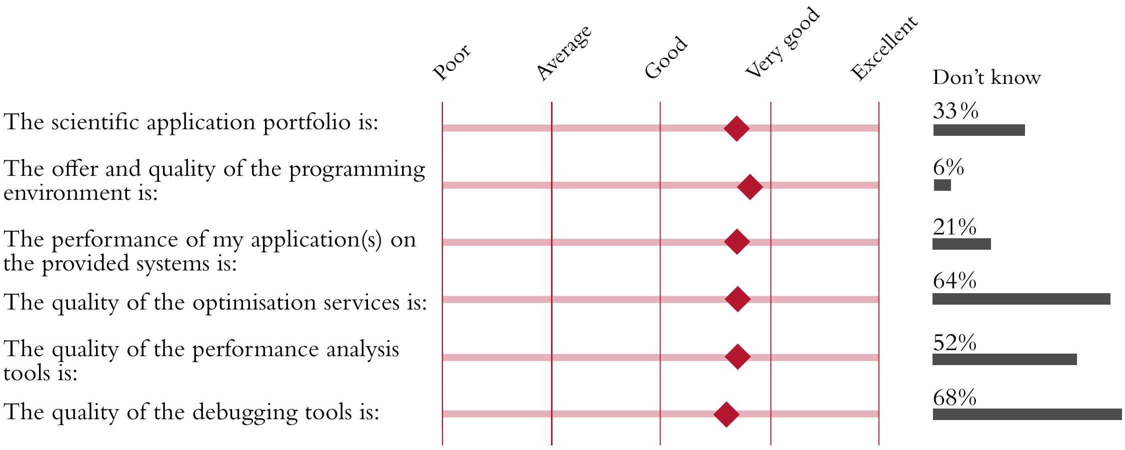




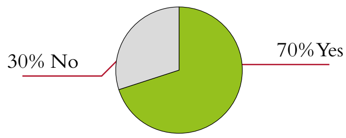
System Availability, Stability and Usability



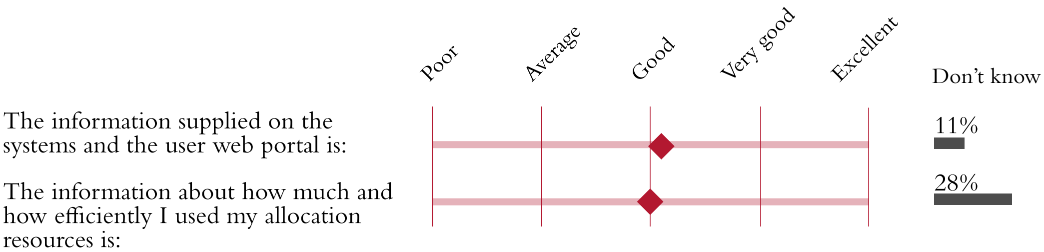
Application and Development Tools



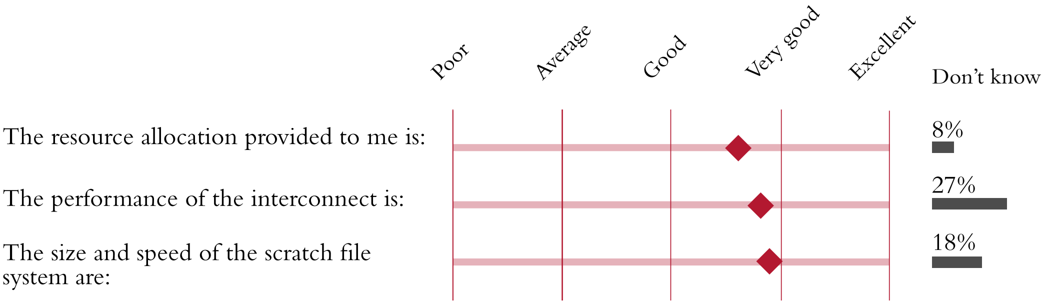
Do you measure the performance of your application code?



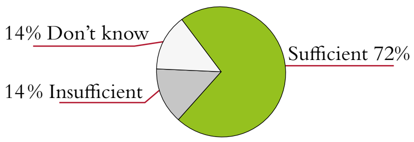
Information and Communication



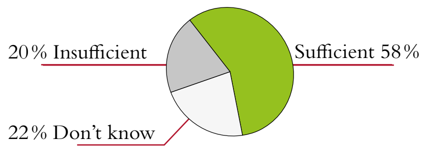
Adequacy of Allocated Resources



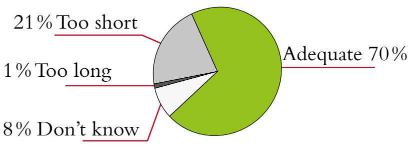
The amount of available memory per core is:



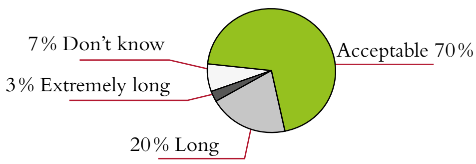
The storage capacity is:



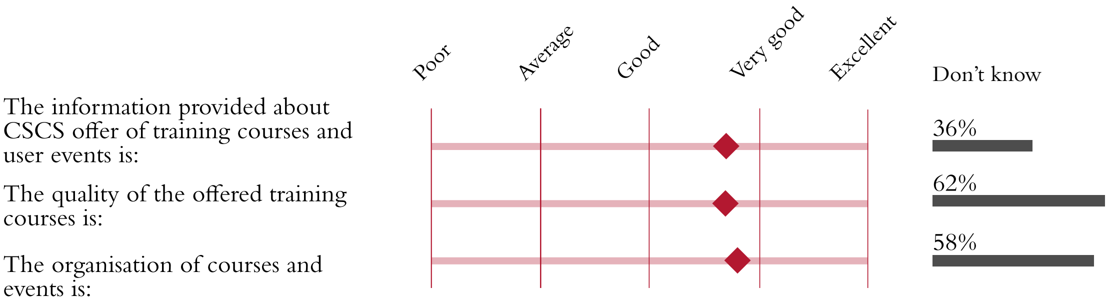
The run time limits for batch jobs are:



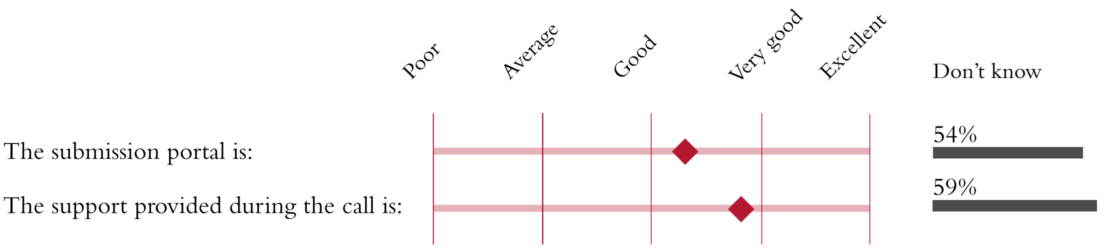
The job waiting time in the queue is:



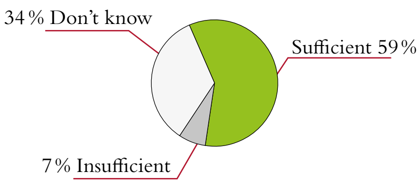
Training Courses and Events



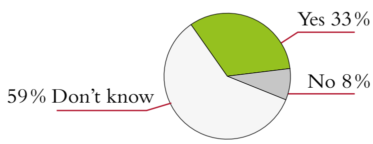
Proposal Submission Process



Two allocation periods per year are:



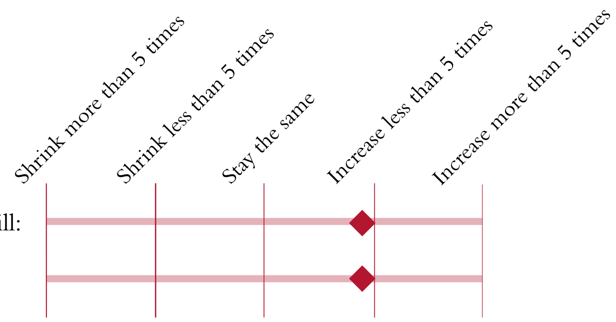
Is the review process transparent?



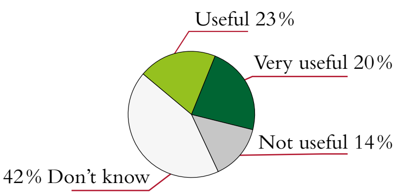
Expectations and Requirements

In the next 3 years, my computing requirements in terms of CPU hours will:

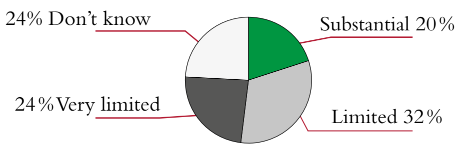
In the next 3 years, my data storage requirements will be:



To me GPU computing would be:

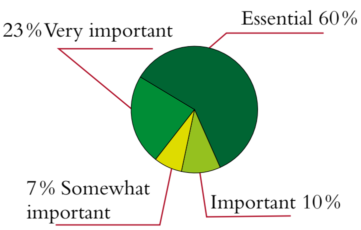


My need for assistance with code optimisation will be:

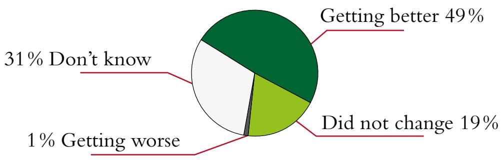


Perception of CSCS

For my research, CSCS resources are:



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



Impressum

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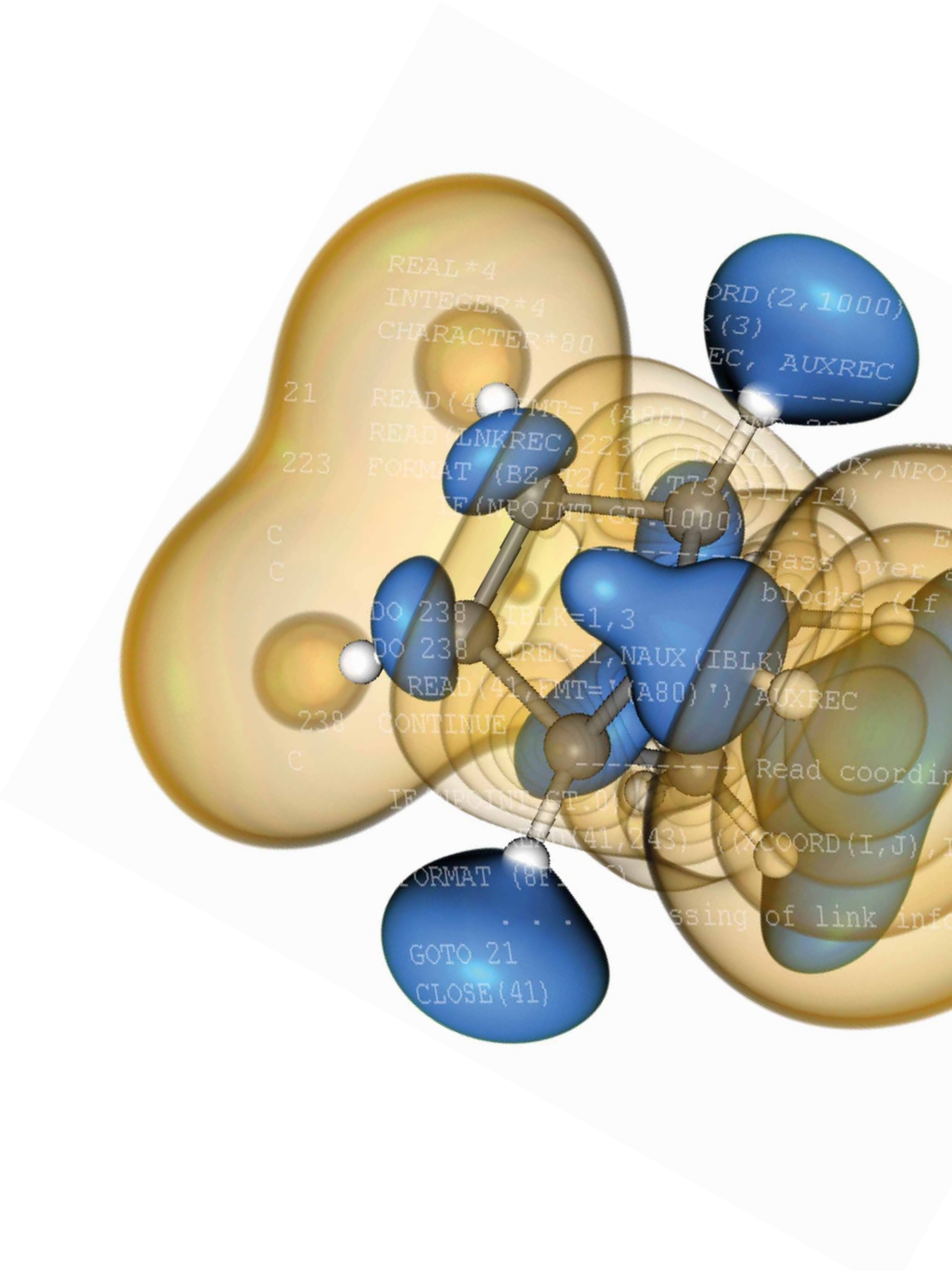

REAL*4
INTEGER*4
CHARACTER*80
21 READ(4
READ(LNKREC,223
223 FORMAT (BZ,
IF(NPOINT.GT.1000)
Pass over
blocks (if
DO 238 IBLK=1,3
DO 238 IREC=1,NAUX(IBLK)
READ(41,FMT='(A80)') AUXREC
238 CONTINUE
Read coordin
FORMAT
ssing of link info
GOTO 21
CLOSE(41)