CSCS
Swiss National Supercomputing Centre

Annual Report 2004

Content

Activity Report

Introduction

2004 has been an important and decisive year in defining the role of CSCS as an “autonomous unit of ETH Zurich”. The increased autonomy that the centre now enjoys is a major element in the implementation of its development plan, which constitutes its road map towards the next period (2008–2011), allowing it to realize the growth necessary for developing and supporting national projects requiring state-of-the-art HPC resources.

Increased investment capacities granted during 2004 have reinforced the duties and responsibilities of the centre and had a major impact: it has been necessary to streamline a certain number of processes and administrative tasks in order to ensure that the value of the work produced by CSCS’s specialists, working on HPC infrastructure, state-of-the-art scientific applications and advanced IT tools, could be fully appreciated. Major advances were made in this area in 2004, and they will be fine-tuned and further extended in 2005.

In 2004, the basis was laid that will enable us to attain the goals formulated in the current performance agreement with our funding bodies over the next three years. Major investments were made and important collaboration projects were initiated. During the year we welcomed 10 new members to the CSCS team, blending their talent, experience and enthusiasm to the already established group.

The profile of our centre can now be summarised in the following three definitions:
– service centre for the highest IT resources for scientific computing in Switzerland
– pioneer centre for exploring new, promising technology (hardware and software) and bringing it into production as a leadership class scientific instrument together with the dissemination of this knowledge to the wider community
– competence centre, with a head count of 31, comprising 18 university engineers, scientists and

computer scientists (6 PhD, 12 university degrees ranging from MSc to BSc).

2004 also saw the completion of Eurogrid and Prism, two European projects in which CSCS participated. This event coincided with CSCS becoming the main Swiss partner of EGEE at the start of 2005, a good premise for further international collaboration.

2005 will see the realization of our two major infrastructure projects: Horizon and Zenith. The first phase of the national Grid effort will be deployed and the R&D platform consolidated. Networking and collaboration with first class national and international institutions will be increased, reinforcing the position of CSCS as the national service and development centre for evaluating, benchmarking, bringing into production and maintaining a complex IT infrastructure as an advanced scientific instrument at the disposal of the most demanding scientific projects of our nation.

The CSCS team is looking towards the future with confidence, well positioned as an enabler of scientific discovery at the highest level.

Dr. Marie-Christine Sawley
CEO

Swiss centre for LHC Computing Grid (LCG)

The main purpose of the LCG project is to establish a stable computing infrastructure for scientific simulation, processing and analysis of the data produced by the new particle accelerator built at CERN, known as the Large Hadron Collider (LHC).

The impossibility of funding and installing all needed resources at one single site led to the choice of implementing the LCG computing service as a geographically distributed computational Data Grid. Several regional computing centres, in various countries, will be connected by fast network links. A special software suite, the LCG Grid middleware, will hide much of the complexity of this environment from the user, giving the illusion that all of these resources are available in a single virtual computer centre.

CSCS and CHIPP (Swiss Institute of Particle Physics) initiated a partnership in 2003 to set up the only regional computing centre for Switzerland outside of CERN. As a direct consequence CSCS assumed the role of single provider of computing and storage resources for Monte-Carlo simulations, physics events reconstructions and data analysis for the entire Swiss physics community.

The first prototype of an LCG cluster, installed in 2003, was replaced by a newer system in August 2004. Since then an increasing usage of the facility has been registered, both in terms of CPU hours and storage space.

CSCS and CHIPP recently consolidated their cooperation with an agreement for the purchase and installation of additional hardware resources. This is the result of an intensive and fruitful discussion that defined the minimum performance requirements and the scope of the new system. This enlarged cluster will be completely dedicated to HEP simulation/reconstruction/analysis and will be accessible only through the Grid.

During the first half of 2004, CSCS reinforced its staff by employing a full-time IT specialist as the local coordinator of LHC Computing Grid. This new collaborator has taken responsibility for installation, upgrade and maintenance of the computing infrastructure and for regular participation in meetings and committees related to Grid deployment activities.

The local LCG group has also taken great advantage of the newly established Swiss Bio Grid group. The synergy between the two groups constantly improves thereby creating the solid foundations for a Grid competence group within CSCS.

Gian Luca Volpato

For more information:
http://www.cscs.ch/lcg-project
http://www.chipp.ch

Swiss Bio Grid

The Swiss Bio Grid (SBG) is an initiative of national scope. Its aim is to support large-scale computational applications in the fields of bioinformatics, biosimulation, chemoinformatics and bio-medical sciences by providing access to distributed high-performance computing resources, high speed networks, and massive data collections and archives.

The intent of forming a Swiss national-level computing grid dedicated to life sciences was expressed by the signing of a declaration of interest on January 2004. Founding partners in this initiative are: CSCS, Biozentrum of the University of Basel, Functional Genomics Centre in Zurich, Friedrich Miescher Institute in Basel, Novartis, and the Swiss Institute of Bioinformatics.

The tasks of coordinating technical aspects of the future grid infrastructure, including evaluation of currently existing middleware solutions were assigned to the CSCS. The coordinating CSCS team was formed in the second quarter of 2004.

A proof-of-concept (PoC) study was established to explore the functional requirements for a computational grid for bio-medical applications, and to evaluate the ability of the presently shared resources to meet these requirements. SBG partners have agreed to provide resources to the PoC study. As scientific content for the PoC study, the project "Grid-based Virtual Screening of Dengue Virus Target Proteins" proposed by T. Schwede and M. Podvinec (Biozentrum Basel) and M. Peitsch (Novartis) was selected.

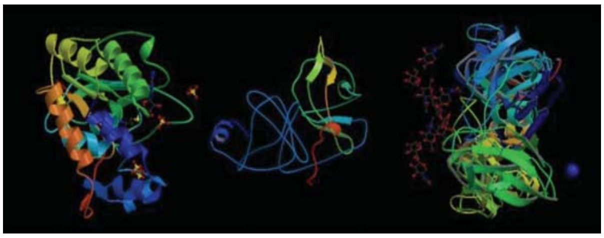
The SBG proof of concept has the following goals:
- Demonstrate collaboration between the SBG partners, including industry - Foster contribution and sharing of resources.
- Encourage broad participation by partners in the proof of concept.
- Develop concepts that ensure a trustworthy environment for participation.
- Explore requirements, both in workflow and in resource availability and management.

The proof of concept has objectives in three areas:
- Infrastructure:
  To establish a test bed that will evolve towards a dynamic infrastructure providing access to resources across institutions and disciplines, delivering services enabling compute-intensive applications and data sharing. Partners develop and analyze solutions based on public and open standards to identify the requirements for, as well as the challenges of a heterogeneous computational grid infrastructure.
- Science:
  To obtain innovative and scientifically valuable results by the use of resources exceeding what any individual institution could have provided on its own. The partners at the Biozentrum have assembled the fundamental tools and data necessary for the virtual screening project chosen as PoC. The outcome of calculations on the grid will be carefully evaluated. Compounds considered likely to bind to Dengue virus proteins will subsequently be tested experimentally for activity in collaboration with the NITD - Novartis Institute for Tropical Diseases in Singapore.
- Feasibility:
  To convincingly demonstrate that it is possible to address complex and demanding scientific questions by sharing existing infrastructures in Switzerland with only minimal impact on the normal use of these resources.

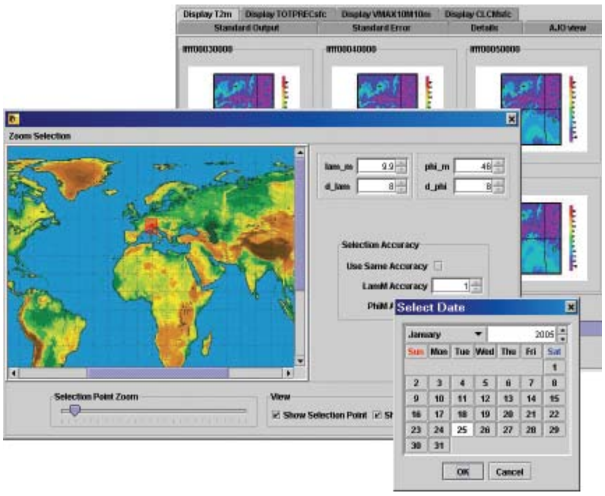
This pilot project has the potential to provide two sustained benefits: The public computational ligand-finding platform can be applied in drug development against other neglected disease targets. The functionality of the established compute grid in Switzerland can be applied to other computationally intensive problems in the life sciences.

Patrick Wieghardt
Sergio Maffioletti

For more information:
http://www.swissbiogrid.org



3 proteins to be run against Dengue targets



Overview of the graphical user interface of the LM plug-in

HPC Benchmarking and Development

Performance issues related to HPC are a key component of the activities of the group. During 2004 there has been further development on the established CSCS performance environment, targeting not only detailed real time system monitoring but also static a-posteriori analysis and statistics through the use an in-house Java application which is increasiingly becoming a reliable and essential tool for investigation, analysis, and decision-making. In addition, the group has started the definition of the “CSCS Benchmarking Suite” which will be composed of a collection of representative applications that cover a range of technical aspects of HPC such as MPI, OpenMP, high memory bandwidth and distributed algorithms, and based on next-generation problem sizes. The goal is to use this suite to explore and assess current and forthcoming HPC systems.

Involvement in international projects such as EUROGRID and ENACTS, both of which closed in 2004, gave the group an opportunity to explore GRID technologies. EUROGRID implemented a grid infrastructure, today available as Open Source, which enabled seamless, secure access to HPC resources and demonstrated the suitability of this approach for brokering resources and running distributed codes from different application areas including biomolecular simulations, weather prediction and coupled CAE simulations. EUROGRID was appreciated particularly for its contribution in defining grid standards and for middleware development. Besides being part of the grid testbed, CSCS was able to develop a new product based on the *LM* regional weather forecast code which can deliver weather forecasts on demand in a GRID environment, a tool which is now available on the CSCS web site. The ENACTS project officially closed on 31 December 2004, with all the studies successfully completed and the reports publicly available on the ENACTS web site (including «Grid Enabling Technologies» by CSCS and FORTH, 2002).

Mauro Ballabio

Fundamental and User Services

During 2004, the section supported

- the production of over 99 000 h∗cpu on the NEC SX-5/16 and 1770 000 h∗cpu on the IBM SP4/256,
- the management of over 400 user accounts,
- the setting up of the new classroom of CSCS.

The highest-priority goal of the Fundamental and User Services section is to make available the most adequate HPCN-resources (systems, networks, data management and storage) to the CSCS end-users community in a reliable, performing and easy-to-use fashion. Furthermore, the Section ensures a reliable, efficient and secure access to all CSCS IT resources internally and from remote (universities, governmental agencies and industry) and manages the CSCS technical infrastructure.

The CSCS HPCN-environment (see Figure) is built on a tight integration of supercomputers, high speed networks, data management and pre-/post-processing resources and offers its end-users an application oriented and highly integrated super-computing facility. Its architecture and exploitation concept have been designed to accomplish the criteria of high availability and reliability, high security and resilience, functionality, performance and ease-of-use, as well as support for quality of service and manageability.

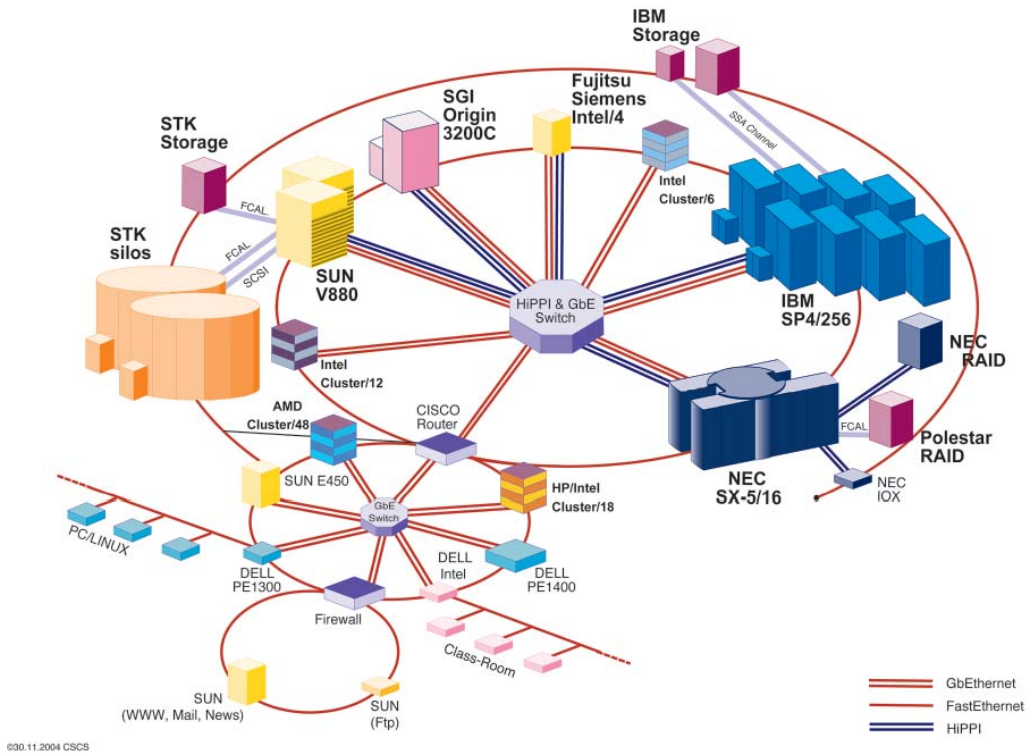
Following fields have been the focus of the section's activities in 2004: The significant reinforcement of the high-performance production network and front-end upgrade, and the implementation of the state-of-the-art teleconferencing, as well as the installation of SWITCHmobile, allowing wireless access to the Swiss academic network. As a part of the continuous pro-active evaluation of new HPCN-technologies, as well as for the permanent assessment of the current and future users' requirements, two IA-64 Linux clusters have been installed and are being extensively tested.

Storage capacity extension, including its improved integration with the computational servers, has been carried out, enabling for the increasing adoption of data-intensive end-user applications, either for data stored on disks or for archival data stored on tapes.

In addition to ensuring the highest production operational standards, a major step in resource monitoring and accounting has been performed in 2004, with the implementation of a new powerful tool capable of supplying the data with the necessary granularity and precision. Furthermore, the permanent optimization of the job scheduling, load balancing, controlling, accounting and overall throughput performance has been a major focus of the Section activities.

Djordje Maric

For more information:
http://www.cscs.ch/b-display.php?id=7



CSCS HPCN production environment

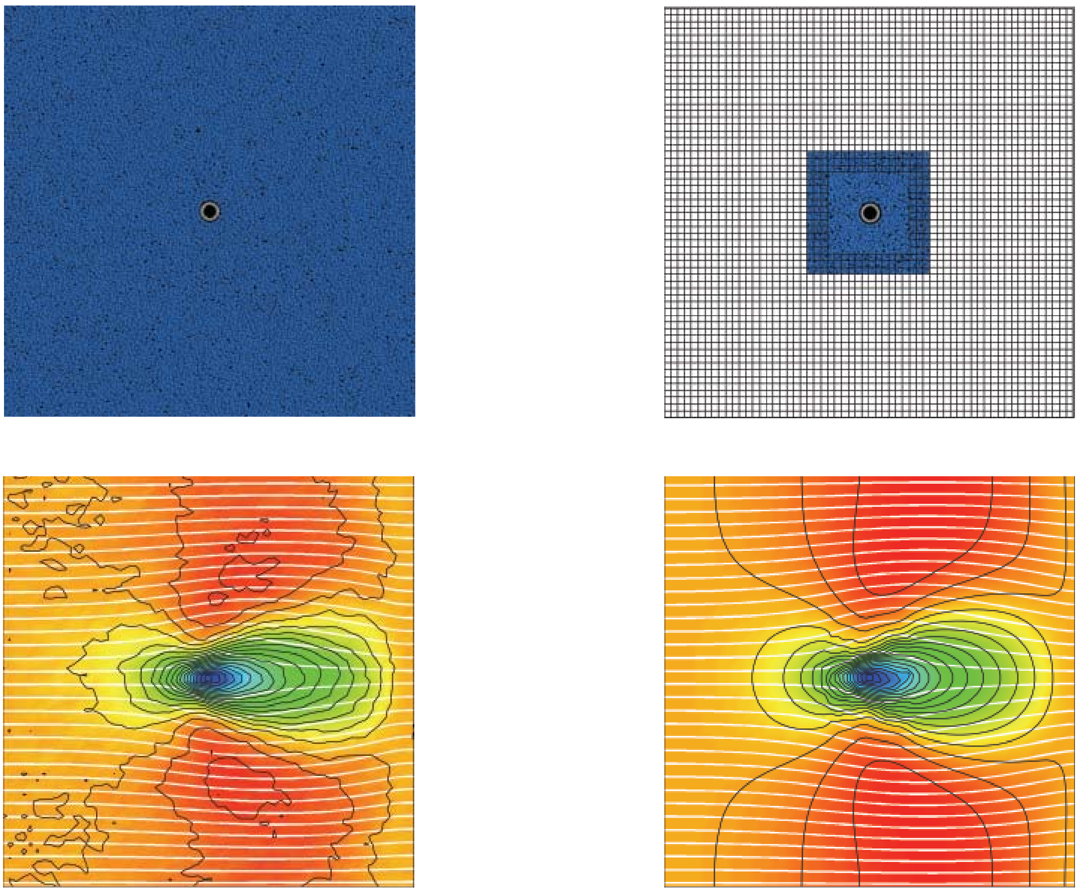
Scientific Application Support

Computational sciences and engineering are focussing on ever more complex systems and phenomena, aiming at becoming able to perform highly accurate simulations of realistic systems. By their nature, such complex simulations require an integrated, multidisciplinary and multi-physics approach.

This multi-scale and multi-physics approach generally implies very large computational requirements in terms of CPU power, central memory and I/O. Users are most often constrained in their research by the 'size' of their computational facility in terms of memory, number of CPU, disk space, etc. and by the relative efficiency of their application on the facility itself, often also referred to as 'sustained performance', the main factor determining 'time to solution'.

Meanwhile, data intensive applications are also gaining momentum and we have noted a constantly increasing rate of data transfer between the archive and the computing servers in several application fields, and especially so in CFD, meteorology and climate. CSCS acts as one of the main computational laboratories for the NCCR Climate community.

This community sets new and challenging requirements not only related to efficient high-end comput-



a) b) c) d)

Multiscale simulations of a dense fluid flowing past a carbon nanotube. The reference solution is obtained using molecular dynamics simulations covering the entire computational domain (a). The hybrid atomistic/continuum computational approach (b) replaces a large portion of the atomistic systems with a continuum description through the incompressible Navier-Stokes equations. Both computational domains have an extent of 30 x 30 nm. c) Velocity field for the reference solution averaged over 4 ns. The white lines are streamlines, and the black lines are contours of the speed ($|\mathbf{u}|$). d) Velocity field of the hybrid solution after 50 iterations. The black square marks the interface between the atomistic and continuum domains. Image courtesy by Prof. P. Koumoutsakos Group (ETH Zürich).

ing, but also to data archiving and data pre/post-processing. Large data sets, spanning several TB, are not only archived, but are also regularly accessed for data analysis and data verification experiments. MeteoSwiss, the Swiss national weather service, has been carrying out all its production and research computations at CSCS for several years now. The computation of its numerical model, a slightly adapted version of LM, named aLMo, which simulates the atmospheric evolution over a domain covering most of Western Europe is the most important task outsourced to CSCS. The aLMo numerical model, along with the entire weather forecast suite, must be regularly adapted to support the constantly evolving requirements and the regular cycle of software engineering maintenance issues.In this context our group plays an important support role in a well-established collaboration with MeteoSwiss experts.

The main use of these simulations, starting twice a day from the state of the Earth atmosphere at noon and midnight, is the daily weather forecasts issued by MeteoSwiss. Beyond this, the results are also used as input for follow-up models computing the dispersion of air particles and the dispersion of pollutants for the National Emergency Operations Centre (NEOC) located in Zurich, as well as hydrological runoff forecasts at the Swiss National Hydrology Survey in Ittigen (BE). Model results are also sent to the Swiss Federal Institute for Snow and Avalanche Research in Davos, for assessing the risk of avalanches over the following 3 days. In addition to these governmental institutions, model results are also disseminated to a large number of users, such as PhD students, researchers, and several companies in the private sector.

Aiming at an efficient and effective use of the overall HPC facilities, the Scientific Applications team continued the consolidation and completion of the CSCS computational (bio-)chemistry framework, as well as the support and maintenance of mathematical and numerical libraries. The available software portfolio now covers a wide spectrum of algorithms and methods, including specific architecture optimized libraries and development tools, along with the most widely used computational (bio-) chemistry application suites.

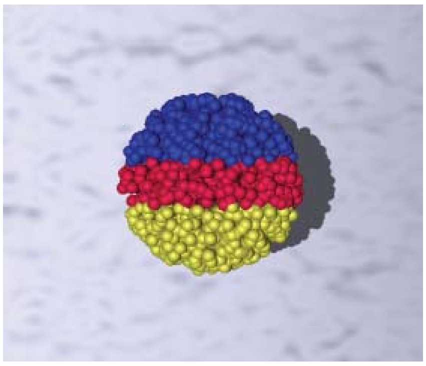
The Scientific Applications group has also been involved in the European project PRISM (Program for Integrated Earth System Modelling), a pilot infrastructure project for the establishment of an EU climate research network. The primary task of CSCS was the definition of a set of recommendations and rules defining the software engineering process, coding rules and code quality standards. Part of this effort was included in the PRISM System Specification Handbook and proved to be a great opportunity for CSCS to acquire and share new competencies on code portability and code quality standards across multiple platforms. This project ended in November 2004 after 3 years.

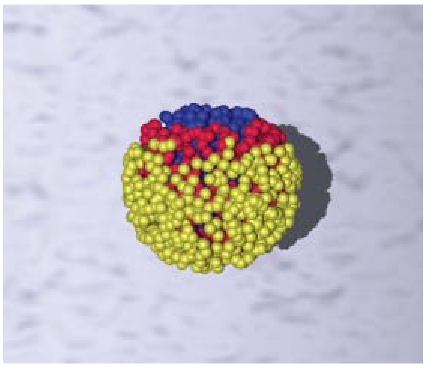
Finally, a considerable effort was spent in processing user support requests on a daily basis, as well as in consolidating and regularly updating the technical documentation made available on the CSCS user web portal.

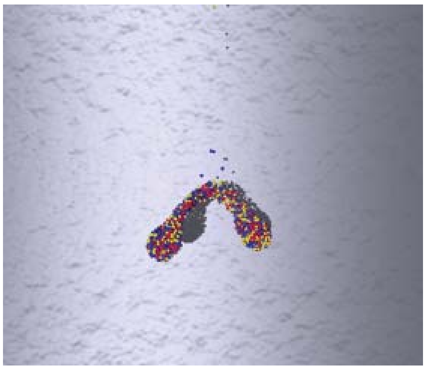
Angelo Mangili

For more information:
http://www.nccr-climate.unibe.ch
http://prism.enes.org
http://www-users.cscs.ch

Scientific Visualization







T. Bosse, C. Härtel, E. Meiburg, L. Kleiser, „Numerical simulation of finite Reynolds number suspension drops settling under gravity", Phys. Fluids 17, 3 (2005)

This year was marked by a large increase of use of a new visualization environment called ParaView. ParaView is based on the VTK toolkit and provides most standard visualization needs. ParaView also serves as the basis for our benchmarking activities centered on parallel data extraction and visualization and we can now offer customized parallel data reading and visualization to CSCS users. This new emphasis does not however diminish our involvement in the AVS suite of softwares. We maintain a lead expertise available to the academic community at large and our success is confirmed with the publication of the book chapter called "AVS and AVS/Express" published in "The Visualization Handbook", edited by Profs. C. Hansen and C. Johnson of University of Utah.

We contributed to a major development and release of the ParaView open-source application in the hands of our industrial partner VA TECH HYDRO in Vevey who specializes in hydro-electric power supply and the design of water turbines. We specialized ParaView with a set of source code macros to be used for Pelton turbines.

We also placed a great emphasis on the evaluation of Scientific Data Management procedures aimed at the selection of the best archiving formats and tools. We applied our results for several projects among which we find one initiative combining experimental data (from measuring devices) and numerical results from model simulations in the industrial water turbines field; one project in optimizing archiving and graphical representations of particle data; and our first tutorial held during the annual CSCS User Day, with a presentation on Data Management practices for the CSCS users.

We greatly improved our support for particle-based simulations. A very large investment was made in improving visual perception of time-dependent particle sets. The use of boundary wall textures, shadows, velocity field textures, 3D labels, color and linked multiple views greatly improved the state of the art of particle rendering and made great impression at the November 2004 APS conference, where it was selected as one of the four winning videos of the Gallery of Fluid Motion.

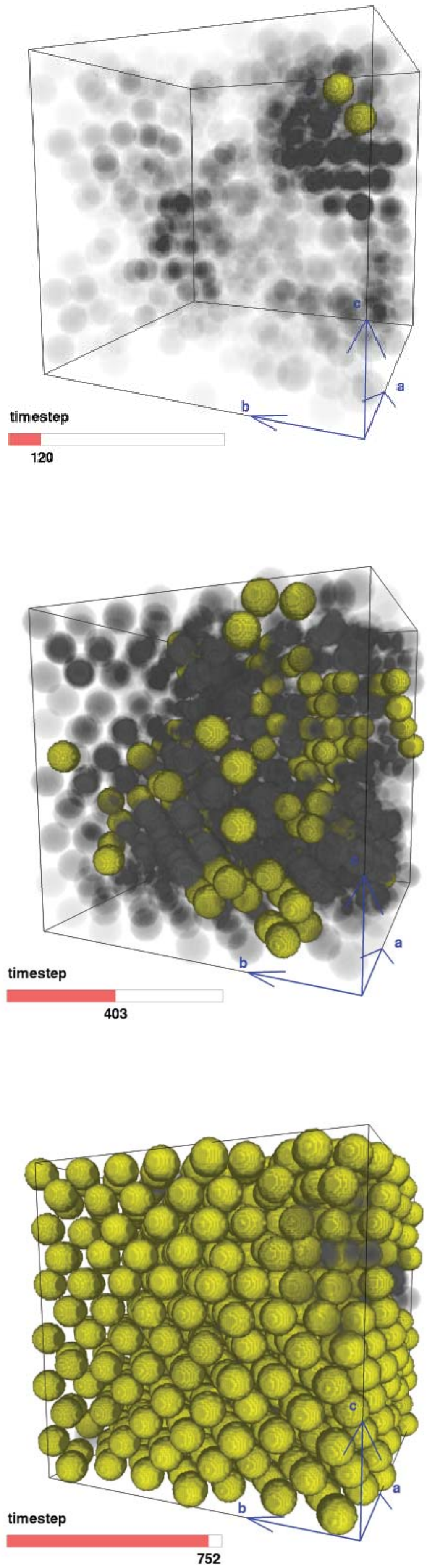
We contributed several software modules to the VTK open-source community. An interface for FLUENT GAMBIT data, for AVS UCD data and the Lagrangian Eulerian Velocity Texture class developed for our daily visualization of the Swiss Meteorology forecast. It is now available in source code, and was demonstrated by Kitware staff at the 2004 IEEE Visualization conference.

A substantial improvement in visualization of crystallography in collaboration with the ETH-Zürich group of Prof. Oganov also marks our continued involvement with visualization for atomistic and molecular simulations initiated with the support of Prof. Parrinello's research group.

Our group was reinforced at the end of 2004 with the addition of a numerical simulation expert (specialist in industrial fluid flows), and of a Graphics and Visualization expert (specialist in imaging).

Jean M. Favre

For more information:
http://www.cscs.ch/gallery/images-d.php



Classical molecular dynamics simulation of argon atoms freezing.

An order parameter is computed for each atom. When this parameter value moves above a threshold the atom freezes.

The chosen visualization technique renders atoms below the threshold as transparent clouds to reduce display clutter and to make frozen atoms visible. Atoms whose parameter approach the thresholds turn less and less transparent; they turn solid yellow when frozen.

Federica Trudu, Computational Science, Department of Chemistry and Applied Biosciences, ETH Zurich.

Images done with STM3 toolkit by the CSCS Visualization group.

Development of CSCS' compute infrastructure

The current inadequacy of the available supercomputing power for the Swiss researchers is today all too obvious. Whilst Swiss universities rank top of the list of leading research universities worldwide (ETH Zurich reached position 27 in the last Shanghai ranking of the top 500 universities), the systems of the Swiss National Supercomputing Centre have, since June 2004, ceased to appear in the TOP500 list of the most powerful computers in the world. This mismatch between demand and offer of resources is also apparent in the fact that the number of research projects proposed to CSCS that receive approval from the regular Large User Project evaluation amount to double the capacity of the centres' computers. If we were to include those research projects that are never proposed because the scientists already know that CSCS does not have the compute power to host them, it can safely be said that a lot of good science remains unexplored due to lack of resources at CSCS.

CSCS therefore developed a technology strategy in 2004 which pursues two major goals: firstly, to ensure the provision of the necessary number and quality of cycles and storage resources for Swiss researchers, and secondly, to bring newest leading-edge supercomputing technology to our customers and making it mature for production, thus, providing a competitive advantage for Switzerland. The technology strategy maps the compute portfolio on an innovation cycle that has two coordinate axes, "scientific output productivity" and "support effort" (which from a user point of view represents "time to solution", see Figure 1). In our strategy, CSCS will host at least two systems in the right-hand half of the diagram, which depicts systems with high scientific productivity of different maturity. Given that the current computer portfolio is inadequate to satisfy our customers' needs, we concluded in May 2004, that the portfolio must be renewed and restructured in two major, and closely consecutive procurement projects:

– The "Horizon" project targets a message-passing, massively parallel system with a minimum of 1024 efficient scalar processors and scalable, low latency/

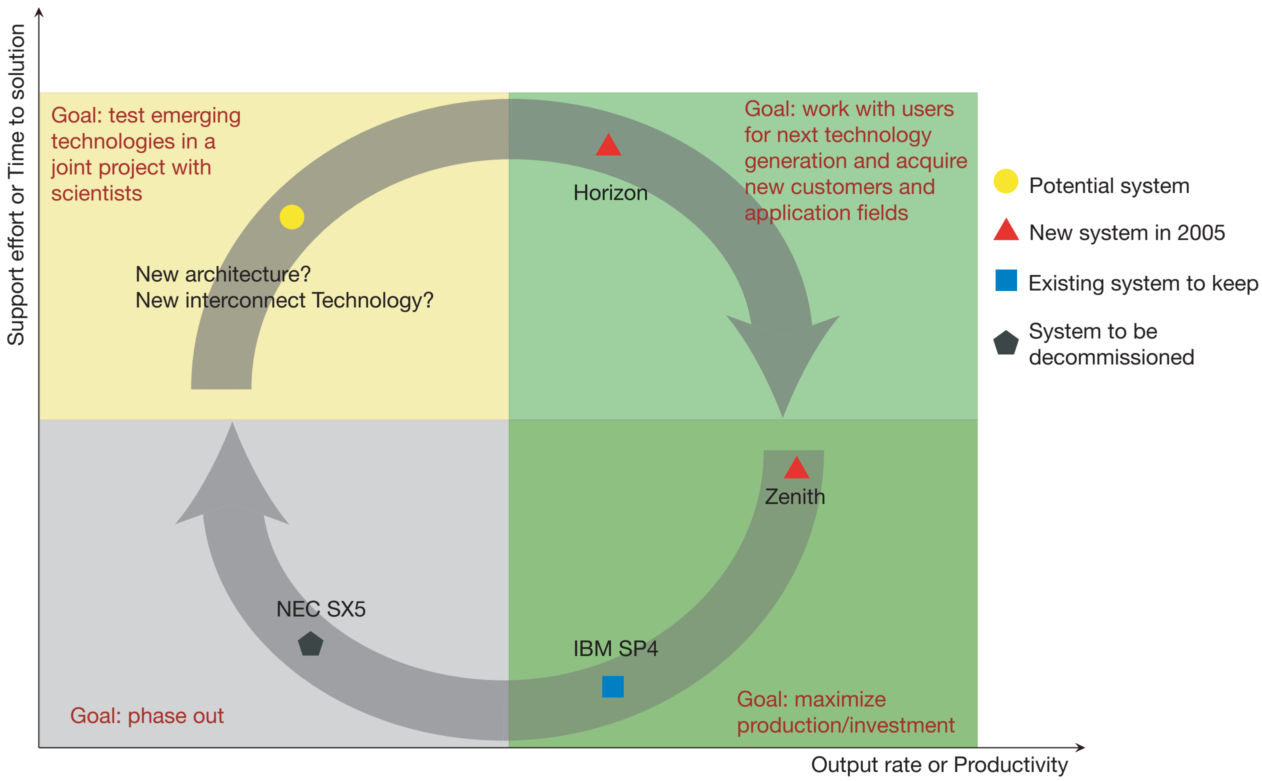


Figure 1: CSCS innovation cycle

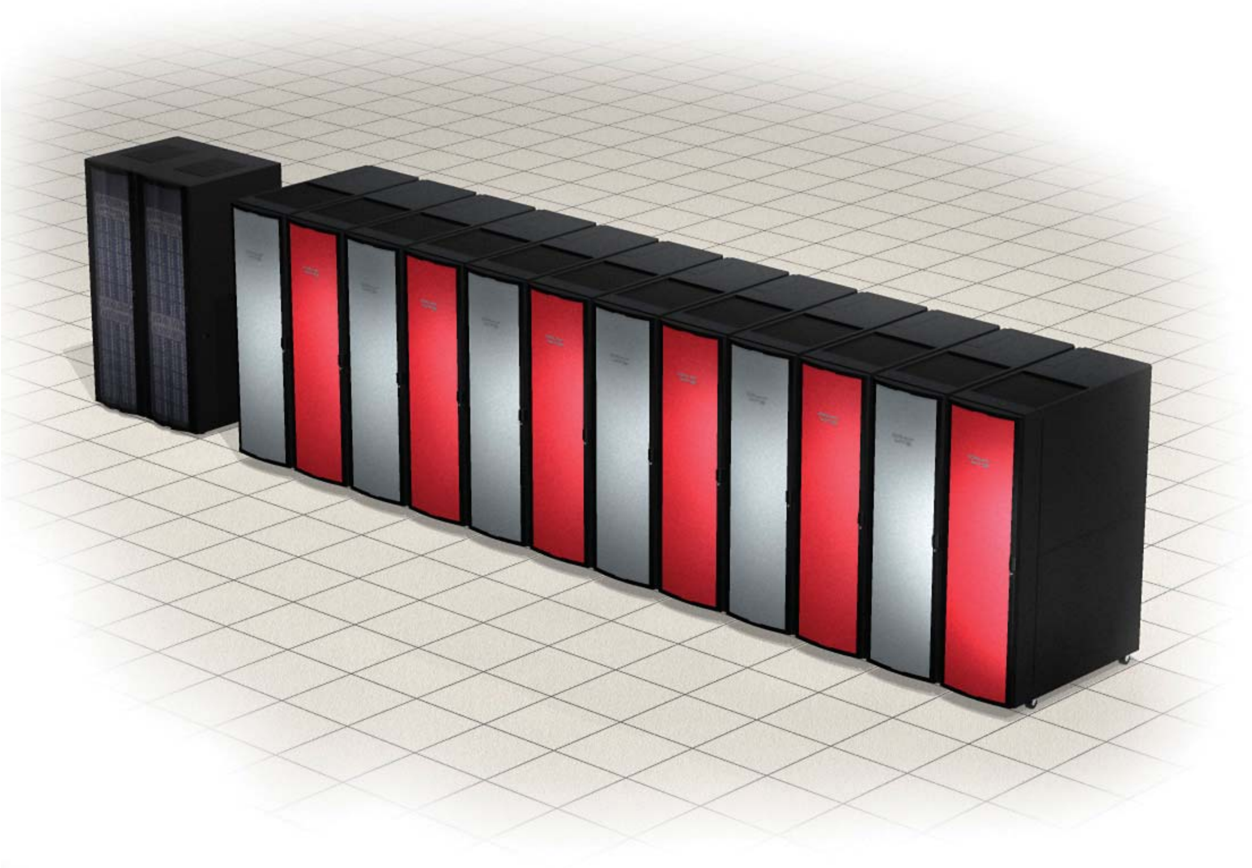


Figure 2: A computer rendered view on the coming Horizon installation

high bandwidth interconnect. The system is based on a cluster approach but targets at a true capability computing architecture that scales for big computing jobs requiring thousands of processors, thus combining the compute capabilities of an MPP architecture with the economic advantage of cluster architectures.
– The “Zenith” project, is focussed on a system with powerful processors, less parallelism but higher shared memory capability, thus providing a system that is closer to the experience of CSCS’ present users and complementary to the architecture of Horizon.

The CSCS Steering Board approved this technology strategy in May 2004 and CSCS immediately started implementing it by issuing a call for tender for the Horizon system in late summer 2004. The result of this call for tender shows the effectiveness of our approach: In January 2005, CSCS selected the offer for a Cray XT3 system for the award.
The XT3 is the commercial product developed from the Red Storm project at Sandia National Lab and the installation at CSCS will be the first in Europe, after US American installations at Sandia National Labs, Oak Ridge National Labs, and Pittsburgh Supercomputing Centre. It will provide a system of 1’100 compute CPU with a theoretical peak of 5.9 Tflop/s, or 5.9 trillion calculations per second (see Figure 2). We plan to install the system by June 2005. After the finalisation of these steps, when the architectural features of Horizon are completely defined, CSCS will issue the second call for tender for Zenith, which will be designed to be maximally orthogonal, or complementary, to Horizon.

Dominik Ulmer

Extension of the building infrastructure

2004 marked a turning point in the infrastructure development of CSCS. Since 1991, when CSCS opened, the technical building infrastructure, especially the capacity for electrical power and cooling, has remained unchanged. This infrastructure has run successfully and reliably, experiencing no power supply interruption of more than 2.5 minutes during all of 2004. However, with increasing parallelism of the high-performance computing systems, the energy requirements of modern supercomputers are ever larger, and other compute centres have adapted to this demand accordingly. CSCS' electrical capacity is about half that of comparable HPC centres in Europe..

CSCS and the building department of ETH Zurich therefore started an infrastructure project in September 2004 to improve the situation:

- in a first step, the electrical and cooling capacity of CSCS will be almost doubled by the summer of 2005 in order to enable CSCS to host the new supercomputers Horizon and Zenith. The extension will rely on the existing technical installation as much as possible without any new building investments.
- in a second step, envisaged for 2008, the building situation of CSCS will be revised. The technical infrastructure for electricity and cooling will be brought to a standard comparable of that of other European supercomputing centres. Also, office space and rooms for teaching, meetings and teleconferencing will be increased.

Currently, two different scenarios are being investigated for this step: the first consisting of a remodelling of the current premises of CSCS and inclusion of other space within the Galleria 2 building, the second is the construction of a new building for CSCS, possibly in collaboration with the Canton of Ticino and the Università della Svizzera Italiana. We hope to decide on these two options by mid-2005 and initiate the building project by the end of the year.

Dominik Ulmer

User events

In order to present the new CSCS organisation and get feedback on the needs of our users, a User Event was held on 14th May at Bern University.

The traditional annual User Day was held on 27th-28th of September at CSCS. 48 users were welcomed on site for this event during which the projects supported by CSCS resources were presented in posters and a selected number of talks.

Outreach and education

One of the main shortfalls of CSCS underlined by the task force study of 2003 was its insufficient integration into the academic scene of Switzerland. When comparing CSCS to other national HPCN centres, at the time the very low training and educational activity was striking. Hosting or offering courses and summer schools certainly requires a major effort, but is also a good opportunity to hear about different experiences and mindsets, as well as for us to present CSCS and its activities to a young public. In a sense, it is also an extremely efficient way to acquire new customers by making CSCS known to a wider public.

These are the reasons why in 2004, after a three year pause, we were pleased to welcome, under the new organisation of CSCS, Prof. Bally, from the University of Bern, for the summer school on computational chemistry followed by a workshop on computational physics by Prof. Troyer from ETH Zürich. Both courses boasted a high participant count as well as internationally renowned speakers.

In October the COST action D23 tutorial , coordinated by Hans Peter Lüthi from ETH Zürich was held at CSCS in collaboration with ZIB, Perugia University, AEI and the CSCS Grid specialists.

All three events were able to take full advantage of the new classroom infrastructure, installed in a very short time by the specialists of the Fundamental and User Service Section, with the help of the application specialists for the scientific support: this classroom hosts a cluster of 20 new Intel P4 processors with standard Linux workstations with one main management and administration station. The classroom also offers local printing facilities and wireless LAN access also via SWITCHmobile and standard high quality equipment.

Additional application software can be installed and configured to meet the specific purposes of each session. We look forward to jointly coordinating further educational activities with you in the future! Should you be interested in organizing a summer school/ workshop/ tutorial at CSCS, please do not hesitate to visit the relevant pages on our website or directly contact Ms. Ladina Gilly who will be pleased to discuss the possibilities with you.

Marie-Christine Sawley
Ladina Gilly

http://www.cscs.ch/a-display.php?id=105

Research Digest

Editorial

2004 – a year marked by intense and fruitful work realized with passion and collaboration by everyone: that is the balance of CSCS's first year of management as an independent unit of ETH Zurich.

2004 was also characterized by the creation of the conditions necessary to realize the next investment steps in infrastructure and resources.

Thanks to the invaluable collaboration of the Vice President of ETH Zurich Ulrich Suter and the determination of the CEO Marie-Christine Sawley, CSCS's management has, during this first "trial" year, been successfully reoriented on the basis of its four-year performance mandate with ETH Zurich.

As the independent management with a separate budget became a reality, a new definition of financial and qualitative control mechanisms were put in place, allowing the measurement of the achieved goals.

The management of CSCS can rely on the support of both its Scientific Advisory Board and Steering Board and a Resource Allocation Committee will soon be formed.

Thanks to the formation of a Financial Audit Committee – a subset of the Steering Board led by Dr. Stephan Bieri – the tools for risk management are being fine-tuned; the 4th quarter of 2004 even saw a financial audit by an external company.

CSCS is on the starting line towards new goals, in particular the realization of two important procurement projects, the first, a fine granular, message passing type of system (cluster), called Horizon (in collaboration and thanks to PSI) and the second, a highly- integrated large shared memory system, called Zenith.

These two projects, which were developed in 2004, will lead to considerable but necessary investments allowing the centre to increase the quality and quantity of its offer towards users.

Beyond the proven technical and scientific capacities of CSCS employees and its growing and adapting infrastructure, CSCS possesses all the qualifications necessary to be a centre of national importance with employees from eight different countries ensuring communication in no less than nine languages.

I would like to thank all members of CSCS and all those who, in different ways, have trusted in CSCS, making this leap forward possible.

Dr. Monica Duca Widmer
Chair of the Steering Board

Editoriale

Il 2004 è stato caratterizzato da un lavoro proficuo ed intenso, svolto da tutti con passione e collaborazione: questo il bilancio del CSCS nel suo primo anno di gestione quale unità indipendente del Politecnico di Zurigo.

Un 2004 ancora caratterizzato dalla riorganizzazione e dalla creazione delle condizioni quadro necessarie alla realizzazione dei passi successivi, quelli di investimenti sia nell'infrastruttura che nelle risorse.

In questo primo "anno di collaudo" si è riusciti, complice anche la preziosa collaborazione del vice presidente per la ricerca dell'ETH Zürich Ulrich Suter e la determinazione della CEO Marie-Christine Sawley, a riorientare la gestione del CSCS sulla base del mandato di prestazioni quadriennale con l'ETH Zürich.

La gestione indipendente, con un budget separato, è divenuta realtà ed è cresciuta parallelamente alla definizione delle modalità di controllo - sia finanziario che qualitativo - della verifica del raggiungimento degli obietti.

Il management del CSCS può contare sul supporto del Scientific Advisory Board oltre che dello Steering Board e nominerà rapidamente di un Resource Allocation Committee.

Tramite l'istituzione di un Financial Audit Committee – sotto gruppo dello Steering Board pilotato dal Dr. Stephan Bieri - anche gli strumenti di gestione del risk management sono in corso di affinamento; si è già pure provveduto ad effettuare una revisione esterna delle finanze per il 4 quartale del 2004.

Il CSCS è sulla linea di partenza verso nuove mete, in particolare larealizzazione di due progetti molto importanti per l'utilizzo di applicazioni HPC parallele e distribuite: il primo, chiamato Horizon, basato su un' architettura a memoria distribuita (cluster) e realizzato anche grazie alla collaborazione con il PSI ed il secondo, chiamato Zenith, basato su un' architettura integrata a memoria condivisa .

I due progetti elaborati nel corso del 2004, comporteranno investimenti rilevanti ma necessari al Centro per ampliare la propria offerta all'utenza, sia dal lato qualitativo che da quello quantitativo.

Oltre alle provate capacità tecniche e scientifiche degli operatori del CSCS e ad un'infrastruttura in via di adattamento e ampliamento, il CSCS possiede tutti i requisiti necessari di un centro di valenza internazionale, con operatori provenienti da ben otto Paesi, che assicurano la comunicazione in nove lingue.

Grazie a tutti i collaboratori e a chi ha dato fiducia al CSCS contribuendo – in forme diverse – ad aver reso possibile questo balzo in avanti!

Dott. Monica Duca Widmer
President dello Steering Board

Presentation of three Large User Projects
by David Bradley, Science Base, UK

We propose here a special insight into the work of three scientists, who carried out their research using computing resources from CSCS. The reader can find the list of all the 2004 projects in page 28.

Going with the flow
(Prof. Leonhard Kleiser, Institute of Fluid Dynamics, ETH Zürich)

A numerical simulation of flowing particles by researchers at the Swiss Federal Institute of Technology Zürich (ETH Zürich) reveals trailing droplets and breakaway doughnuts. The research could have implications for understanding phenomena as diverse as avalanches and sandstorms and even improve efficiency in the chemical industry.

Physicists use statistics to explain the behaviour of gases, liquids and solid, but, granular materials present a different problem. Sometimes they behave as solids, sometimes fluids and explaining their bizarre behaviour is difficult. Consider a snow-covered peak. In settled times, the snow particles behave like a solid, but as soon as they start flowing downhill as happens during an avalanche, the flowing snow behaves more like a liquid. Pharmaceutical tablets behave similarly during packaging - in a container they act solid, but flow like a liquid. The concept of particle flow becomes even more complicated when one considers mixtures of more than one type of particle, or phase, such as oil droplets suspended in a solvent, bubbles in a fluid, or solid particles flowing with a liquid.

Thorsten Bosse of ETH Zürich's Institute of Fluid Dynamics explains that such two-phase flows range from large-scale phenomena, such as dust particle transport in the atmosphere to small-scale phenomena such as the formation of fatty deposits inside blood vessels. He adds that many engineering problems in the pharmaceutical and chemical industries, including mixing, drying, and transport processes, can involve such phenomena.

Bosse is using enhanced computational fluid dynamics (CFD) under the supervision of ETH Zürich's Leonhard Kleiser to study an example of two-phase flow: the settling of particles in suspensions. This phenomenon is observed in rain drops in the atmosphere, river sedimentation, and in chemical reactors and separators, for example.

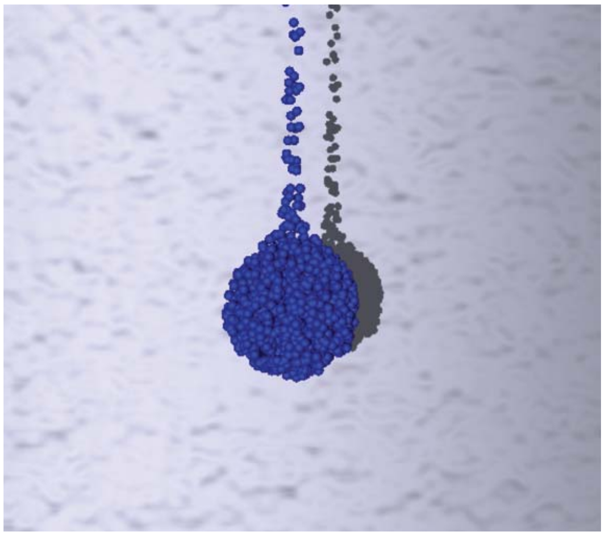
Chemical engineers need to understand the behaviour of two-phase flow if they are designing settling tanks for separating particles from a fluid and reaction vessels. To produce the best design, they need to know how much time the particles need to settle out, the average settling velocity in other words.

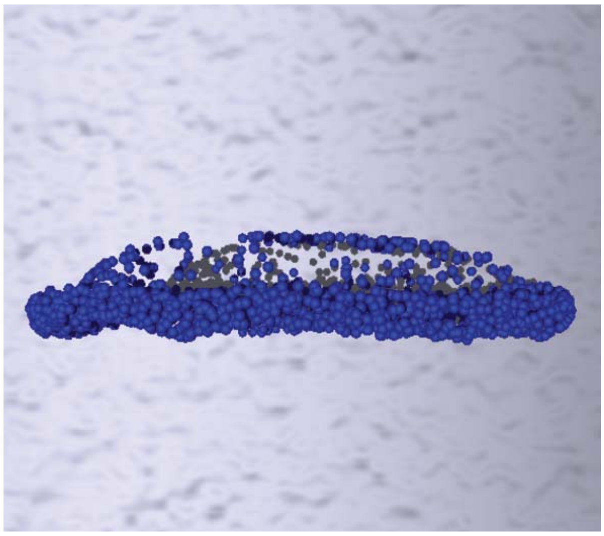
Bosse and his colleagues have carried out numerous investigations to help them understand the behaviour of solid particles in fluids. Their first project involves the settling of so-called "suspension drops" (initially spherical clouds of particles suspended in a still fluid). The second deals with an initially random particle suspension in a turbulent flow in which particles are uniformly distributed throughout the fluid at the beginning of a simulation. "Both projects are fundamental research," explains Bosse, "and we want to understand what happens in such systems and why."

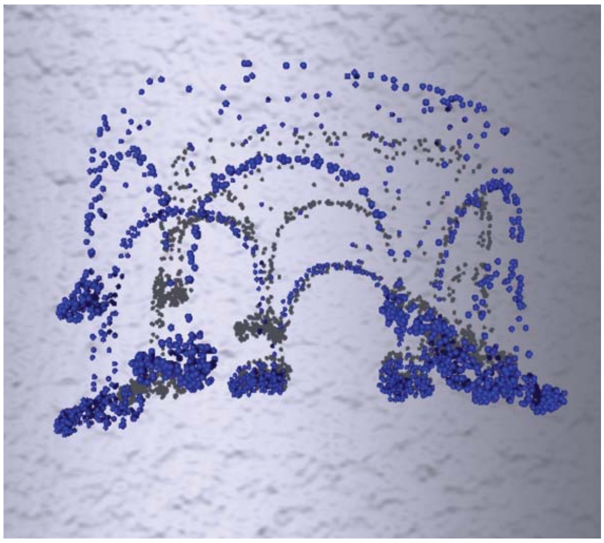
Their simulations revealed that when suspension drops settle in a very viscous fluid they retain their spherical shape but a tail of leaked particles forms behind them, explains Bosse. The second type of behaviour is far more complex. When suspension drops settle in a less viscous or "thinner" fluid or when the particles are heavier, the initially spherical droplets assume a shape resembling a doughnut, a torus. This torus becomes unstable and eventually breaks up into secondary blobs.

The second investigation involving turbulent flow has implications for chemical reactors and separators, says Bosse. Common sense suggests stirring a mixture would mix it evenly, but Bosse's results suggest this is not always the case.

While relatively light particles tend to go with the flow and are evenly mixed and much heavier particles simply sink to the bottom as expected, particles of a certain size and weight in between behave differently. Particles that are interacting more readily with turbulent eddies in the fluid are actually "de-mixed" from the fluid forming structures of very high particle concentration and large regions in between which are almost particle-free. This implies that straightforward mixing may not necessarily produce an even distribution of all particles in a fluid.







Global confirmation of the greenhouse effect
(Dr. Martin Wild, Institute for Atmospheric and Climate Science, ETH Zürich)

A high resolution computer model of the Earth's climate running at Swiss Center for Scientific Computing (CSCS) is allowing ETH researchers to make clearer predictions about the effects of local geography, such as mountain ranges, on climate change across the globe and to confirm the effect of greenhouse gases on the global climate.

Three-dimensional computer models are the most powerful tools for investigating the potential impact of human activities on the Earth's climate, according to Martin Wild, an atmospheric scientist at ETH Zurich. Models such as the global climate model known as ECHAM5 help researchers to predict climate changes on a timescale lasting decades on the basis of changing levels of atmospheric gases, aerosols or particulates, and other parameters, including cloud cover.

Wild and Atsumu Ohmura and their colleagues are running the ECHAM5 model on computers at CSCS and producing incredibly detailed predictions over the entire globe that can better account for the effects of individual surface features, such as mountain ranges.

The ETH Zurich researchers have focused on the climate effects near the earth's surface from the global scale down to the European and Alpine scales. They are looking at how the greenhouse effect affects near surface climate and hydrology. For instance, they are studying how topography affects surface solar radiation as well as thermal emission from the atmosphere radiating back to the surface. This, explains Wild, is the most direct effect to be felt at the surface as atmospheric greenhouse gas levels change.

Wild points out that an additional focus of his team's work is investigating the impact of greenhouse warming on the frozen parts of the Earth's surface, the "cryosphere" of snowy regions, mountain glaciers, and polar ice sheets, and their effects on sea levels. Because the surface detail included in the climate model they are running on CSCS computers is so high, they can make very detailed predictions about how changes in the cryosphere might affect sea levels. They can now more realistically simulate the accumulation of snow and so model mountain glaciers and polar ice sheets more effectively.

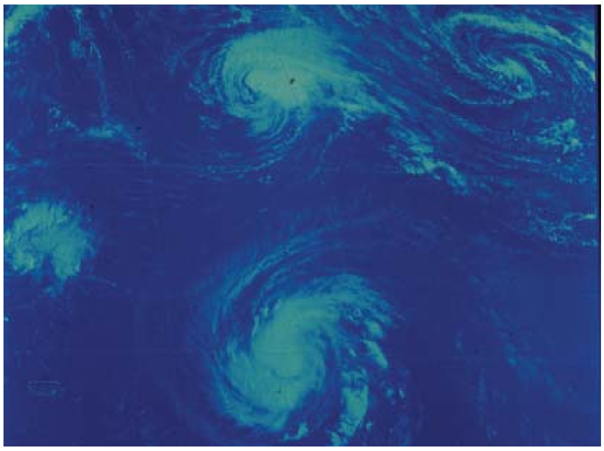
The experiments carried out at CSCS formed the key for the estimates of future contribution of polar ice sheets to sea level changes publishes in the third assessment report of the Intergovernmental Panel On Climate Change (IPCC).

The researchers are also using their model to understand the issue of "global dimming", the fall in solar radiation at the earth's surface that was first observed in the late 1950s but apparently ceased around 1990. Their research puts global dimming in a wider context linking the decline in solar radiation with long-wave radiation, surface temperature and water evaporation. A study of the period 1960 to 1990, using the climate model and real data suggests that global dimming may compensated for the greenhouse effect up to the 1980s and reduced evaporation from land surfaces between the 1950s and 1980s, so that changes that could lead to global warming were masked during this period.
We are now in a period of "global brightening" and Wild suggests that the ETH Zurich studies could help fine-tune the climate models so that the origins of these changes can be understood.

The team has also collaborated with Rolf Philipona on NCCR project 2.4 to focusing on how long-wave downward radiation has changed over time. This surface effect is the most obvious change observed as greenhouse gas levels change, Wild explains.
The scientists can now correlate changes in greenhouse forcing predicted by global climate models

to worldwide surface measurements of long-wave radiation. This means they could detect the greenhouse effect at the earth's surface earlier than by measuring temperature alone.

ECHAM running on CSCS computers has already demonstrated that an increase in long-wave downward radiation is linked with changes in rainfall and evaporation. The ECHAM predictions correlate directly with recorded temperature changes, says Wild, and help validate the model's ability to predict future changes due to the greenhouse effect.



Pictures: NOAA Photo Library

A model solution for biology
(Prof. Ursula Röthlisberger, Laboratory of Computational Chemistry and Biochemistry, EPF Lausanne)

Ursula Röthlisberger and Stefano Piana of the Institute of Molecular and Biological Chemistry, at the Federal Institute of Technology, EPFL, Lausanne, Switzerland are using the computing power of CSCS systems to allow them to simulate the behaviour of an important group of enzymes known as the procaspases. These enzymes are heavily involved in controlling the life cycle of the cell and when they go wrong, cancer and foetal abnormalities can be one of the results.

According to Röthlisberger, molecular dynamics simulations which work from the first principles, ab initio, of so-called density functional theory (DFT) have become a rather powerful tool for the study of physical and chemical systems with up to 1000 atoms and are now widely used by physical scientists. The idea of applying these powerful techniques to biological problems, such as protein folding, have only very recently come to the fore and are, she says, still in their infancy.

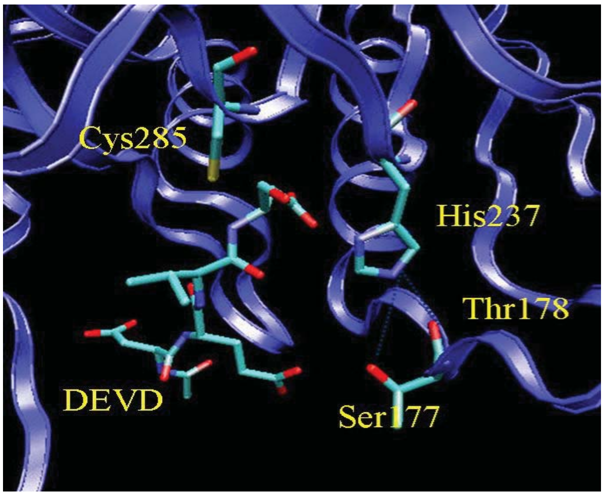
The EPFL team has found that they can extend the remit of ab initio DFT methods to systems containing many more atoms, such as enzyme systems and other proteins. They have devised a hybrid approach that blends the best of quantum and classical approaches - a QM/MM hybrid scheme. This approach is capable of undertaking in situ investigations of biochemical reactions by treating the reactive site of the system at the quantum mechanical (QM) level and the protein environment at the molecular mechanics (MM) level using DFT.

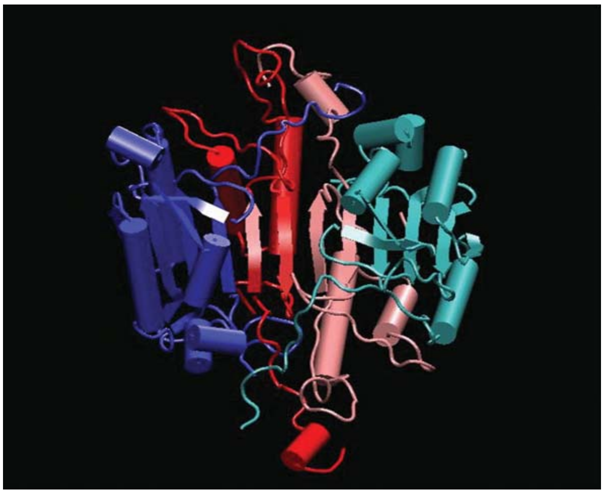
The team has applied this approach to the study of caspases and their precursor proteins, the procaspases. Caspases are a family of enzymes that play a central role in the process of programmed cell death, or apoptosis. Apoptosis is one of the processes by which our individual cells die when they come to the end of their useful life or when they have been damaged beyond repair. They accumulate in the cell in the form of relatively inactive proenzymes, which fold into their mature and active form following a cascade of biochemical reactions, which then instigates the apoptosis pathway. Consequently, procaspase regulation is crucial to the cellular life cycle. When the procaspase enzymes go awry, a variety of disorders such as deformities, nerve damage, and cancer can ensue.

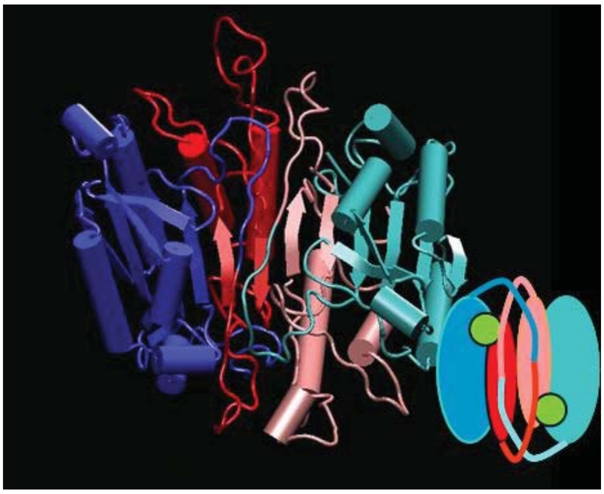
In 2004, Röthlisberger and Piana together with colleague Zoe Taylor of Curtin University of Technology in Perth Australia, published results showing how they had used related techniques to show that the folding pathways of procaspase 3 and 7 are very similar and have monomeric (one enzyme molecule) and dimeric (two enzyme molecules joined) intermediates. A third procaspase, procaspase 8, on the other hand, is more stable in the dimeric form than the monomeric and the way two copies of the enzyme are joined is very different from that seen in either of the dimers of procaspase 3 or 7. The researchers suggest that this difference could be very important in the initiation of apoptosis.

In a second paper, Piana and Röthlisberger team simulated two forms of caspase 3 and procaspase 3, the monomer (one enzyme molecule) and the dimer (two enzyme molecules joined together). They confirmed the validity of their simulations with X-ray crystallographic results, which measure the position of each atom in a molecule and found that the computer simulations provide a reliable picture of the enzyme in solution. Their first of two studies reveals that the way the procaspase enzyme is folded determines whether or not it is active and that only when it is reorganized by the cell's biochemistry does it trigger the cell death pathway.

These results and others obtained by the team with computational support from the CSCS are providing scientists with vital new clues about the involvement of protein enzyme folding in programmed cell death. They could ultimately open up new pathways to drugs for side-step problems with the system goes wrong.







List of Large User Projects 2004

Name	Organiszation	Project Title
Arbenz P.	ETH Zürich	Large scale eigenvalue problems in opto-electronic semico ductor lasers and accelerator cavities
Avellan F.	EPF Lausanne	Unsteady flow analysis in hydraulic turbomachinery
Baiker A.	ETH Zürich	Hydrogenation reactions in heterogeneous enatioselective catalysis and homogeneous catalysis in supercritical CO2
Baldereschi A.	EPF Lausanne	Structural and electronic properties of solids and surfaces
Beniston M.	Uni Fribourg	Global and regional climate modelling
Bey I.	EPF Lausanne	Coupling tropospheric chemistry and aerosols in the general circulation model ECHAM
Böckmann R.	Uni Zürich	Nanodynamics of MHC/peptide complexes and its dependence on MHC polymorphism
Bürgi Th.	Uni Neuchâtel	Structure and enantiospecificity of chiral nanoparticles and interfaces
Cooper W.A.	EPF Lausanne	Computation of stellarator coils, equilibrium and Sstability
Davies H.C.	ETH Zürich	ERA40 for NCCR-Climate
Fäh D.		ETH Zürich Site effects assessment using earthquake and seismic ambient vibration simulation
Fichtner W.	ETH Zürich	Computational science and engineering in microelectronics and optoelectronics
Folini D.	EMPA	Inverse modeling to monitor source regions of air pollutants in Europe
Gödecker St.	Uni Basel	Structure of large clusters, surfaces and biomolecules
Hasenfratz P.	Uni Berm	Hadron spectroscopy in QCD with 2+1 light flavours
Hauser A.	Uni Genève	Photophysics and photochemistry of transition metal compounds: Theoretical Approaches
Hutter J.	Uni Zürich	Development and application of ab-initio molecular dynamics methods
Keller J.	PSI	Air quality modeling in Switzerland
Kleiser L.	ETH Zürich	Numerical simulation of transitional, turbulent and multiphase flows
Koumoutsakos P.	ETH Zürich	Simulations using particle methods. Optimization of real world problems using evolutionary algorithms
		Multiscale modeling, simulation and optimization of complex systems
Leriche E.	EPF Lausanne	Direct numerical simulation ot the buoyancy-driven turbulence in a cavity: The DNSBDTC project
Leutwyler S.	Uni Bern	Proton transfer and hydrogen bonding in microsolvent clusters and nucleic acid base pairs: theroy and dynamics

Name	Organization	Project Title
Leyland P.	EPF Lausanne	Aerothermodynamic simulations in aerospace and aeronautic applications
Lüthi H.P.	ETH Zürich	Computational quantum chemistry of large molecules
Mareda J.	Uni Genève	Studies of uncatalyzed and antibody catalyzed reactions: modeling of cation-olefin cyclizations
Meuwly M.	Uni Basel	Electronic structure calculations for molecular dynamics simulations of iron-containing, reactive centers of biomolecules
		Theoretical investigations of iridium-catalyzed reactions
Moore B.	Uni Zürich	Computational cosmology
Ohmura A.	ETH Zürich	Global climate change: modelling atmosphere/ocean variability on decadel time scales
Parrinello/Deubel	ETH Zürich	Quantum chemical studies on the interaction of anticancer drugs with biological targets
Pasquarello A.	EPF Lausanne	Disordered network-forming materials
Quack M.	ETH Zürich	Quantum mechanical simulation of molecules and molecular clusters
Röthlisberger U.	EPF Lausanne	Mixed quantum mechanics / molecular mechanics study of systems of biological interest
Samland M.	Uni Basel	The Milky way and its satellite dwarf galaxies
Schär Ch.	ETH Zürich	Modelling weather and climate on european and alpine scales
Sennhauser U.	EMPA	Nanoxid
Steurer W.	ETH Zürich	Minerals and planetary materials
Stocker Th.	Uni Bern	Monalisa: modelling and reconstruction of north Atlantic climate system variability
Troyer M.	ETH Zürich	Simulation of quantum phase transitions
Van Swygenhoven H.	PSI	Modelling of nanostructured materials
Vogel P.	EPF Lausanne	New organic chemistry with sulfur dioxide Electron releasing homoconjugated carbonyl group
Weber J.	Uni Genève	Computational quantum chemistry of increasingly complex systems
Yadigaroglu G.	ETH Zürich	DNS and LES of multiphase flows

Facts & Figures

Income & expenditure flow (1.1.2004-31.12.2004)

Expenditures		Income	
Investments	**632'267.07**	**Basic Budget**	**10'420'000.00**
		Contribution ETH Zurich	6'720'000.00
Materials, Goods & Services	**7'438.79**	Contribution ETH-Board	3'700'000.00
Personnel	**3'390'970.64**		
Payroll	2'776'523.75		
Employer's contributions	365'818.00		
Other	248'628.89	**Third-party contributions**	**632'817.05**
		Meteo Swiss	556'568.85
Other material expenses	**3'081'919.78**	KTI/CTI	73'000.00
Floor space	39'926.65	Other third-party	3'248.20
Maintenance	117'773.31		
Energy & media	385'788.01		
Administrative expenses	17'593.95		
Hardware, software, services	2'440'788.02		
Services & remunerations	76'808.08		
Other	3'241.76		
Internal payments	**163'641.05**		
Contributions to ETH Zurich	33'144.90		
Administrative expenses	30'144.50		
Infrastructure duties	100'381.65		
Expenses total	**7'276'237.33**	**Income total**	**11'052'817.05**
Balance			**3'776'579.72**

– All figures are given in CHF.

– The balance is rolled over to the 2005 budget, according to the decision of the Steering Board.

Cost Distribution

Cost element	Q1	Q2	Q3	Q4	Total
Costs of goods & services	7'606	39	50-		7'595
Costs of personnel	758'533	794'648	824'585	1'015'406	3'393'172
Costs of administration and building infrastructure	*75'546*	*264'408*	*183'229*	*186'241*	*709'425*
Costs of hardware, software, services	*558'066*	*745'383*	*547'362*	*520'923*	*2'371'735*
Other costs	*20'123*	*5'911*	*5'306*	*49'868*	*81'209*
Losses from outstanding claims		*33'145*			*33'145*
Depreciation of investments	*1'268'173*	*1'243'630*	*1'268'385*	*1'267'139*	*5'047'327*
Total costs of materials	1'921'909	2'292'476	2'004'283	2'024'171	8'242'840
Internal payments to ETH Zurich & other extraordinary costs		26'478		2'868	29'347
Total costs	**2'688'048**	**3'113'641**	**2'828'819**	**3'042'446**	**11'672'954**

Compute infrastructure

Vendor & Model	CPU Type	No. Of Processors	No. Of Nodes	Interconnect type	Interconnect bandwidth per partition (MB/s)	Interconnect typology	Total memory size (GB)	Year of installation plus upgrade history	Peak Performance (Gflop/s)	LINPACK Perfomance (Gflop/s)	Actual TOP500 position	Total File System Size (TB)	Annual direct costs in 2004 (CHF)
NEC SX-5/16	NEC custom	16	1	N/A	N/A	N/A	64.00	2000	128.00	125.80	-	1.00	1’505’050.00
IBM pSeries 690 Turbo	Power-4 1.3GHz	256	8	Double Colony	400.00	Star	768.00	2002	1’380.00	736.60	-	4.00	4’463’350.00

Usage statistics

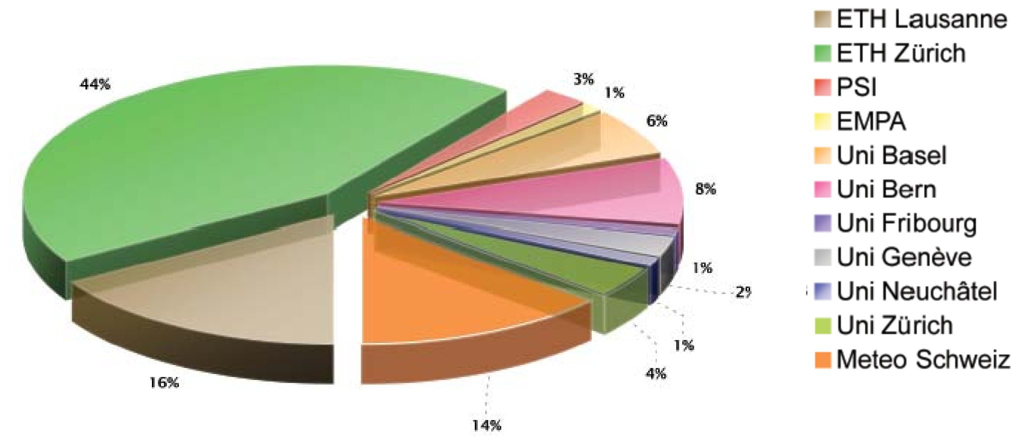
Usage by research fields

	Chemistry	Engineering	Environment	Material Sciences	Physics	Other	Internal
NEC	9%	3%	44%	7%	30%	2%	5%
IBM	64%	3%	8%	12%	11%	0%	2%

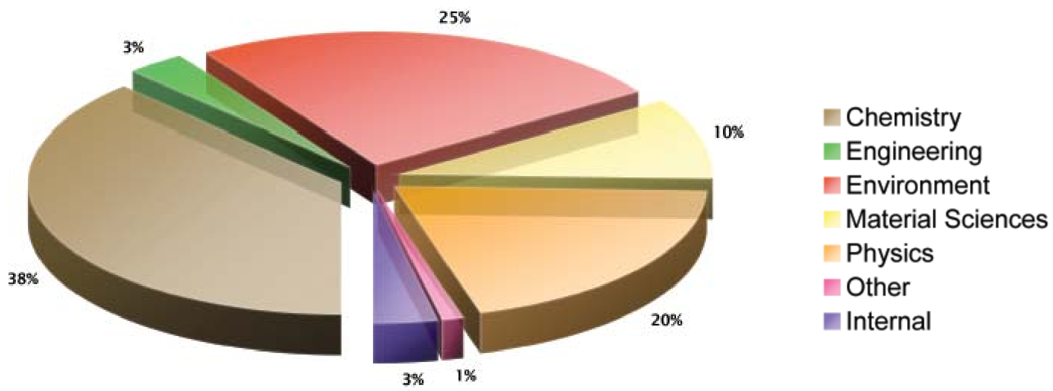
Usage by customer

	ETH Lausanne	ETH Zürich	PSI	EMPA	Uni Basel	Uni Bern	Uni Fribourg	Uni Genève	Uni Neuchâtel	Uni Zürich	Meteo Schweiz	CSCS	NEC
NEC	9%	40%	0%	1%	9%	0%	1%	3%	0%	3%	28%	3%	3%
IBM	22%	46%	5%	0%	2%	16%	0%	1%	2%	4%	0%	2%	0%

Cost of machines per institution based on total cost of ownership of HPC systems



Cost of machines per discipline based on total cost of ownership of HPC systems



Cost analysis

Cost coverage by customer

	ETH Lausanne	ETH Zürich	PSI	EMPA	Uni Basel	Uni Bern	Uni Fribourg	Uni Genève	Uni Neuchâtel	Uni Zürich	Meteo Schweiz	CHIPP*	VATech (KTI)	CSCS	NEC	Total
Proceeds																
Total	**0**	**6'720'000**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**556'568**	**0**	**73'000**	**3'703'248**	**0**	**11'052'817**
Direct costs																
Directly assigned staff	0	0	0	0	0	0	0	0	0	0	180'522	46'721	18'199	2'365'527	0	2'610'970
Compute server costs (incl. sys admin staff)	1'117'391	2'655'161	223'167.50	15'050	224'721	714'136	15'050	89'785	89'267	223'685	421'414	0	0	134'418	45'151	5'968'400
Other costs	0	0	0	0	0	0	0	0	0	0	154'981	0	0	2'938'601	0	3'093'583
Total	**1'117'391**	**2'655'161**	**223'167**	**15'050**	**224'721**	**714'136**	**15'050**	**89'785**	**89'267**	**223'685**	**756'918**	**46'721**	**18'199**	**5'438'547**	**45'151**	**11'672'953**
Costs after redistribution of cost of remaining scientific personnel to LUP customers																
Redistributed staffing costs	65'826	65'826	65'826	65'826	65'826	65'826	65'826	65'826	65'826	65'826	0	0	0	-658'260	0	0
Total	**1'183'217**	**2'720'987**	**288'993**	**80'876**	**290'547**	**779'962**	**80'876**	**155'611**	**155'093**	**289'511**	**756'918**	**46'721**	**18'199**	**4'780'287**	**45'151**	**11'672'953**

*Swiss Institute of Particle Physics

Cost coverage by research field

	Chemistry	Engineering	Environment	Material Sciences	Physics	Other External Research	Grid	Visualization	Internal	Total
Proceeds										
Total	**0**	**0**	**556'568**	**0**	**0**	**0**	**0**	**73'000**	**10'423'248**	**11'052'817**
Direct costs										
Directly assigned staff	95'231	0	180'522	0	108'438	0	174'382	252'814	1'799'581	2'610'970
Compute server costs (incl. sys admin staff)	2'991'998	179'052	1'019'290	640'955	942'483	30'101	0	0	164'519	5'968'400
Other costs	0	0	154'981	0	0	0	0	0	2'938'601	3'093'583
Total	**3'087'230**	**179'052**	**1'354'794**	**640'955**	**1'050'921**	**30'101**	**174'382**	**252'814**	**4'902'702**	**11'672'953**

FIDIREVISA
Società di revisione e consulenza

An den Vorstand (Steering Board) des
CSCS SWISS NATIONAL
SUPERCOMPUTING CENTRE
6928 Manno

Lugano, den 18. Februar 2005/GZ/GG/zn

Sehr geehrte Damen und Herren,

auftragsgemäss, haben wir das Management Reporting (4. Quartal 2004/Jahresabschluss) des CSCS SWISS NATIONAL SUPERCOMPUTING CENTRE für das am 31. Dezember 2004 abgeschlossene Geschäftsjahr geprüft.

Für das Management Reporting (4. Quartal 2004/Jahresabschluss) ist der Vorstand (Steering Board) verantwortlich, während unsere Aufgabe darin besteht, dieses zu prüfen und zu beurteilen. Wir bestätigen, dass wir die gesetzlichen Anforderungen hinsichtlich Befähigung und Unabhängigkeit erfüllen.

Unsere Prüfung erfolgte nach den Grundsätzen des schweizerischen Berufsstandes, wonach eine Prüfung so zu planen und durchzuführen ist, dass wesentliche Fehlaussagen im Management Reporting (4. Quartal 2004/Jahresabschluss) mit angemessener Sicherheit erkannt werden. Wir prüften die Posten und Angaben des Management Reporting (4. Quartal 2004/Jahresabschluss) mittels Analysen und Erhebungen auf der Basis von Stichproben. Ferner beurteilten wir die Anwendung der massgebenden Rechnungslegungsgrundsätze, die wesentlichen Bewertungsentscheide sowie die Darstellung des Management Reporting (4. Quartal 2004/Jahresabschluss) als Ganzes. Wir sind der Auffassung, dass unsere Prüfung eine ausreichende Grundlage für unser Urteil bildet.

Wir empfehlen, das vorliegende Management Reporting (4. Quartal 2004/Jahresabschluss) zu genehmigen.

Mit vorzüglicher Hochachtung
FIDIREVISA SA

G. Zwahlen G. Ghesa
Leitende Revisoren

Beilagen:
Management Reporting (4.Quartal 2004/Jahresabschluss)

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Tel. +41 (0)91 913 32 00
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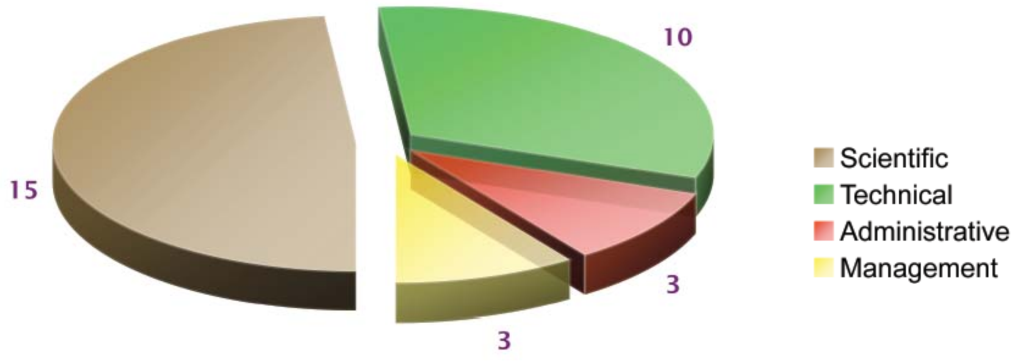
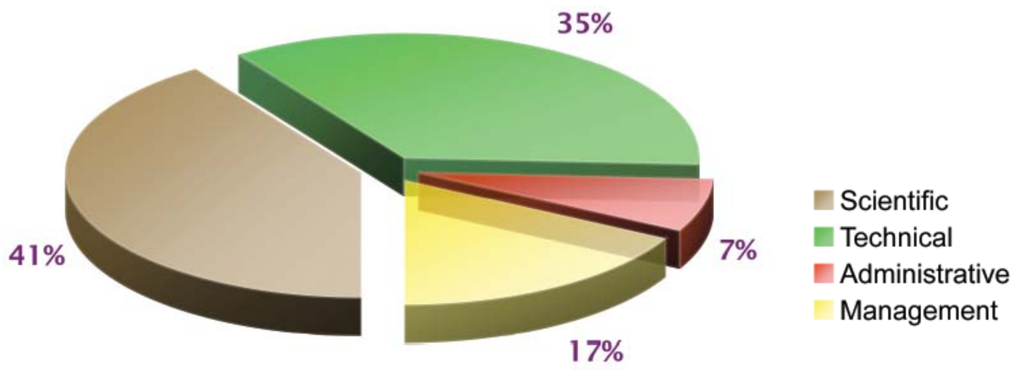
Personnel

Head Count (as of 31st December 2004)



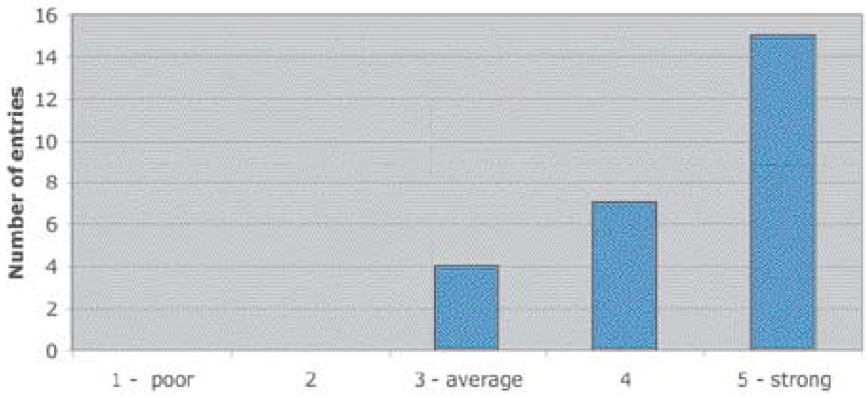
Staffing Costs (total for 2004)



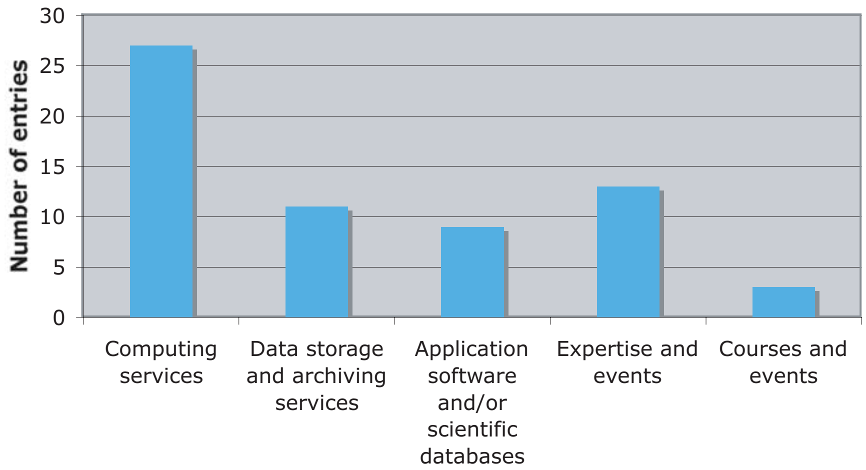
Customer satisfaction (March 2005)

The following customer survey results are based on responses of 70% of the groups that run large projects on CSCS systems.

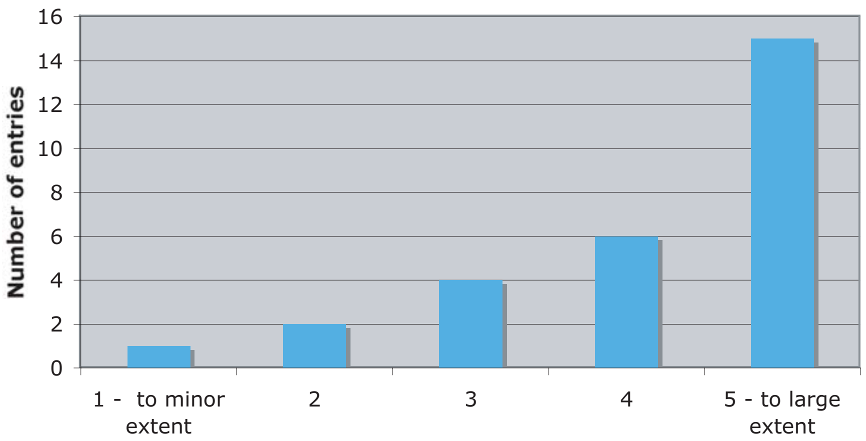
Quality of computer support services



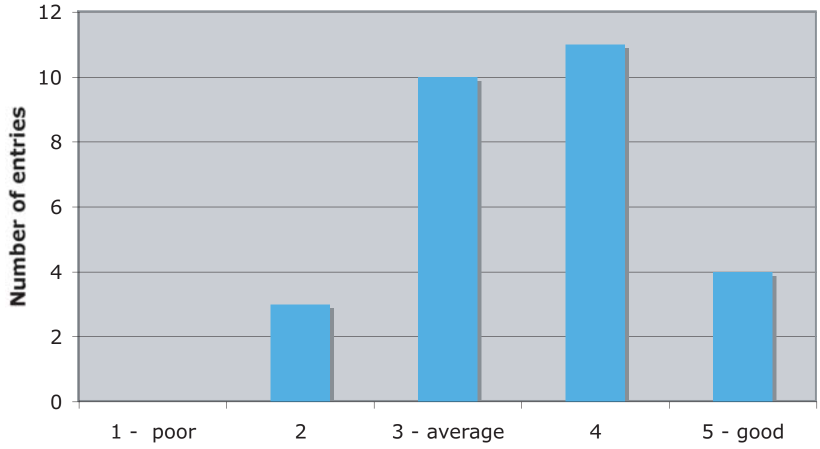
Q: Which services of CSCS are important in your work?



Q:To what extent have CSCS services enabled your scientific work?

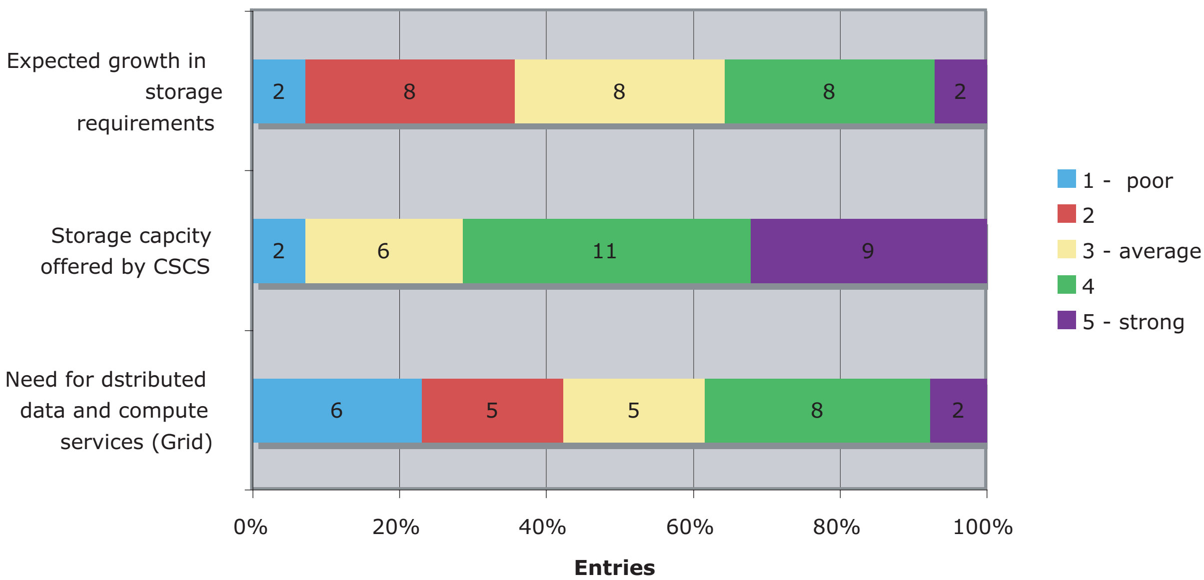


Q: Did the performance of computer environment at CSCS meet your expectations?



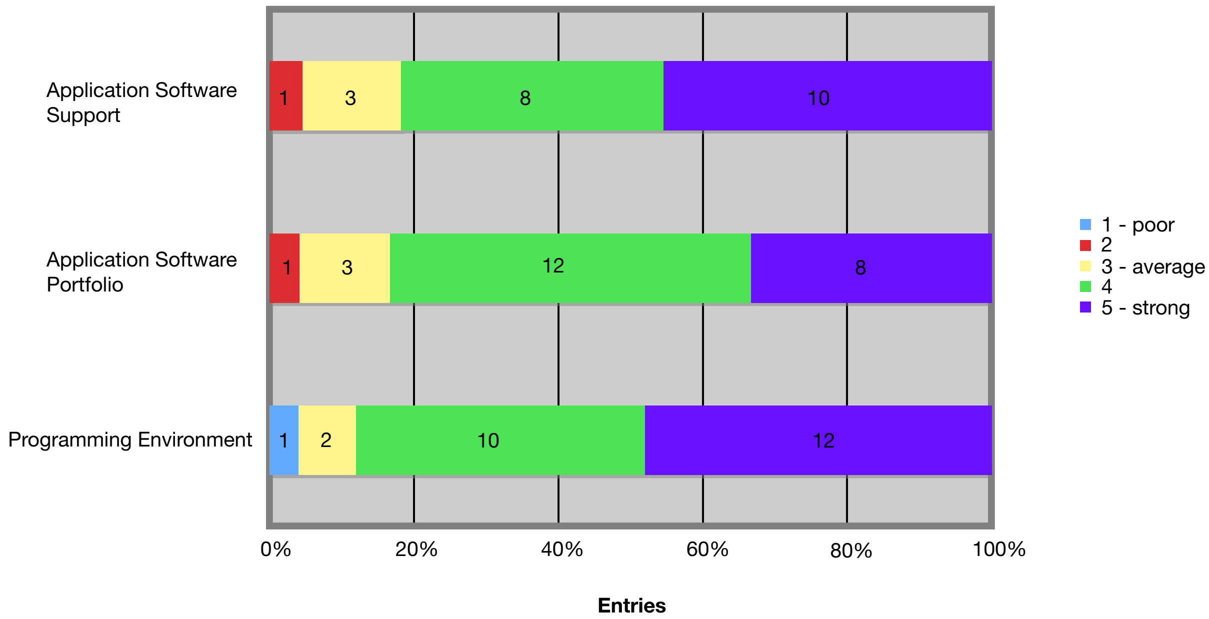
Need for technical resources

(Number in bars indicate the absolute number of entries per category)



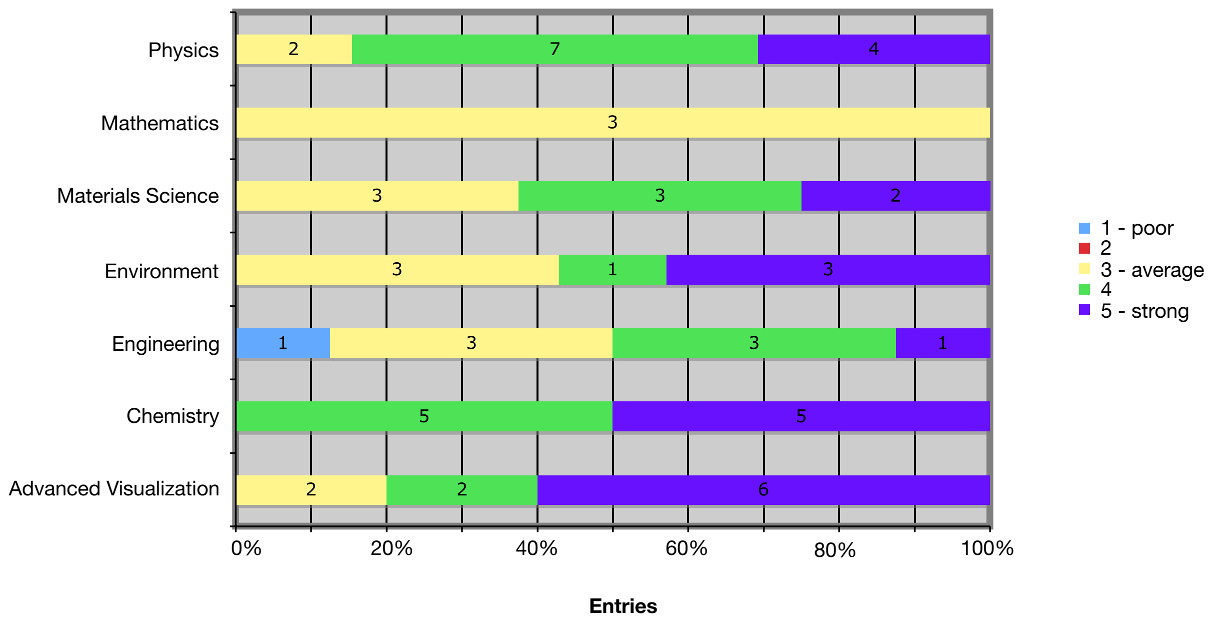
Quality of application software

(Number in bars indicate the absolute number of entries per category)



Quality of research support services

(Number in bars indicate the absolute number of entries per category)



Publications

Awards won by collaborators CSCS

The Division of Fluid Dynamics of the American Physics Society selected the visualization "Settling and Break-up of Suspension Drops" as one of four winners of the Gallery of Fluid Motion of the 2004 Conference held in November 2004 in Seattle.

"Settling and Break-up of Suspension Drops", Thorsten Bosse, Swiss Federal Institute of Technology, Zurich, Eckart Meiburg, University of California at Santa Barbara, Leonhard Kleiser, Swiss Federal Institute of Technology, Zurich & Jean Favre, Swiss National Supercomputing Centre (CSCS)

The award includes publication in the September 2005 issue of "Physics of Fluids"

Papers published by collaborators CSCS

"Introduzione alla visualizzazione scientifica", Marmo R., Valle M., Zannoni C., Eds Il Rostro 2004

"Large Data and Distributed Visualization with The Visualization Toolkit (VTK)", Favre J. M., EPFL Supercomputing Review 2004, http://sic.epfl.ch/SA/publications/SCR04/scr_14.pdf

"Numerical flow analysis in a Pelton turbine bucket", PerrigA., Farhat M., Avellan F., Parkinson E., Garcin H., BisselC., Valle M., Favre J. M., 22nd IAHR SYMPOSIUM on Hydraulic Machinery and Systems, June 2004, Stockholm, http://www.swedpower.se/iahr2004/authors_papers.htm

"AVS and AVS/Express", book chapter in The Visualization Handbook, Eds Hansen C. & Johnson C., Elsevier Academic Press, ISBN 0-12-387582-X

Papers published by users of CSCS

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Design, Production:
Dorothea Gerhardt, CSCS
Consultant: Andretta Grafik

Printing
Hürzeler AG, Regensdorf

Print-run:
550