CSCS
Swiss National Supercomputing Centre

Annual Report 2005

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Meetings of Steering Board (SB), Financial Audit Committee (AC) and Scientific Advisory Board (SAB) in 2005

3.2.2005, SB and AC at CSCS, Manno
11.4.2005, AC at CSCS, Manno
17.5.2005, SB and AC at PSI, Villigen
16.9.2005, SB/SAB and AC at ETH, Zurich
21.11.2005, AC at ETH, Zurich
2.12.2005, SB and AC at CSCS, Manno

Content

Prof. Mario Botta, photo by Beat Pfändler

Carte Blanche

Avere la possibilità di esplorare comprendere e visualizzare i significati e i comportamenti di eventi sconosciuti alla nostra ragione è un anelito naturale che motiva il nostro stesso operare.

Indagare i meccanismi delle leggi fisiche o biologiche presenti in natura, fa parte dell'istinto dell' uomo, così come la necessità di condividere con l'intera umanità il sapere acquisito è la ragione stessa del vivere civile. La somma delle conoscenze che si sono accumulate lungo l'arco della storia è un patrimonio collettivo che connota l'identità e la crescita delle differenti comunità. Per questo possiamo affermare che a un maggior sapere corrisponde anche una più avanzata civiltà. E così ogni qualvolta ci giunge notizia di una nuova conquista nell'ambito del sapere abbiamo la sensazione di sentirci più ricchi, riconosciamo di appartenere ad una più vasta collettività e ritroviamo una nuova serenità rispetto alla storia travagliata del nostro tempo.

Questi pensieri mi sono passati nella mente dopo una recente visita negli spazi del CSCS a Manno. Certo, il "supercomputing" si presenta come strumento e come tale può svolgere unicamente un servizio rispetto alle intelligenze, alle ricerche, alle intuizioni che la società è in grado di elaborare; ma sapere che esiste un centro pionieristico e intuirne le potenzialità ci rassicura come studiosi e ci spinge ad affrontare con maggiore speranza le sfide e le insidie del nostro tempo.

La complessità sempre più estesa delle interrelazioni che caratterizzano il "villaggio globale" e la rapidità delle sue continue trasformazioni, comportano, per il cittadino come per lo scienziato, l'esigenza di un impegno teso a comprendere e razionalizzare il sapere nel tentativo di penetrare i differenti fenomeni che sorreggono la vita.

Il Centro Nazionale Svizzero di Calcolo è una potente struttura di produzione e divulgazione di dati disponibili per i programmi di ricerca e per le spinte creative che il paese saprà elaborare. D'altra parte è la nostra stessa condizione di nazione ricca e privilegiata nell'ambito della cultura occidentale che ci richiede di assumere questa responsabilità nello studio e nella ricerca: le idee sono le premesse indispensabili per trasformare le attese in nuove realtà. In tal senso è possibile interpretare la società anche come somma di intelligenze che interagiscono in un contesto storico. È questa una bella immagine che ci suggerisce di valutare il CSCS come strumento di crescita sociale oltre che di progetto tecnico dove le elaborazioni matematiche, le simulazioni scientifiche e le visualizzazioni virtuali che si rendono possibili nei differenti programmi diventano anche speranze concrete per migliorare la qualità della vita.

Come architetto mi sembra di riconoscere come la complessità delle relazioni che caratterizzano questo strumento e le potenzialità delle indagini presentano molte analogie con l'infinita rete di comportamenti (mobilità di uomini e cose, problemi sollevati dalla scarsità dalle risorse energetiche, nuovi equilibri ambientali) che oggi caratterizzano l'organizzazione del territorio.

La speranza è che anche gli operatori territoriali (architetti e ingegneri) possano accedere alle ricerche del CSCS. La rete dei problemi dettata dalla nuova globalizzazione potrà forse allora meglio interpretare anche i valori di storia e memoria del nostro contesto e concorrere così ad organizzare una migliore qualità dello spazio di vita dell'uomo.

Mario Botta

Carte Blanche

Having the opportunity to examine and understand, as well as visualise the meanings and behavioural patterns of events as yet unknown to our reasoning, is a natural yearning that motivates the way we operate.

The investigation of mechanisms of physical or biological laws that are present in nature is part of human instinct, just as the necessity to share acquired knowledge with the whole of humanity is civilised life's very reason for being. The sum total of knowledge accumulated throughout history is a collective heritage, which describes the identity and growth of the various communities. Therefore, we can affirm that greater knowledge corresponds with a more advanced civilisation. In this way, when every now and then a new conquest in field of knowledge comes our way, we feel richer and confirmed in our role as part of a greater collective, and we gain a new serenity with regard to the troubled history of our times.

These thoughts occurred to me after a recent visit to the grounds of CSCS in Manno. Supercomputing is a tool and as such can only develop a service with respect to the understanding, research and insight that society is able to formulate. The knowledge of the existence of a pioneering centre and to feel its potential reassures us as scholars and pushes us to confront the challenges and dangers of our times with greater hope.

The ever-expanding complexity of the interrelations that characterise the "global village", and the rapidity of its continuous transformations, involves – for the citizen as well as the scientist – the need for a commitment that is aimed at understanding and rationalising knowledge in the attempt to comprehend the various phenomena that support life.

The Swiss National Supercomputing Centre is a powerful structure of production and data distribution made available to research programmes and for creative thrust that the nation hopes to develop. On the other hand, it is a condition of our status as a rich, privileged nation within the ambit of Western culture demands that we assume this responsibility in study and research: ideas are the essential basis for transforming expectations into new realities. In this sense, it is also possible to interpret society as a sum total of acquired knowledge that interacts within an historical context. This is an attractive prospect which suggests to us that CSCS should be valued as a tool of social growth as well as a technical project where mathematical processes, scientific simulations and virtual displays that are made possible also become specific goals for improving the quality of life.

As an architect I feel that I am able to recognise how both, the complexity of relations which characterise this tool and the capacity of the research, present many analogies with an endless network of behavioural patterns (the mobility of man and things, pro-blems raised by the scarcity of energy resources, new environmental balances) which today our special planning.

The hope is that those involved in the planning of space (architects and engineers) can also gain access to CSCS's research. The network of problems dictated by the new globalisation may then also help to better interpret the importance of history and recollection of our context, and in this way contribute to organising a better quality of living space for man.

Mario Botta

Activity Report

Introduction

When I have the chance to give presentations about scientific computing to the younger generations, I always insist on the intrinsic beauty in creating or visualizing virtual experiments, cutting through complex data, simulating physical objects and complex phenomena with the power of mathematical modeling. Yes, mathematics can be fun, elegant as well as an excellent tool for diving into the complexity of nature, and for making scientific progress. For every young person interested in considering a scientific career the long-term potential benefit resulting from the created innovation, economic value and knowledge must be considered. As a publicly funded institution, such dialog with the members of the public is our duty.

We have the honor to have the 2005 edition of the activity report prefaced by Prof. Mario Botta, who has captured the value and the beauty of the possibility to visualize and “move through” the data scientists and engineers deal with. He is an excellent advocate of the indispensable need to knit the relation between scientific work and the human intuition, creativity, and memory.

The Steering Board of CSCS, who oversees the activities of the centre and guides it in accordance with the performance agreement set out in 2004, was initially elected for 2 years. ETH-Board confirmed all members of the Steering Board for the next 2-year period in December 2005. At the same time Prof. Ulrich Suter stepped down as Vice President of Research to be replaced by Prof. Dimos Poulikakos, author of this years introduction to the research digest. We look forward to working with the new Vice President over the coming years.

The restructured resource application process was put into action in the fall of 2005 for the call for project for the first half of 2006. The newly formed Scientific Review Committee met in Zurich in

October for the scientific evaluation of the 44 submitted projects. During 2005 the CSCS resources served 38 large projects from most academic institutions of Switzerland. The existing IBM and NEC systems continued to yield good efforts as stable production systems. The newly acquired CRAY XT3 “Horizon” system proved to be an invaluable addition for satisfying the growing needs of our users and facing the challenges of future breakthroughs. As of July the first early users were allowed on to the yet unstable system to test their codes and the efficiency of the machine. First results obtained by these early users proved to be an exciting taste of the possibilities yet to come once the system would reach full production and stability. Horizon passed its acceptance test in December and was sent into production as of January 2006. In order to maintain the level of compute power equivalent to the worldwide ranking of ETH and the quality science performed in Switzerland CSCS put out a request for purchase (RFP) under the code name of “Terrane”, published with agreement of the Steering Board in September, that would complement the existing architectures available at CSCS and replace the outgoing technology. We hope to bring the Terrane system into production in time for the resource allocations for the 2nd half of 2006.

The acquisition of the Horizon system allowed us to form a working partnership with the Paul Scherrer Institute (PSI) leading to an enriching and challenging exchange between the two institutions. Other existing partnerships with CERN’s LCG project and the Swiss Bio Grid have continued to unfold throughout the year. We were also able to sign a new contract with MeteoSwiss for the continued support of their compute needs by CSCS.

CSCS has continually been involved with educational activities, workshops and conference activities throughout 2005 – confirming the trend set out in the previous year. 2006 will see these activities progress further.

As the Swiss National Supercomputing Centre CSCS will over the next two years develop its specific branding around HPC software capable of bridging a number of hardware platforms, data intensive applications and the introduction of new leadership class capability computing resources.

Just like a competitive sailing team CSCS has spent the first 2 years of its performance agreement working towards an optimal tuning of its resources that would allow it to achieve the best results. Given the rapid development in our sector we continually have to adapt to new challenges in order to best serve our users and the scientific community of Switzerland.

We hope you enjoy your sail through CSCS’s 2005 achievements!

Dr. Marie-Christine Sawley
CEO

Computer Resource Allocation at CSCS – The Important Role of the Scientific Review Committee

In spring 2005, the Steering Board of CSCS gave a mandate to CSCS to establish a scientific review committee (SRC) to give scientific advice to CSCS for the resource allocation process, i.e., the selection of the end-user projects to which computational resources will be assigned. CSCS appointed the following scientists to serve on the committee: Rudolf Aebersold (ETH Zurich, bioscience), Martin Beniston (University of Fribourg, environmental sciences), Peter Hasenfratz (University of Bern, physics), Jari Järvinen (CSCS, mathematics), Leonhard Kleiser (ETH Zurich, engineering), Hans-Peter Lüthi (ETH Zurich, chemistry) and Michael Posternak (EPF Lausanne, materials science).

The SRC started its three years mandate (September 1, 2005 – August 31, 2008) in October under the chairmanship of Hans Peter Lüthi. This was in parallel with CSCS' Call for Proposals (CFP) for computational resources. By the deadline, CSCS received 68 proposals, of which 45 were handed over as large project proposals to the SRC. Proposals are categorized as large projects, if computational requests exceeded specified thresholds in CSCS' computing environment, i.e., 1000 CPU hours/month on the IBM SP4, 3000 CPU hours/month on the Cray XT3 or 100 CPU hours/month on NEC SX-5. Requests falling below these thresholds were considered as small projects, and they were reviewed by CSCS directly.

The total requests for resources expressed in CPU hours per month in large project proposals were 144506 (on IBM SP4), 1056320 (on Cray XT3), and 8190 (on NEC SX5). The available resources at CSCS were only 86512, 400000 and 4019 CPU hours/month, respectively. The SRC was therefore forced to propose cuts, which amounted to 40% on SP4, 62% on XT3, and 51% on SX5.

In the review process, the large project proposals were rated according to their scientific and computational merit. Apart from their previous record, the committee also considered the research funding situation of each proposal. Many of the projects had obtained grants from national and international funding organizations, and had therefore been subjected to a review process already. The SRC also honored the technical aspect of the project based on the pre-evaluation of CSCS (e.g. computational methodologies, software development efforts, level of parallelism and suitability of software on specific architectures). As a result of a very dedicated review process, where at least two reviewers were assigned to a project proposal, nearly no linear cuts had to be applied.

Following the recommendations of the SRC, CSCS assigned allocations for the first six months in 2006. CSCS informed the end-users on the allocations the week before the Christmas and they were effective in January. Based on feedback of end-user, the review process was accepted in the user community. The only concern was the tight schedule for this first review process. This was also the first time that CSCS applied electronic applications forms in resource requests.

Jari Järvinen

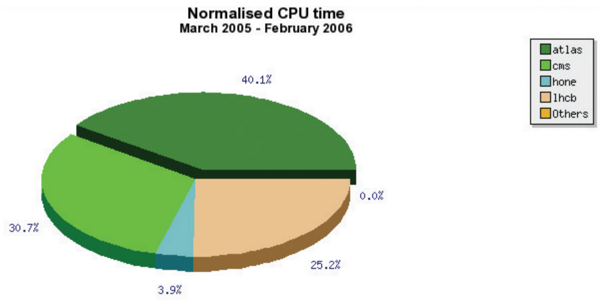
Swiss Grid Initiative at CSCS
LHC - LCG

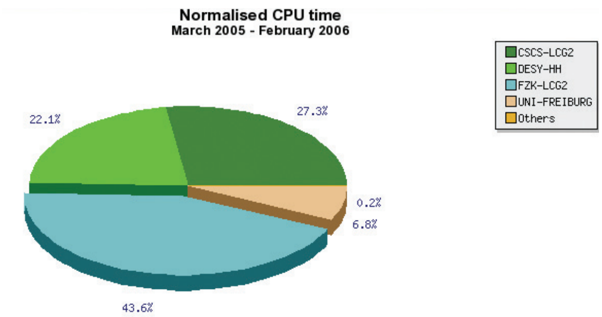
The main purpose of the LCG project is to establish a stable computing infrastructure for scientific simulation, processing and analysis of the data produced by the new particle accelerator built at CERN, known as the Large Hadron Collider (LHC).

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 event reconstructions and data analysis for the entire Swiss high energy physics community.

In 2005, the new computing infrastructure named 'Phoenix' has started to provide significant resources to the CHIPP community. With an aggregate peak of 180 Gflops and with a total storage capacity of 8TB, Phoenix is only the first building block of the LCG infrastructure foreseen to be put in place by the end of 2008 at CSCS.

CHIPP is participating in three of the four LHC experiments: ATLAS, CMS and LHCb. The Phoenix cluster runs the basic LCG middleware with all the necessary additions to support the applications of these three experiments. CSCS has provided continuous support during 2005 to maximize the availability and efficiency of Phoenix. Later in the year, support for H1 was added on the request of CHIPP. H1 is an experiment running on the HERA collider at DESY, the German national high-energy physics laboratory located near Hamburg.





Coexisting with the Grid middleware that every LCG Tier-2 site must support, Phoenix provides an additional NorduGrid interface that enhances its flexibility in terms of Grid services provided.

During 2005 Atlas has already produced a large amount of scientific results that have been published in "The Swiss ATLAS Computing Prototype", presented at SUN High Performance Computing Consortium Europe 2005.

Gian Luca Volpato

Swiss Bio Grid

CSCS is participating in the Swiss BioGrid project that has the aim to support large-scale computational applications for bioinformatics, biosimulation, chemoinformatics and biomedical sciences. The partners are among the most prominent research institutions both in education and industry in Switzerland. The Swiss BioGRID will make use of the available distributed high-performance computers, high-speed networks, large data collections and archives, and has the goal to integrate the necessary tools and services to establish a collaborative platform, addressing the key scientific challenges of life science.

In 2004 a preliminary roadmap for the project has been written. As a first step, a proof-of-concept study was foreseen to demonstrate the feasibility of a collaborative framework between the partners.

In 2005 this study has begun to show results. The partners at the Biozentrum have assembled the fundamental tools and data necessary into an in-house implementation called ProtoGRID aimed to ensure the minimal connectivity between sites participating to the Proof of Concept phase. The proof-of-concept has demonstrated that by pooling the resourc-es in the Swiss BioGrid it is possible to exceed the capabilities provided by each individual institution alone.

In parallel with the development of the ProtoGRID, partners in the Swiss BioGRID project with the leadership of CSCS have started to gather requirements for a more general Grid infrastructure. The Grid middleware that has been selected as the baseline for this first next level Grid service framework is called NorduGRID. This infrastructure is currently running at CSCS, Vital-IT, and the University of Zurich. The next step will be to extend this infrastructure and to federate it with the ProtoGRID to provide a homogeneous and comprehensive solution to the applications.

Sergio Maffioletti

Intelligent Grid Scheduling System

The Intelligent Scheduling System (ISS) has the ambitious goal to provide a Grid service capable of locating the most suitable resource to execute an application on the Grid.

The ISS would rely on information and monitoring data collected from the distributed infrastructure, taking into account and learning from application behavior and performance. The user launching an application can specify the requirements in terms of resource usage, dependencies and also performance and the ISS will decide which resource should be used, improving from experience in time.

Current Grid schedulers have no adaptive learning capability yet, taking into account application characteristics. The ISS may become the first scheduler of this kind, improving the throughput of the Grid as a whole.

The ISS has three partner institutes, the Ecole d'Ingenieurs de Fribourg (EIFR), the EPF Lausanne and CSCS. The project will be realized in three phases. During the first phase, current Grid middleware solutions that the ISS could make use of are being evaluated. This evaluation has already begun and UNICORE was choose as the base infrastructure to be used for this phase. This infrastructure is being deployed on the currently available resources at EIFR and EPF Lausanne.

During the first phase, only static monitoring information is being taken into account for scheduling. In order to make the best use of UNICORE, there has been a very fruitful collaboration with the Research Centre Juelich in Germany.

For the second phase it is planned to adapt ISS to a second Grid infrastructure and to test it with additional applications. In this phase already dynamic monitoring data will be collected during and after the execution of each application.

Finally, the third phase will concentrate on the statistical evaluation of the data collected over extended periods of time so that resources can be optimized and adapted to the demand of the applications. For example, overloaded resources can be identified early and measures can be taken to avoid bottlenecks.

Sergio Maffioletti
Nello Nellari

SEPAC

The SEPAC project (Southern European Partnership for Advanced Computing) has been initiated in 2004 as an evolution of the previous international TAPAC project (Trans-Alpine Partnership for Advanced Computing) where the partners involved are by CILEA, ETH Zurich and HP.

Three new important European groups, leaders in advanced technologies, associated with University of Zurich, CSCS and SPACI, joined the group in order to cooperate in the achievement of the following tasks:

- Setting up a basic Grid infrastructure based on the Globus Toolkit middleware on designated high performance computing resources;
- Analysis of the state of art of Grid tools from a supercomputing environment point of view;
- Test of selected applications and user interfaces in an heterogeneous Grid environment;

The international character of the project, the heterogeneous nature of the working group, a synergy between academy and industry, and the variety of the involved resources, constitute the strength point and the surplus value of the project.

Sergio Maffioletti

EGEE German-Swiss Federation and EGEE2

In 2005 CSCS joined the Germany/Switzerland EGEE federation (DECH). The EGEE federation Germany/Switzerland is heavily involved in the EGEE activity SA1, "Grid Operations, Support and Management".

This responsibility includes middleware certification, deployment, as well as day to day operations and user support. A lot of responsibility for these activities within the regional federations rests with the Regional Operations Centres (ROCs).

The Regional Operations Centres are the heart of the operational support for the Grid infrastructure. They have a key role as sources of expert advice and technical support in the process of building and operating the infrastructure. The ROCs have the expertise to assist the growing number of Resource Centres in joining the infrastructure, through the deployment of middleware releases and the development of procedures and capabilities to operate those resources. Resource Centre requires close support, including on-site assistance where required. This support is provided by the ROC team.

In 2006, CSCS will be involved as an active member of the "Grid Operations, Support and Management" activity, as well as Networking Activity 3 (NA3) - User Training and Induction where CSCS will collaborate in reaching the following goals:

- To produce a portfolio of training material and courses from introductory to advanced user material.
- To use this material to train a wide variety of users both internal to the EGEE consortium and from external user groups from across Europe who will make use of this infrastructure.
- To engender team spirit across the EGEE activities.

CSCS is willing to strength its role and participation in the EGEE through the German-Swiss Federation and it formalized its active participation within EGEE phase 2 that will start in 2006. CSCS will be a funded partner of EGEE2.

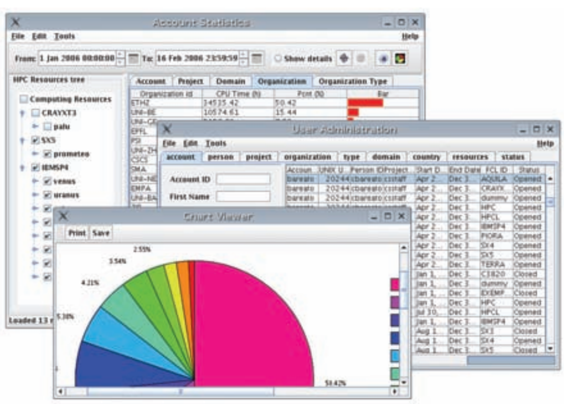
Gian Luca Volpato
Sergio Maffioletti

HPC Benchmarking and Development

Performance issues related to HPC play a central role in the activities of the group. This is reflected in the main developments conducted in 2005.

During the year there has been a major development step of the already established CSCS performance environment with the official release of the newly developed user administration and performance monitoring tools and the final migration from the old user accounting system based on C/Motif and Oracle. This process was done in a very tight collaboration with people from the fundamental and user service (FUS) section who gave significant contribution to the final design of the MySQL database structure and in the definition of the major tool requirements and products. Further improvements have also been done on the low-level components of the tool in order optimize the gathering of performance and usage statistics of large HPC clusters. The integration of the new Cray XT3 system within the official accounting process has also started as well as some feasibility studies for global and real time monitoring of jobs and applications. PerfMon has already demonstrated to be a reliable and essential tool for investigation, analysis, and decision-making.

From the HPC applications side, besides the established and regular support on the already available HPC systems, there has been a significant effort in providing dedicated support to CSCS users during



Performance Monitoring & User Administration

the installation and migration phase on the new Cray XT3 system. This support involved working closely with the applications group to port codes to the new system and attempting to maximize performance and scalability for individual codes, as well as working with members from the FUS section to look at system-wide issues such as the implementation of a batch scheduling policy and the partitioning of the high performance file system. Also a quite deep and extensive benchmarking study based on the public RAPS version of the weather forecast code LM was done on various HPC platforms (Cray X1, NEC SX-8, IBM p690, SGI Altix) and results were presented at the RAPS Workshop 2005.

Mauro Ballabio

Scientific Applications Group

In the year 2005 much effort was spent in assisting the scientific community with the multiple facets of software engineering and those of application integration within the CSCS production environment. The aspects ranged from application porting, compilation and debugging, to high level algorithmic optimization. In the last semester these activities have been mainly focused on the Cray XT3 architecture, which was undergoing acceptance and being prepared for production.

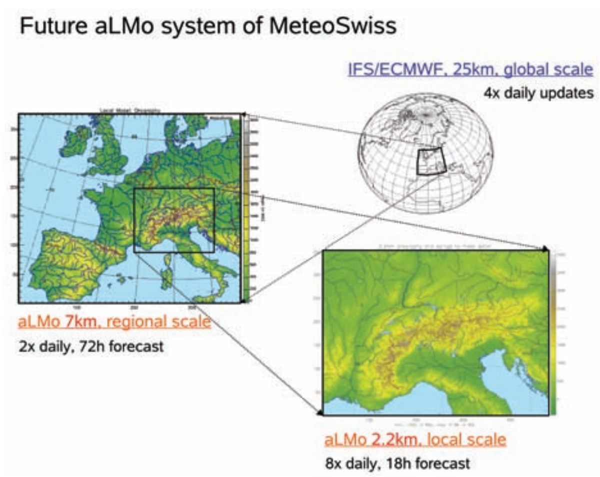
Aiming at an efficient and effective use of the overall HPC facilities, the Scientific Applications team continued the consolidation and the completion of the CSCS computational (Bio-) Chemistry Framework, the deployment of several widely used climatological applications, as well as the support and maintenance 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.

Beside pure computational application, data intensive applications are also gaining momentum, a constantly increasing data transfer rate between the archive and the computing servers has been definitely observed, this applies to several application fields, and especially so in CFD, meteo and climate. It has to be noted that CSCS is acting as one of the main computational laboratory for the NCCR-Climate community (http://www.nccr-climate.unibe.ch). This community sets new challenging requirements not only related to efficient high-end computing, but also to data archiving and data pre/post-processing. Large data set, spanning several TB, are not only archived, but are also regularly accessed by data analysis and data verification experiments.

A considerable effort was spent in processing User support requests coming in on a daily basis, as well as in consolidating and regularly updating the technical documentation made available on the CSCS User Web Portal.

Key account MeteoSwiss

MeteoSwiss, the Swiss national weather service, has been carrying out all its production and research computations at CSCS for several years now with its numerical weather prediction model aLMo (the Swiss implementation of the LM of the consortium COSMO), which simulates the atmospheric evolution over a domain covering most of Western Europe.



Future aLMo system of MeteoSwiss: the actual NWP system will be extended by a nested, very high resolution model for short range, local forecasts

Many internal and external MeteoSwiss clients critically depend on the timely production and dissemination of aLMo output; in particular, some important issues related to the security of the Swiss population are based on the results produced by MeteoSwiss. As an example the aLMo results are used by models computing the dispersion of air particles and of pollutants for the National Emergency Operations Center (NEOC), as well as hydrological runoff forecasts at the Swiss National Hydrology Survey. Model results are also sent operationally to the Swiss Federal Institute for Snow and Avalanche Research, where they help to assess the risk of avalanches in the forthcoming days.

With aLMo, MeteoSwiss takes a significant part in the national and international R & D effort to improve the quality of weather forecasts. Over the past five years, many scientific collaborations with Swiss high schools and federal institutions have been developed, for the benefit of all partners. aLMo is currently entering in a new challenging phase with the development of a new version with a higher resolution at the kilometric scale, targeting a further increase of the quality of the forecasts, especially in complex topography like in Switzerland and the Alpine region. To meet this new challenges, MeteoSwiss needs adequate computing infrastructure, software environment and computing support services. In this frame a new agreement has been recently signed and we are now starting implementing all this ambitious but stimulating goals. Our group played and will play an important support role in this well established collaboration with MeteoSwiss experts.

Angelo Mangili

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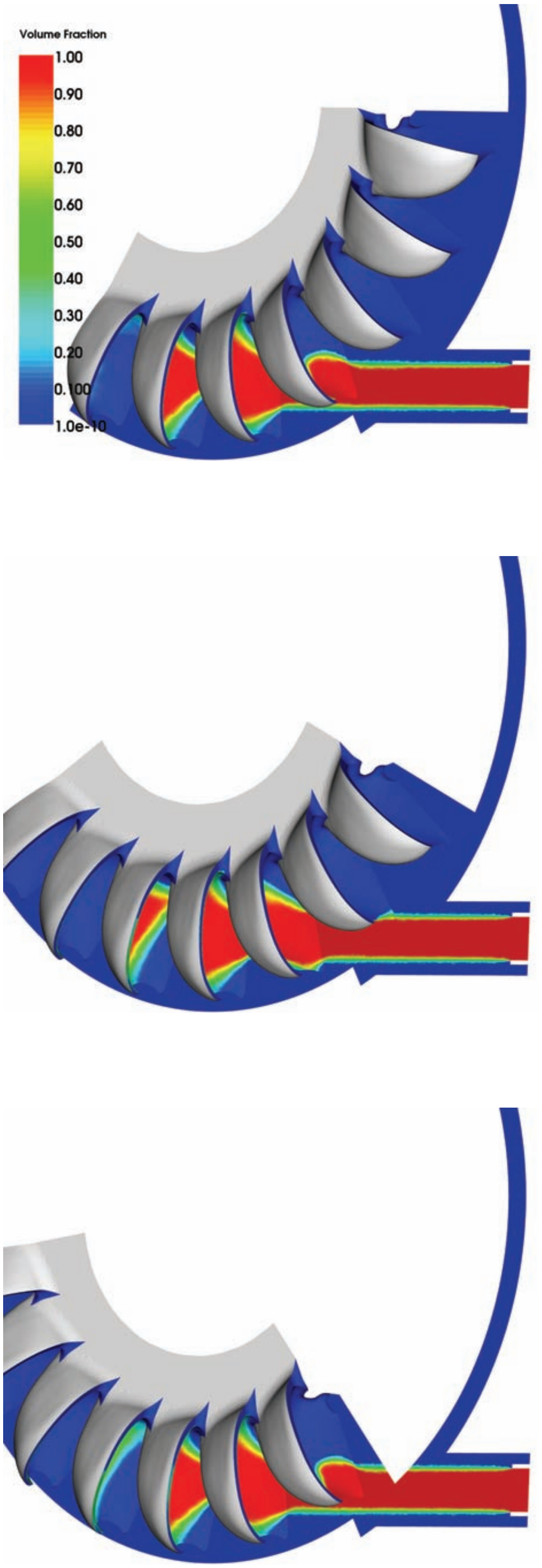


Water jet driving a Pelton Turbine. Simulation by VA TECH Hydro

Data management, analysis and visualization

The visualization group has continued and reinforced its support for activities related to the production of images and animations. Visualization depends on reliable and efficient access to data, and its goal is to provide means to achieve understanding and discovery of features in the data. After internal discussion the group has chosen the name “Data Management, analysis and visualization” to better reflect our activities and how we rely on these related multi-disciplinary fields.

The whole group participated with great enthusiasm to promote CSCS and its numerous achievements at the 2005 OpenDay, an integral part of the ETH-Zurich 150th anniversary. The group led the overall event management and demonstrated the following activities emphasizing then throughout the year. We highlight here a few of our accomplishments.

Fluid Dynamics Computations and Visualizations with industry-leader VA TECH HYDRO of Vevey and EPFL - Laboratory for Hydraulic Machines

We were able to apply and demonstrate our multi-disciplinary skills in this complex industrial simulation project marked by the sheer size of the data (a full Pelton turbine two-phase simulation of over 40 millions cells) coupled with experimental data acquired in laboratory reduced-scale models. The group was responsible for the parallel run of the simulation and all the post-processing development, including a parallel visualization environment to support the CFD results (CFX5 interfaces, and algorithms specific to the Pelton turbines), and image processing of the endoscopic camera images. A related activity was developed to process meshless data (particle data) which are seen as a possible future simulation track to avoid the extremely complex unstructured geometry seen in the hydraulic machine simulation field. This led to the development of state-of-the art rendering methods available now for all CSCS users with particle simulations.

Molecular Dynamics and Chemistry Visualizations

Our AVS/Express-based "STM3" molecular visualization environment continues to mature at a steady pace. The development of new features is driven by our user community, more actively by the groups of Prof. Parrinello and Prof. Oganov. For example, we have created an interactive environment for their new crystal structure determination code. Our expertise was also extended to the VMD software, to provide a much needed pluggin for VMD to cache molecular surfaces computation to speed up molecular animations. In fine, work has begun on a new version of Molekel which will hopefully address the majority of problems that existing users have experienced. The primary objective has been to rewrite and consolidate the code such that it is possible for others to contribute to the project. A new GUI has been added and the core code has been restructured so that it can be extended and improved.

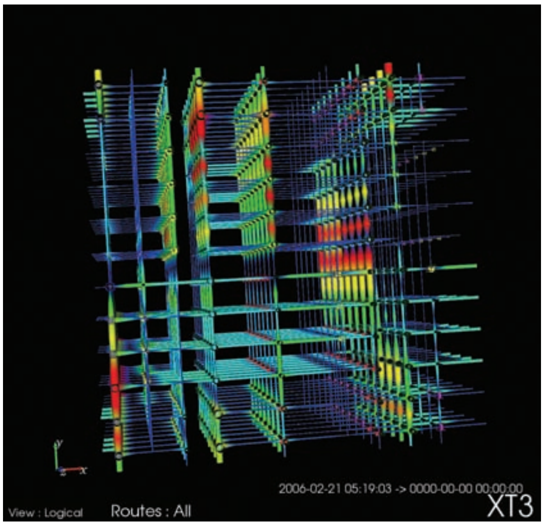
Parallel Visualization

We made numerous experiments to gain practical experience and understanding of parallel visualization issues, including parallel file reading, parallel feature extraction, parallel rendering to multiple frame buffers and to a prototype tiled display (a 3x3 mosaic of computer screens) with the open-source ParaView software. This is invaluable experience to help us define requirements for the 2006 purchase of a graphics cluster. Further, large display surfaces (large pixel count) were evaluated to cover the needs of multi-media conferencing and collaborative (several persons) visualization.

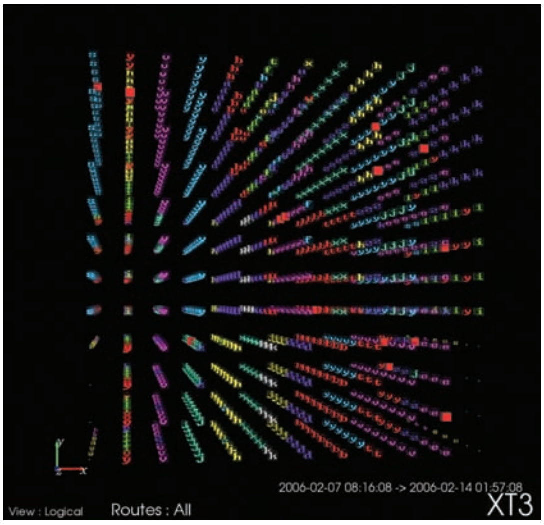
Visualization at the front-end of the introduction of CSCS's new Cray supercomputer

A dedicated visualization tool was created to help diagnose early installation problems with the newly installed Cray. The tool has proved interesting as a means of examining the state of a large parallel machine and has been extended to use the systems SQL database to query not only the current state of the machine, but the state at any point in the past.

Jean M. Favre



Visual representation of the network traffic between compute nodes within the Cray XT3



Visual representation of the jobs running on each node within the Cray XT3

Fundamental and User Services

The main activities of the Fundamental and User Services Section in 2005 have been
- the operation and maintenance of our HPC servers, data management and storage systems, networks, and dedicated pre- and post-processing systems
- the commissioning and test of the new Cray XT-3 HPC server
- improvements to the capability, accessibility, and availability of CSCS infrastructure.

All our HPC servers are now accessible through a new front-end computer. Besides providing increased computer power and storage, the new CSCS front-end provides world-wide accessibility through a secure SSH connection to our computing resources as well as to all related documentation and real-time information on the status of all resources.

In addition to the existing communication line to Zurich, SWITCH, the operator of the Swiss education and research network, has installed a new line connecting Manno to Lausanne. The new line improves the availability and reliability of our connection to our users. Preliminary tests on operating these connections at a speed of 10GB/s have been made in preparation for increased future requirements.

The CSCS-internal network has been adapted to meet new requirements of the grid community (cf. the descriptions of the BioGrid and LCG grid projects in this report). New security requirements stem from the fact that – contrary to the users of our HPC servers – not all members of a grid community are known and registered with CSCS.

The throughput and stability of our archive system have been improved through the addition and reconfiguration of high speed/high capacity tape drives. The performance for small files and for multiple file access in a directory has been significantly improved through the installation of a SamFS/QFS disk archive.

We have installed group videoconferencing equipment allowing us to strengthen communication with

Cray XT3, Photo by Simon Norfolk ©

some of our user communities. In order to streamline this communication, we have also reorganized all user data and consolidated it in a single database.

Finally, fast computers consume plenty of power and produce plenty of heat. In order to meet the gross power and cooling requirements of the Cray XT-3 installed in 2005 and of other HPC server extensions planned for 2006, we have increased the power supply of CSCS from 750kVA to 1200kVA. The capacity of the backup battery system has been increased accordingly.

Paolo Conti

Development of the high-performance computing infrastructure

2005 was a milestone in the development of the computing infrastructure at CSCS. The procurement project Horizon started in autumn of 2004 and ended up in the delivery of a Cray XT3. This massively-parallel computer, the first installation of its kind in Europe and the fourth in the world, consists of 1’100 AMD Opteron processors, which are interconnected by a custom very high-bandwidth, low-latency network with a 3D-torus topology. The new computer is able to deliver 5.8 Tflops or 5.8 trillion floating point calculations per second. It offers a total memory of 2.2 TBytes and a global shared parallel file system of 28 TBytes. It operates a special software stack, including a micro-kernel on the compute part of the system, which yields very high efficiency for computational experiments involving hundreds or thousands of processors in parallel. Horizon went through a period of intense testing and verifications by CSCS and a large number of pilot users in late 2005, and it finally went into general production in January 2006.

With Horizon, CSCS has entered a new level of parallel computing, going from tens of processors on the previous NEC and IBM computers, to up to 1’000 processors per single experiment. This new level of parallelism enables CSCS’ researchers to carry out scientific research they were not able to do before. Already during the pre-production period in 2005, two research groups at CSCS reported that they have run computational experi-

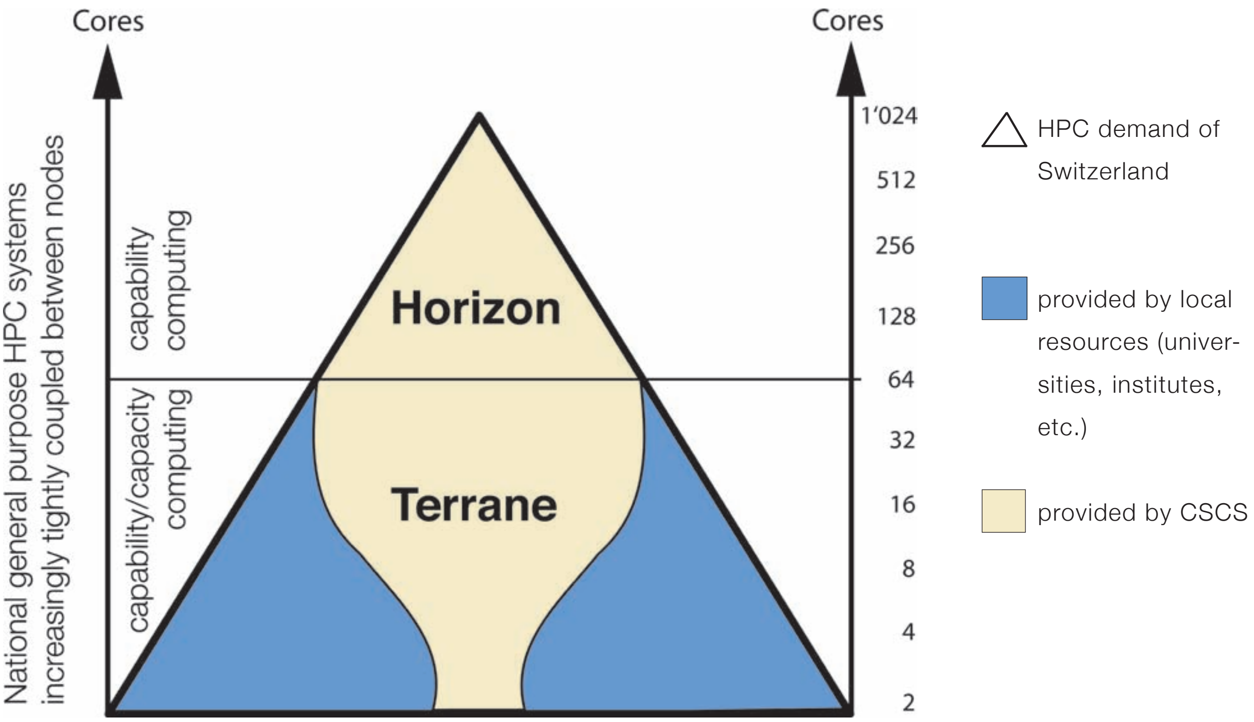


Figure 1: Two-tier computer portfolio strategy of CSCS (January 2006)

ments they could not run before. New users, coming from new institutions, have applied for working on Horizon and we expect exciting scientific results from this machine in the near future.

As Horizon extended significantly the capabilities of CSCS computing infrastructure, the next development step was designed to increase the capacities of the systems of the centre. CSCS identified the importance of offering our users compute facilities for lower level of parallelism, with some shared memory capacity, and with a high level of compatibility to other systems. Thus, CSCS stays flexible and open in terms of technology and application portfolio and it has economic solutions for all kinds of computational need. The strategy also takes into account the fact that every computational research project, even if it targeted at running big, massively parallel experiments, requires heavy computational resources on a lower level of parallelism for preparing, validating, and complementing the large-scale experiments. If a proposed research project is evaluated by the CSCS Scientific Review Committee as scientifically sound and to be supported, CSCS must offer the full spectrum of services for fulfilling all computational requirements of the project. Of course, resources of lower-level parallelism are also available at other institutions in Switzerland. CSCS will therefore not cover the full national need for these kinds of facilities but share this offering with compute services at the universities and research sites (see Figure 1).

Consequently, CSCS launched the Terrane procurement with a public call for tender in late 2005. In addition to the requirements concerning the level of parallelism, we targeted at a system that has some shared memory capacity, offers a sound performance per node, i.e. strong single processors, and is easy to use and to migrate to. Therefore, we followed our strategy already published in the Annual Report 2004, which envisaged a system of current HPC market standards to be inserted into CSCS' HPC portfolio in 2006 (Figure 2). Terrane is expected to arrive at CSCS in summer 2006 and to be open to our users for early access, porting, and testing during the second half of 2006.

Dominik Ulmer

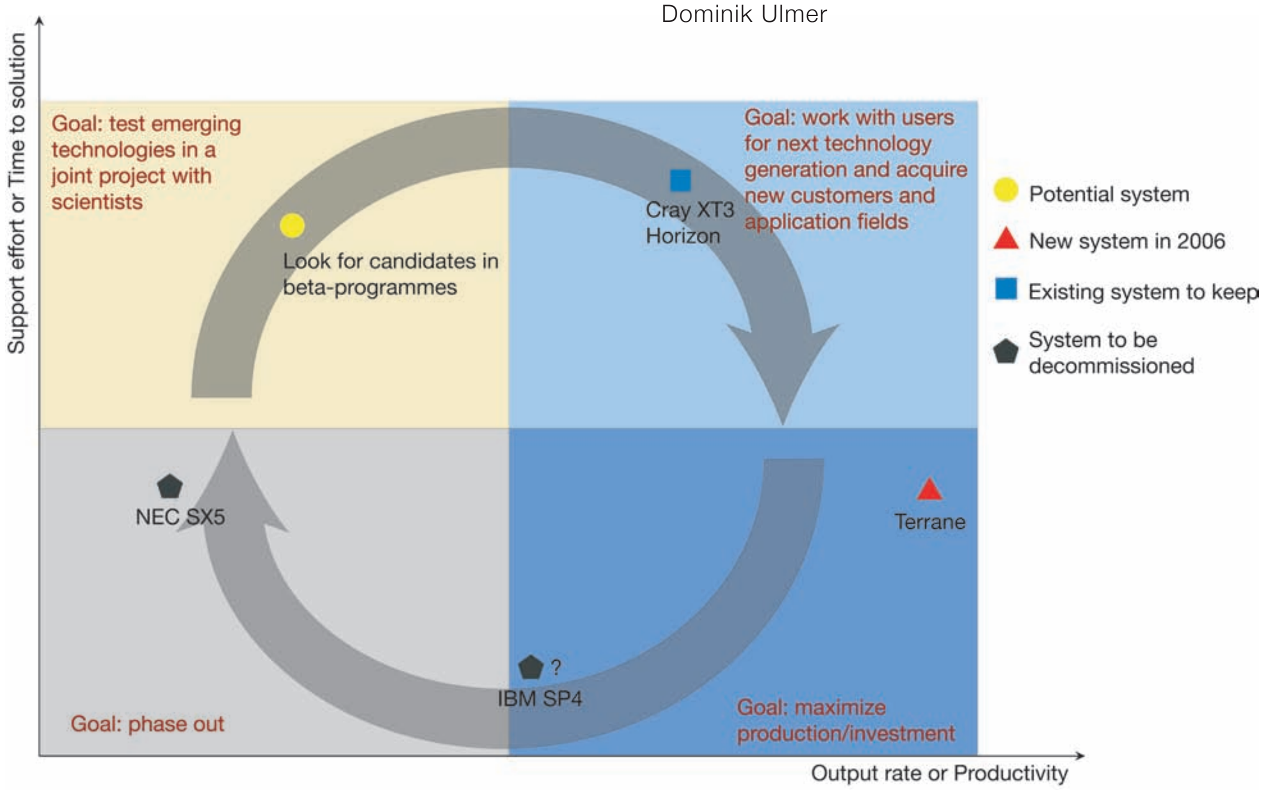


Figure 2: CSCS innovation cycle 2006

Outreach

2005 has proven to be a truly eventful year for CSCS! Ideas and intentions that were formulated during the first year of the new management began to take shape, confirming their importance within the annual calendar of CSCS.

Interacting with our users

Having set out to improve the exchanges between users and CSCS, management decided to add a second user-event to the annual User Day. This lead to the first *User Assembly* meeting taking place in Bern in the summer of 2004. In 2005 this event was repeated and again very well attended. Based on positive feedback received from users, this event has become a fixed feature of the annual CSCS calendar to be held in May/June. During this event CSCS employees travel to a more central location within Switzerland to meet their users, thus providing a good balance to the annual User Day held on CSCS premises.

User day 2005

The already long established annual *User Day* took place on 26-27th of September and was attended by approximately 70 users. This event, conceived around the presentation of user achievements via talks or posters and complemented by CSCS presentations is currently being rethought in order to better accommodate for user requests and wishes and increase the value of the exchange for both parties. The addition of a keynote speech, as held this year by Dr. Wolfgang Sell – former Director of DKRZ, will be continued. The 2006 event, to be held on 25th - 26th Sept will reflect these changes and we look forward to receiving feedback from our users.

Educational activities at CSCS

The need for educational activities to be organized and given by CSCS was clearly stated in the current performance agreement. First efforts in this sense were made during 2004 when we hosted courses in *Computational Chemistry* (Prof. Bally, Uni Fribourg) and *Computational Methods for Strongly Correlated Systems and Nanomagnetics* (Prof. Troyer, ETH Zürich) as well as the annual COST Action D23 (chemistry) meeting. During 2005, activity in this area increased with the organisation of two courses on *Advanced Visualization* and Data Management taught by our own visualization specialists (Dr. Jean M. Favre, Mario Valle, John Biddiscombe, Theophane Foggia) and a course in *Parallel Programming* taught by Dr. Rolf Rabenseifner from HLRS. In addition, first introduction courses to the new machine Horizon were held in May and July and the Grid group were able to host the *German – Swiss Federation EGEE workshop* in June as well as a *Swiss Grid workshop* in July.

User day 2005

Special events

The leap in compute time provided by the arrival of the Cray XT3 machine – Horizon – was celebrated with an ***inauguration party*** on September 15th attended by our partners, our users, politicians and decision makers from ETH domain and industry

Horizon inauguration, 2005

alike. The arrival of this new machine – joint venture with the Paul Scherrer Institute – led to CSCS hosting the Cray Advanced Technical Workshop Europe with 70 participants from international Cray sites.

The President of ETH Zurich with the CEO of CSCS

An active exchange with other international compute centres lead to a ***visit by a delegation from the Finnish Supercomputing Centre – CSC***. This visit proved an excellent opportunity for members of the CSCS Steering Board and ETH Board to meet with our Finnish counterparts and exchange on views and projects.

When Filippo Lombardi stepped down as President of the ***Commission for public building of the cantonal parliament***, CSCS was honoured to host the last meeting of the commission that is traditionally held in the home canton of the outgoing President. The biggest event of the year – and most important for ETH Zurich – was without doubt the ***CSCS Open Day*** held as part of the festivities around the 150th anniversary of ETH Zürich on May 7th. During this event, it was our pleasure to represent ETH Zurich in Ticino and give the general public the opportunity to get to know CSCS. All employees were involved with the preparation of contributions ranging from posters, visualization demonstrations, presentations, guided tours of the machine room and the

CSCS employees interacting with the VIP guests at the Open Day

general set-up and functioning of the event. During the morning the VIP guests were addressed by the CEO Marie-Christine Sawley before enjoying a guided tour of the exhibits of visualization demonstrations, posters and the machine room. Thanks to the mild and sunny weather the ensuing aperitif and lunch buffet took place in the gardens where the guests were able to exchange on the development of CSCS. When the time came for opening the doors to the public we were overwhelmed to find people already patiently waiting in front of the main entrance. It was delightful to see how the event attracted people of all ages and walks of life. Over 300 guests were given an insight into CSCS on the day and went away with a clearer view of the work we do. The feedback received from visitors was most rewarding and confirms the value of such events in communicating with the general public.

CSCS on the road

CSCS again reached out to the local Ticino public at the *Ticino Informatica* trade fair held in October in Lugano. The close collaboration with the University of Italian-speaking Switzerland – USI – and the technical college – SUPSI – were mirrored by grouping the stands of all three institutions in the same area of the fair. Several employees of CSCS gave presentations and informal Q & A sessions took place at the stand with the various specialists who were on site.

2005 has also been the year in which CSCS ventured into hosting larger international conferences by hosting the ***9th SOS meeting*** that was held in March in Davos. SOS is a series of yearly workshops attended by worldwide experts in leading edge scientific computing. The workshop was attended by 90 people and sponsored by 6 providers to the HPC industry. This branch of activity will be further reinforced with the organization of the ***2006 Cray User Group*** meeting that will be held in Lugano from the 8-11th of May.

CSCS at TicinoInformatica, Lugano

We at CSCS have thoroughly enjoyed the exchange and challenges that these interactions brought in the past year and very much look forward to new and interesting encounters in 2006. We hope to welcome you at one of our numerous events throughout the year!

Ladina Gilly

Research Digest

Editorial

I am glad at the beginning of my tenure as Vice President of Research at ETH Zurich to have the opportunity to write this editorial for the annual report of CSCS, for the year 2005. CSCS is a national computer centre (a national platform for high performance computing) of ETH Zurich.

When I look back over the past 12 months I see significant progress in a number of areas of activity. Regarding renewal of hardware, the new system Horizon a massively parallel processing Cray XT3 computer system, consisting of 1100 processors and a total of 2.2. Terabytes of memory has been installed and is now fully operational and available to the users. In the area of management CSCS is gradually becoming an entity working well with a needed degree of autonomy within the structure of ETH Zürich and successfully fulfilling its mission of covering the high performance computing needs of Switzerland.

Significant research achievements of users were made possible last year with CSCS. To this end a rich palette of success stories can be reported ranging from life sciences to environmental sciences and to engineering, as exemplified by the short summaries in this year's annual report.

Looking into the future, there is a variety of significant activities lying ahead. The acquisition of new needed hardware and the further development of GRID computing are projects that will be advanced further in 2006.

I thank all members and users of CSCS for their efforts and contributions last year and I am looking forward to working with them in my position as VP Research ETH Zurich in the future.

Prof. Dimos Poulikakos
Vice President of Research ETH Zurich and
Member of the Steering Board CSCS

Interview
with Prof. Artem R. Oganov
by David Bradley, Science Base, UK

Prof. Artem R. Oganov is a Senior Researcher in the ETH Zurich's Laboratory of Crystallography and an Adjunct Professor at Moscow State University (Russia). Together with PhD student Colin W. Glass he is developing an evolutionary program to predict the crystal structure of almost any compound at a given temperature and pressure and has demonstrated its efficacy on otherwise inaccessible geological minerals.

What inspired you to become a crystallographer?

When I was a child I wanted to become a chemist, towards the end of school I also developed an interest in mineralogy. The combination of these interests made me a crystallographer right from the beginning of my university studies.

Why is being "international" important to a crytallographer?

My main "homes" are Moscow, London and Zurich. This mobility has given me many extremely useful experiences, both professional and personal. Having gone through these experiences and grown as a scientist and as a person, I feel that now is the time for me to settle down. In Summer 2005, I was offered a Professorship in the US, at Princeton University. However, I think that staying in Switzerland and continuing to build up my research group here is a better idea.

How does your structure prediction program work?

Initially, we create a set of structures - a population - at random and locally optimise them using standard approaches. Their energies are calculated using quantum-mechanical simulations and the worst (i.e. the highest energy) structures are discarded, the others are then used to produce the next generation - through ”genetic” crossover. This new generation is similarly evaluated and a further generation produced and so on. It’s like Darwinian natural selection and quickly finds the best structure. Such an evolutionary algorithm is also self-learning, recognising ”good” and ”bad”, structures, which is key to its success and adaptability.

Does it ever fail?

No, we have not seen any failures in the several dozen tests done so far. Our method can handle very complicated materials, but the current restriction is that you have to specify the chemical composition.

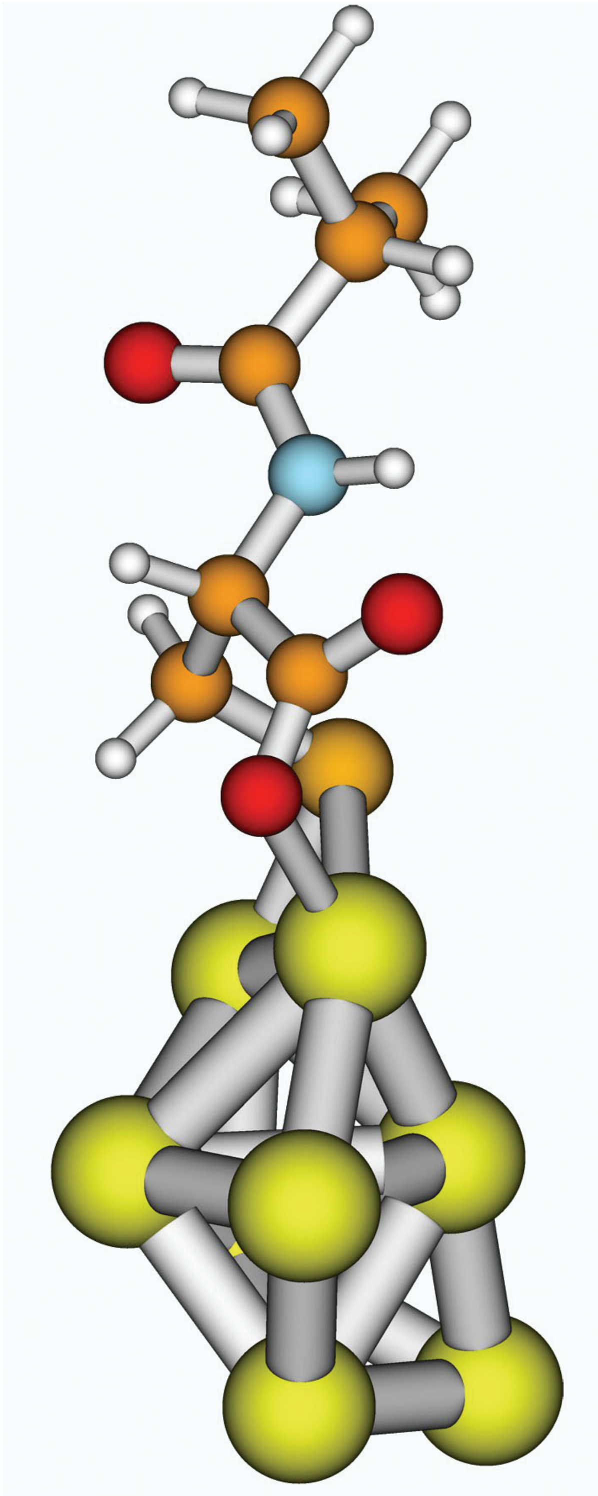
What do you hope to learn about the earth from mineral structures?

Learning about the structures of minerals inside the Earth is the best way to understand their properties, and this is linked to the structure of the Earth, to the way geological processes occur, and ultimately to the evolution of the Earth. Recently, we found a new major Earth-forming mineral, magnesium silicate post-perovskite, which exists in the so-called D” layer at the boundary between the earth’s mantle and the very hot iron core. From what we learned about the structure and properties of this mineral, the D” layer appeared some 4 billion years ago as a result of the cooling of the Earth, and this layer still continues to grow!

It would be extremely difficult and often impossible to solve crystal structures experimentally at high pressures. Yet, this is necessary in order to understand how the Earth and planets work. Our method solves this difficulty. I believe that theory and experiment should complement each other. Therefore, theory will never replace experiment - and experiment will never remove the need to have good theory.

What kind of computing power do you need for structure predictions?

This depends on how complex the chemical composition is. For some simple cases you can do a whole run within 1-2 hours on a personal computer, for more complex cases you need longer calculations and if you want to study a very complex material you need a big supercomputer. This is where CSCS will play a big role.



Structure of N-isobutyryl-cysteine adsorbed on a gold particle as determined by a combination of infrared spectroscopy and density functional theory.

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 2005 projects in page 36.

Getting a grip on molecular handedness

(Prof. Thomas Bürgi, Institut de Chimie, Université de Neuchâtel, Switzerland)

Thomas Bürgi and colleagues at the University of Neuchâtel, Switzerland, have used a combined experimental and theoretical approach on the IMB SP4 CSCS system to gain new insights into how to distinguish between left- and right-handed molecules. Their approach will help chemists improve separation techniques for the pharmaceutical and agrochemical industries as well as lead to novel materials for nanotechnology.

To understand molecular handedness, or chirality, look at your hands – each a non-superimposable mirror image of the other. With molecules and surfaces having different atoms at different positions a similar situation arises. For instance, the molecule alanine has four different chemical groups surrounding a central carbon atom. Swapping any two groups produces a chemically identical molecule with an important difference - the pair cannot be superimposed. The importance of this manifests itself when each form interacts with other chiral molecules.

Chirality is ubiquitous in nature from chiral forms of the same molecule that smell different to drugs that work in one form but are harmful in the other. A chiral pesticide might kill the pest in one form but harm beneficial species in the other. Surfaces can be chiral too because of the arrangement of atoms or chemical groups on them.

Bürgi and colleagues have used spectroscopy to investigate chiral separation and the behaviour of metal nanoparticles coated with a chiral layer. Simulating the spectra helps them understand what happens on a chiral surface at the molecular level, while experimental data feed the computations and improve the model.

The team investigated how a chiral material commonly used to separate handed forms (in chiral chromatography) interacts with the molecules that pass over it. Their studies revealed that the prime mover in differentiating between chiral forms is the so-called hydrogen bond that can form between hydrogen atoms in one molecule and ”spare” electrons on an oxygen atom in another.

The spectra suggest that the right-handed molecule does not form hydrogen bonds with the chromatography material and so is flushed through more quickly by carrier solvent than the left-handed form. This is what is observed in the actual chromatography experiment and is confirmed by the computational model. This result could not have been obtained through chromatography alone, Bürgi explains.

Related studies with another type of spectroscopy on chiral nanoparticles, just a few billionths of a metre across, has revealed important clues about the behaviour of these materials, too. Technologists hope to exploit nanoparticles in biological sensors, chemical catalysis, and electronics, but need a clearer understanding of how nanoparticle protective surfaces affect their properties.

The team studied gold nanoparticles modified with a chiral molecule. To interpret the resulting spectra, they used computational techniques and investigated the properties of gold clusters of different size containing up to nineteen gold atoms. The spectra showed signals due to different-sized gold particle but also that the arrangement of the chiral molecule on the surface of the gold particles did not depend on the particle size. This could be important in making nanoparticles for various applications because they could tolerate variations in manufacturing. More important for the present research, however, is that spectroscopy coupled with simulations allowed the team to elucidate the structure of chiral molecules adsorbed on metal particles.

The common feature of these two threads of Bürgi›s research is that both «surfaces» are chiral and are thus able to discriminate between chiral molecules. The result is improved understanding of discrimination between chiral forms for the chromatography work and of the structure of the chiral ”surface” itself in the cluster research. Bürgi explains that such information is a prerequisite for the rational design of chiral surfaces and particles.

Mapping Emissions
(Dr. Doris Folini and Sandy Ubl, Empa Duebendorf, Switzerland)

Greenhouse gases, ozone-eating molecules, and other pollutants are continually entering the atmosphere. Some come from natural sources, such as volcanoes and oceans, but others are pollutants caused by human activity. Efforts such as the Montreal and Kyoto international treaties attempt to reduce emissions of ozone-depleting chemicals and greenhouse gases, respectively, but monitoring international compliance will be an essential requirement if the treaties are to be successful.

Sandy Ubl and Doris Folini of Empa, Dubendorf explain there are essentially two ways to verify whether a nation is compliant. The 'traditional' way is to compile sales numbers, taxes, etc. However, for many gases this is not feasible and produces only very inaccurate data. An alternative approach would rely on creating a computer model that could work out rates of emissions based on long-term concentration measurements of various gases.

Ubl and Folini are using the MeteoSwiss LPDM (Lagrangian Particle Dispersion Model) to model atmospheric transport of gaseous substances. The model can link emissions with concentration measurements at different monitoring sites and given this connection, provide specific information about emissions. The work was carried out on the NEC SX-5 and the data storage facility (rosa) at CSCS and the SGI from MeteoSwiss (terra) was used to manage the tasks.

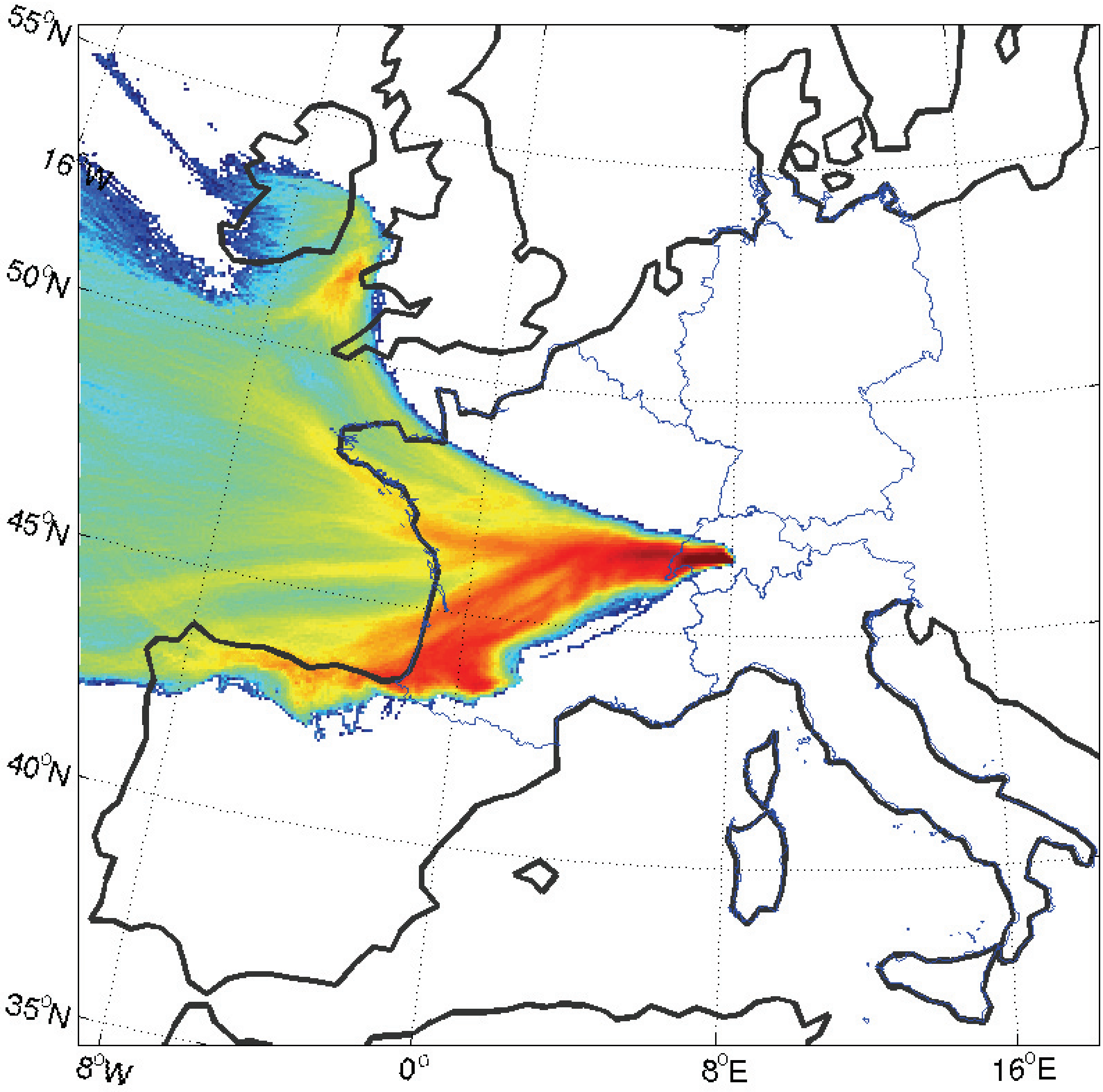
The ultimate goal, the researchers explain, is to derive regionally resolved emission maps for various gases, in particular the halocarbons, some of which are not only greenhouse gases but ozone-destroying compounds and so are controlled by both the Montreal and Kyoto treaties.

Rather than working from source to atmosphere, the team runs the LPDM in backward mode. This uses real measurements from, for instance, the high Alpine station Jungfraujoch, (3580 metres above sea level) and plots the path of a large number of gas particles backward from the measurement site using recorded wind patterns. The result is a three-dimensional map revealing the probability that a particular pocket of air will reach the measurement site during the measurement period. From this 3D data, the team then extract a 2D footprint showing how much air from layers close to the ground will reach the measuring site. This provides them with information on how well that measuring site performs in determining emissions from the geographical region it covers.

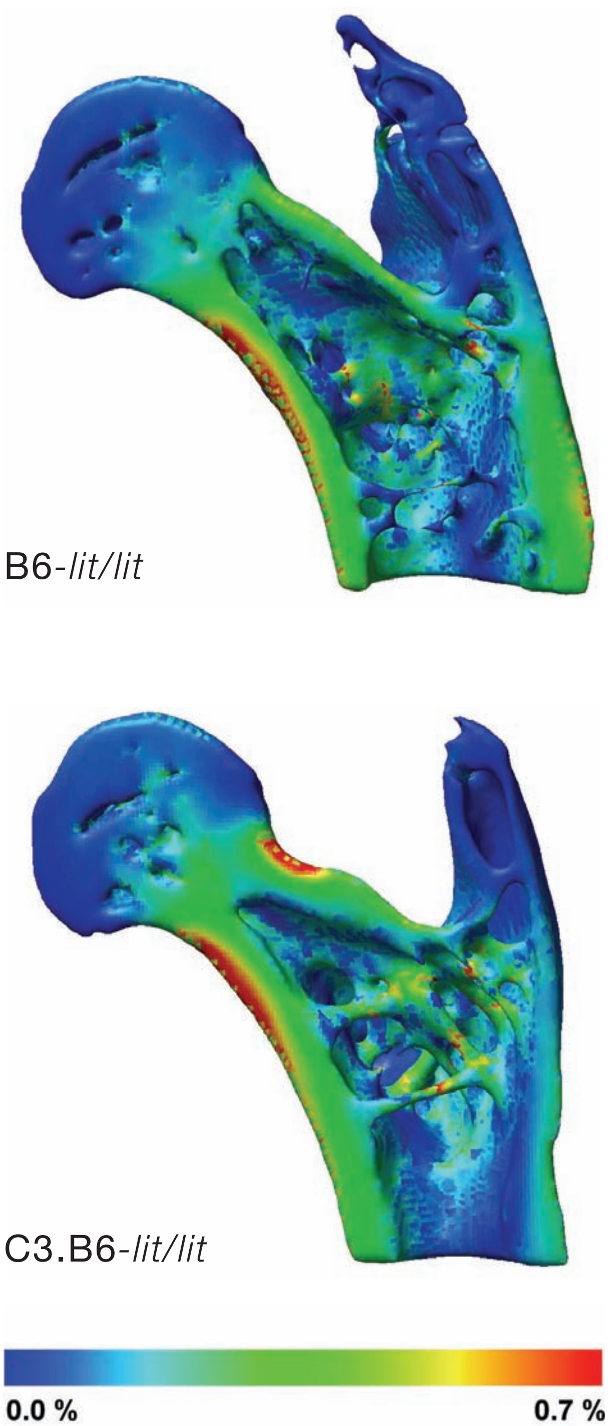
In the real world, the problem is much more complicated because of the complex topography of this region. So, the researchers have tested how well the LPDM itself performs under these conditions by comparing real, measured data with simulated data from the model. The comparison revealed that the average measured and simulated data agree well.

The next step will be to determine the source of particular gases, whether industrial or urban using measured concentration data and the LPDM. A measured concentration value from a particular measuring station can, in principle, be decomposed into a set of contributions from a variety of different sources, explain the researchers. These sources might lie in different places and have different source strengths, i.e. emit a different amount of the substance over a given time. One way to pinpoint such sources is to place a rectangular grid over the map of Europe and to determine the contributions from different grid cells to the measurements. The average emission per time of each cell is the information they seek. The LPDM can be used together with actual measured concentrations to yield such an emissions map by adapting the emission of each cell until there is optimum agreement between the modelled and measured concentration data.

Ubl and Folini›s analysis of the Jungfraujoch data shows that sources up to about 400 km away contribute frequently to the measured concentrations at this station. This suggests that dozens of stations will be needed to monitor the whole of Europe and so provide the fundamental raw data for monitoring emissions and helping Europe to comply with the Montreal and Kyoto protocols.



Footprint for station Jungfraujoch, July 4, 2002, measurement period between 03:00 and 06:00. Measured concentrations during this time contain signatures of sources that are located in the western part of Switzerland and in the central part of France. Red indicates high residence time, blue is low residence time.



Effective strains in the proximal femur of two genetically different mice. The strains resulting from equal loading at the femoral head were determined from micro-finite element models.

Boning up on genetics of osteoporosis
(Dr. Harry van Lenthe with Philip Morley, Romain Voide and Dr. Ralph Müller, Institute for Biomedical Engineering, ETH and University of Zurich, Switzerland)

A study to track down the genes responsible for the debilitating bone disease osteoporosis, which leaves thousands of people at risk of serious fractures, could one day lead to a new treatment for the disease.

Osteoporosis is a debilitating weakening of the bones that leads to breaks (fractures) commonly in the wrist, spine, and hip. It occurs when marrow-filled pores in bone enlarge reducing bone strength. Fractures due to osteoporosis lead to severe long-term pain and physical disability, which affects thousands of people and places a massive burden on health care services. Indeed, osteoporosis is second only to cardiovascular disease as a leading healthcare problem. According to the World Health Organization, one in two women and one in four men will have an osteoporosis-related fracture after their fiftieth birthday.

Studies of how osteoporosis runs in families recently revealed that bone strength is partly genetic. Now, Harry Van Lenthe and colleagues in the Institute for Biomedical Engineering at ETH and the University of Zürich believe they have found a way to assess bone strength computationally and to correlate it with specific genes in a DNA sample.

Using a new bone scanning technique developed at ETH, known as micro-computed tomography, the researchers obtained three-dimensional images of mouse thigh bones and vertebrae without having to cut any bones. The team then converted these images into computer models which could be analyzed mathematically and provide a value for bone strength. They could then simulate the effects of applying a load to the bone in the computer to work out the force needed to break it. The main advantages of using computer modeling are that it is non-destructive and different tests can be carried out on the same bone. Testing a bone to destruction, after all, is not an option in assessing a live patient!

The researchers thus evaluated a large set of bones from mice for which the genetic make-up is known. The tests would also reveal whether there is a difference between males and females in how the genes control bone strength and whether it is regulated differently for different parts of the skeleton.

Their first simulations mimicked a common fracture in osteoporosis sufferers in which the thigh bone breaks at the weakest point, the femoral neck. The team modeled and then tested several bones obtained from an inbred strain of mice with low bone mass and compared it to a strain with high bone mass. The analysis revealed that the structure of the femoral neck was a very important determinant of bone strength. Although one strain had significantly more bone overall in the femur it was found considerably weaker when loaded in the neck. ”This is an intriguing result”, say the researchers, ”as it shows that bone mass alone is not sufficient to have strong bones”.

The researchers also scanned thigh bones of some 2000 descendants of the two previously investigated inbred strains, with a view to pinpointing the genetic culprits for bone weakness. Individual models for each bone are being constructed on the computer for high-throughput testing. They will combine the strength test results with DNA screening results carried out by collaborators at The Jackson Laboratory in Bar Harbor, Maine, USA. This will allow the researchers to home in on relatively small chromosomal regions that influence femoral bone strength and ultimately to pinpoint the specific genes responsible.

The team will carry out similar scans and modeling on the same animals’ vertebrae. Fractured vertebrae in osteoporosis sufferers are notoriously difficult to treat so any new insights could improve the treatment and quality of life for many affected by the disease. ”With the ongoing work we aim to better understand the features that make bones strong”, explains van Lenthe, ”and to better understand the causes of osteoporosis”. He adds that the findings will hopefully aid diagnosis as well as providing clues for new treatments.

List of Large User Projects 2005

Name	Organiszation	Project Title
Arbenz P.	ETH Zürich	Large scale eigenvalue problems in opto-electronic semiconductor lasers and accelerator cavities
Baiker A.	ETH Zürich	Hydrogenation reactions in heterogeneous enatioselective catalysis and homogeneous catalysis in supercritical CO_2
Bakowies D.	ETH Zürich	Atomizations energies from ab-inition calculations without empirical corrections
Beniston M.	Uni Fribourg	Global and regional climate modelling
Besson O.	Uni Neuchâtel	Numerical solution of Navier Stokes equation in shallow domains
Bey I.	EPF Lausanne	Coupling tropospheric chemistry and aerosols in the general circulation model ECHAM
Bürgi Th.	Uni Neuchâtel	Structure and enantiospecificity of chiral nanoparticles and interfaces
Cooper W.A.	EPF Lausanne	Computation of stellarator coils, equilibrium and stability
Deubel D.	ETH Zürich	Quantum chemical studies on the interaction of anticancer drugs with biological targets
Fäh D.	ETH Zürich	Numerical modelling of seismic local effect estimation on complex sites
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
Hasenfratz P.	Uni Bern	Chiral symmetric dirac oparator in lattice QCD
Hauser A.	Uni Genève	Photophysics and photochemistry of transition metal compounds: Theoretical Approaches
Helm L.	EPF Lausanne	Iperfine interaction anysotropy on first and second coordination sphere water molecules, in paramagnetic metal ion solutions
Hutter J.	Uni Zürich	Development and application of ab-initio molecular dynamics methods
Jakob A.	PSI	Molecular modelling of radionuclide mobility and retardation in clay minerals
Joos F.	Uni Bern	Carboclime: modelling carbon cycle climate feedbacks
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 modelling, simulations and optimization of complex systems
Leriche E.	EPF Lausanne	Direct numerical simulation ot the buoyancy-driven turbulence in a cavity: the DNSBDTC project

Name	Organization	Project Title
Leutwyler S.	Uni Bern	Proton and hydrogen atom transfer in solvent clusters and nucleic acid base pairs: theory and dynamics
Leyland P.	EPF Lausanne	Large scale simulation for aerospace applications
Lohmann U.	ETH Zürich	Effect of aerosols on clouds and climate
Lüthi H.P.	ETH Zürich	Computational quantum chemistry of large molecules
Meuwly M.	Uni Basel	Electronic structure calculations for molecular dynamics simulations of iron-containing, reactive centers of biomolecules. Theoretical investigations of iridium-catalyzed reactions.
Oganov A.	ETH Zürich	Computational mineral physics and cristallography
Ohmura A.	ETH Zürich	Global climate change: modelling climate variability on decadel time scales
Parlange M.B.	EPF Lausanne	Large eddy simulation of atmospheric boundary layer flow over complex terrain
Parinello M.	ETH Zürich	Simulating chemical reactions with Car-Parrinello metadynamics
Pasquarello A.	EPF Lausanne	Disordered network-forming materials
Posternak M.	EPF Lausanne	Computational physic in condesed matter
Poulikakos D.	ETH Zürich	Biothermofluidics for Cerebrospinal fluid diagnostic and control-development of a knowledge base Explosive vaporization phenomena in microenclosures
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 warf galaxies
Schär Ch.	ETH Zürich	Modelling weather and climate on european and alpine scales
Sennhauser U.	EMPA	Nanoxid
Stocker Th.	Uni Bern	Monalisa: modelling and reconstruction of north Atlantic climate system variability
Van Lenthe H.	ETH Zürich	Identifying genetic determinats of bone strengh - a high troughput phenomics approach in mice
Van Swygenhoven H.	PSI	Molecular dynamics computer simulation of nanostructured materials
Vogel P.	EPF Lausanne	New organic chemistry with sulfur dioxide. Electron releasing homoconjugated carbonyl group

Facts & Figures

Income & expenditure flow (1.1.2005-31.12.2005)

Expenditures		Income	
Investments	**8'362.79**	**Basic Budget**	**17'070.00**
		Contribution ETH Zurich	11'270.00
Materials, Goods & Services	**3.60**	Contribution ETH-Board	4'800.00
		Contribution PSI	1'000.00
Personnel	**4'297.98**		
Payroll	3'419.20		
Employer's contributions	433.22		
Other	445.56	**Third-party contributions**	**592.96**
		Meteo Swiss	586.06
Other material expenses	**4'267.11**	Other third-party	6.90
Floor space	165.60		
Maintenance	225.31		
Energy & media	558.10		
Administrative expenses	114.97		
Hardware, software, services	2'889.39		
Services & remunerations	314.59		
Other	-0.83		
Expenses total	**16'931.48**	**Income total**	**17'662.96**
Balance			**731.48**

– All figures are given in kCHF.

– The balance is rolled over to the 2006 budget.

Cost Distribution

Cost element	Q1	Q2	Q3	Q4	Total
Costs of goods & services	**1’087**	**2’513**	**0.00**	**0.00**	**3’600**
Salaries	*821’343*	*851’368*	*864’045*	*882’448*	*3’419’204*
Contribution social insurances	*117’237*	*96’397*	*101’951*	*117’634*	*433’219*
Other personnel costs	*51’453*	*142’693*	*83’676*	*167’738*	*445’559*
Total costs of personnel	**990’032**	**1’090’458**	**1’049’672**	**1’167’819**	**4’297’982**
Costs of administration and building infrastructure	*193’799*	*304’792*	*276’867*	*288’487*	*1’063’944*
Costs of hardware, software, IT-services	*588’165*	*842’378*	*727’324*	*731’477*	*2’889’344*
Other services & remunerations	*42’564*	*40’088*	*56’826*	*175’116*	*314’595*
Other costs	*-3’779*	*1’043*	*424*	*1’485*	*-827*
Depreciation of investments	*539’960*	*124’411*	*629’585*	*963’037*	*2’256’994*
Total costs of materials	**1’360’709**	**1’312’712**	**1’691’027**	**2’159’603**	**6’524’051**
Internal payments to ETH Zurich				**502**	**502**
Total costs	**2’351’828**	**2’405’683**	**2’740’700**	**3’327’924**	**10’826’134**

Compute infrastructure

Vendor & Model	CPU Type	No. of Processors	No. of Nodes	Inter-connect type	Interconnect bandwidth per partition (MB/s)	Total memory size (GB)	Year of installation plus upgrade history	Peak Performance (Gflop/s)	LINPACK Performance (Gflop/s)	Actual TOP500 position	Total File System Size (TB)	Millions of produced CPU hours	Average Utilization (%)	Annual direct costs in 2005 (CHF)
NEC SX-5/16	NEC custom	16	1	N/A	N/A	64.00	2000	128.00	125.80	-	1.00	0.11 **	64.93%	1'629'977.00
IBM pSeries 690 Turbo	Power-4 1.3GHz	256	8	Double Colony	400	768.00	2002	1,380.00	736.60	-	4.00	2.06 **	75.81%	1'593'058.00
Cray XT3	AMD Opteron 2.6 GHz	1100	1100	Cray XT3	7600 (per router) 1'400'000 (total)	2,200.00	2005	5,720.00	4,782.00	71	28.00	4.25 **	55.03% *	1'513'523.00

** average utilization for november and december 2005: 78.89%*
*** CPU hours over the whole year (for Cray XT3 since September)*

Usage Statistics

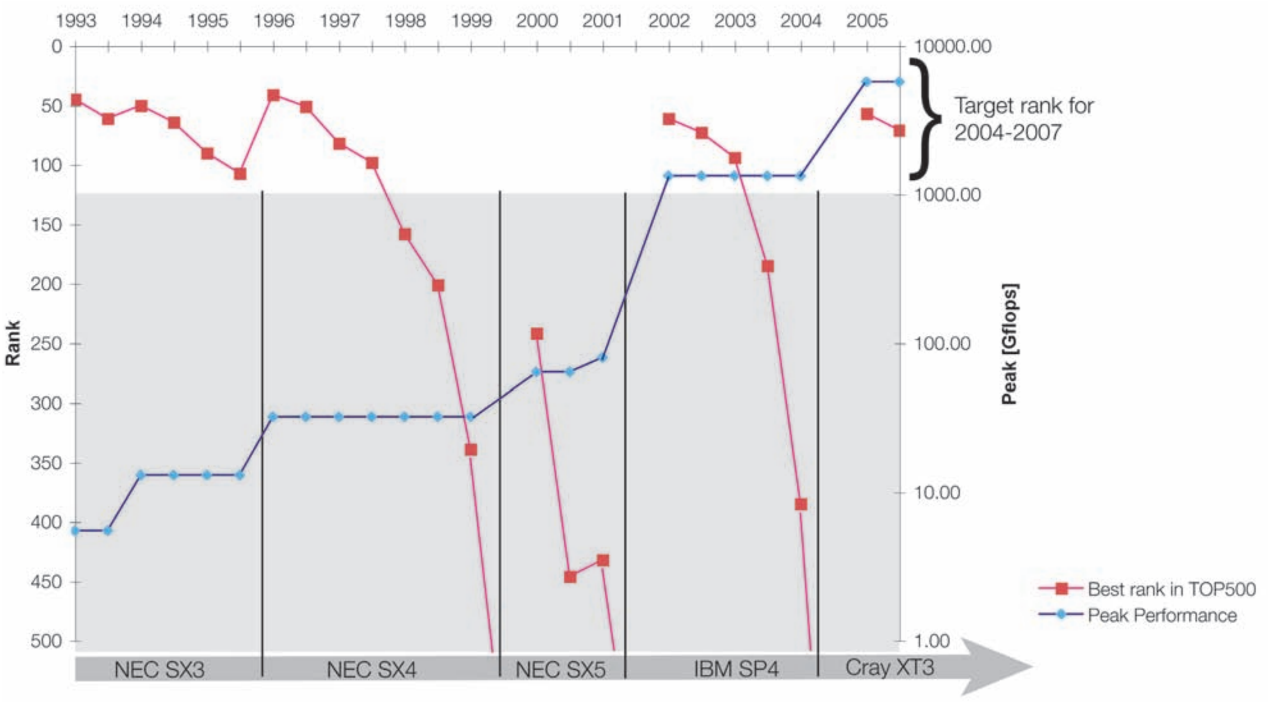
Usage by resarch fields

	Chemistry	Environment	Material Sciences	Physics	Other	Internal
NEC	5.92%	45.53%	16.29%	26.88%	5.38%	0.00%
IBM	64.10%	11.52%	9.34%	10.54%	4.50%	0.00%
Cray	30.04%	2.20%	0.00%	54.85%	0.11%	12.80%

Usage by customer

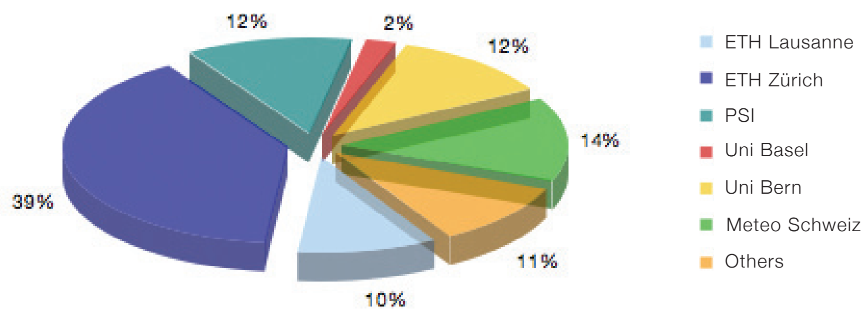
	ETH Lausanne	ETH Zürich	PSI	Uni Basel	Uni Bern	Meteo Schweiz	Others
NEC	10.22%	38.66%	0.00%	5.94%	0.00%	39.85%	5.33%
IBM	18.44%	44.93%	5.14%	0.00%	20.34%	0.00%	11.15%
Cray	4.92%	32.74%	31.66%	0.00%	15.22%	0.00%	15.46%

CSCS in the TOP500

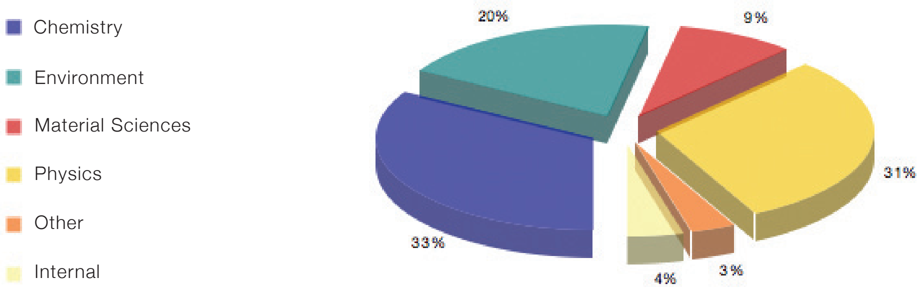


CSCS has committed in its performance mandate 2004-2007 to constantly operate a system in the upper quarter of the TOP500 list.

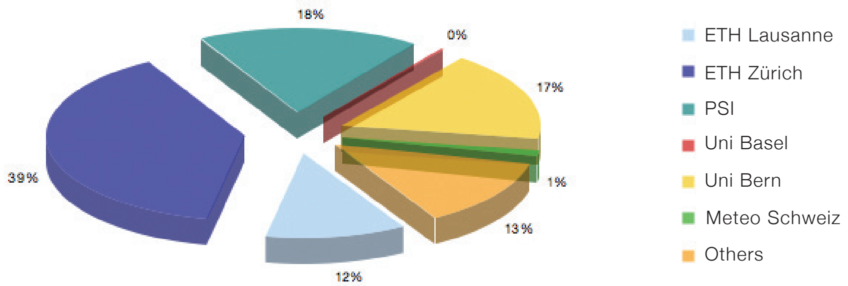
Cost of machines per institution based on direct costs during reporting period



Cost of machines per discipline based on direct costs during reporting period

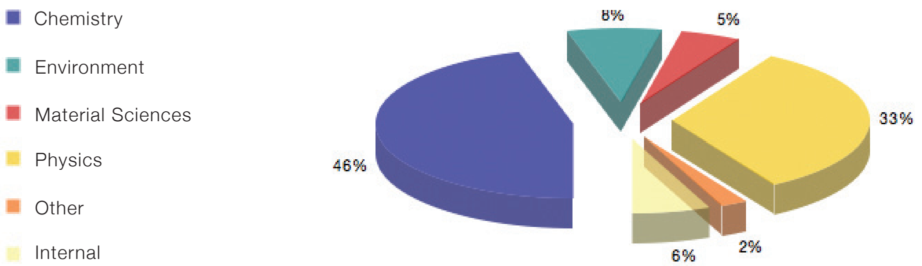


Share of cooperate resources based on produced CPU hours per institution during the reporting period



the field «others» includes broaching, testing and benchmarking of XT3

Share of cooperate resources based on produced CPU hours per discipline during the reporting period



Impact factor for papers listed in the 2004 Annual Report

Publication	Impact factor	Principal investigator	Application field
Oganov A.R. & Ono S. (2004). Theoretical and experimental evidence for a post-perovskite phase of $MgSiO_3$ in Earth's D" layer. - Nature **430**, 445-448	32.182	A. R. Oganov	Earth Sciences/Molecular Dynamics
Schär C., Vidale P.L., Lüthi D., Frei C., Häberli C., Liniger M.A. & Appenzeller C. (2004): The role of increasing temperature variability for European summer heat waves. Nature, **427**, 332-336; doi:10.1038/nature02300	32.182	C. Schär	Atmospheric Sciences
Van Swygenhoven H., Derlet P. M. & Frøseth A.G. (2004): Nanocrystalline metals: stacking fault energies and slip. - Nature Mater. **3**, 399.	13.531	H. v. Swygenhoven	Nanosciences/Molecular Dynamics
Deubel D. V., Frenking G., Gisdakis P., Herrmann W.A., Rösch N. & Sundermeyer J. (2004): Olefin Epoxidation with Inorganic Peroxides. Solutions to Four Long-Standing Controversies on the Mechanism of Oxygen Transfer. - Acc. Chem. Res., **37**, 645	13.153	Deubel/Parinello	Biosciences/Molecular Dynamics
Oganov A.R., Ono S. (2005). New high-pressure phase of alumina and implications for Earth's D" layer. Proc. Natl. Acad. Sci. 102, 10828-10831	10.452	A. R.Oganov	Earth Sciences/Molecular Dynamics
Berger R., Laubender G., Quack M., Sieben A., Stohner J. & Willeke M.; Isotopic Chirality and Molecular Parity Violation; Angew. Chem. Int. Ed. (English), **44**: 3623-3626 (2005)	9.161	M. Quack	Chemistry/Molecular Dynamics
Guidoni L., Spiegel K., Zumstein M. & Röthlisberger U. (2004): Green Oxidation Catalysts: Computational Design of High Efficiency Models of Galactose Oxidase. - Angew. Chem. **116**, 3348-3351.	9.161	U. Röthlisberger	Biosciences/Molecular Dynamics
Raiteri P., Martonák R. & Parrinello M. (2005): Exploring polymorphism: the case of benzene. - Angew. Chem. Int. Ed. 2005, **44**(24), 3769-3773	9.161	M. Parinello	Chemistry/Molecular Dynamics
Šljivancanin Ž. & Pasquarello A. (2004): Nitrogen adsorption on a supported iron cluster.- Vacuum **74**, 173	8.902	A. Pasquarello	Material Sciences/Molecular Dynamics
Bongiorno A. & Pasquarello A. (2004): Reaction of the oxygen molecule at the Si(100)-SiO_2 interface during silicon oxidation.- Physical review Letters **93**, 086102	7.218	A. Pasquarello	Material Sciences/Molecular Dynamics
Derlet P. M. & Van Swygenhoven H. (2004): High-FrequencyVibrational Properties of Metallic Nanocrystalline Grain Boundaries. - Phys. Rev. Lett. **92**, 035505.	7.218	H. v. Swygenhofen	Nanosciences/Molecular Dynamics
Ghose S., Krisch M., Oganov A.R., et al. (2005): Lattice Dynamics of MgO at High Pressure: Theory and Experiment; Phys. Rev. Lett. **96**, 035507	7.218	A.R.Oganov	Earth Sciences/Molecular Dynamics
Giustino F., Umari P. & Pasquarello A. (2003): Dielectric discontinuity at interfaces in the atomic-scale limit: Permittivity of ultrathin oxide films on silicon.- Physical review Letters **91**, 267601	7.218	A. Pasquarello	Material Sciences/Molecular Dynamics
Iannuzzi M. & Parrinello M. (2004): Proton transfer in heterocycle crystals. - Phys. Rev. Lett. **93**, 025901	7.218	M. Parinello	Chemistry/Molecular Dynamics
Martonák R., Donadio D. & Parrinello M. (2004): Polyamorphism of ice at low temperatures from constant-pressure simulations. - Phys. Rev. Lett. **92**, 225702	7.218	M. Parinello	Chemistry/Molecular Dynamics
Micheletti C., Laio A. & Parrinello M. (2004): Reconstructing the density of states by history-dependent metadynamics. - Phys. Rev. Lett. **92**, 170601	7.218	M.Parinello	Chemistry/Molecular Dynamics
Montalenti F., Raiteri P., Migas D.B., von Känel H., Rastelli A., Manzano C., Costantini G., Denker U., Schmidt O.G., Kern K. & Miglio L. (2004): Atomic-scale pathway of the pyramid-to-dome transition during Ge growth onSi (001). - Phys. Rev. Lett., **93** (21), 216102	7.218	M. Parinello	Material Sciences/Molecular Dynamics
Raiteri P., Laio A. & Parrinello M. (2004): Correlations among hydrogen bonds in liquid water. - Phys. Rev. Lett. **93**, 087801	7.218	M. Parinello	Chemistry/Molecular Dynamics
Von Lilienfeld O. A., Tavernelli I., Sebastiani D. & Röthlisberger U. (2004): Optimization of Effective Atom Centered Potentials for London Dispersion Forces in Density Functional Theory. - Phys. Rev. Lett. **93**, 153400.	7.218	U. Röthlisberger	Biosciences/Molecular Dynamics

Source: ISI Web of Knowledge [SM]

Cost analysis

Cost Coverage Calculation per 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**	**11'270'000**	**1'000'000**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**586'058**	**0**	**0**	**4'800'000**	**0**	**17'656'058**
Direct costs																
Directly assigned staff	0	0	0	0	0	0	0	0	0	0	152'518	93'890	143'631	2'730'187	0	3'120'226
Compute server costs (incl.sys admin staff)	480'855	1'310'009	81'246	0	126'649	320'364	0	0	0	0	622'814	0	0	0	280'775	3'222'713
Other costs	0	0	0	0	0	0	0	0	0	0	0	0	0	10'588'540	0	10'588'540
Total	**480'855**	**1'310'009**	**81'246**	**0**	**126'649**	**320'364**	**0**	**0**	**0**	**0**	**775'332**	**93'890**	**143'631**	**13'318'727**	**280'775**	**16'931'478**
Costs after approportioning of remaining scientific personnel to LUP customers																
Approportio need staff	38'330	38'330	38'330	38'330	38'330	38'330	38'330	38'330	38'330	38'330	0	0	0	-383'296	0	0
Total	**519'185**	**1'348'339**	**119'576**	**38'330**	**164'979**	**358'694**	**38'330**	**38'330**	**38'330**	**38'330**	**775'332**	**93'890**	**143'631**	**12'935'430 ***	**280'775**	**16'931'478**

** All investments are accounted under "internal"*

Cost Coverage Calculation per Research Field

	Chemistry	Engineering	Environment	Material Sciences	Physics	Other Research	Grid	Visualisation	Internal	Total
Proceeds										
Total	0	0	836'058	250'000	500'000	0	0.	0	16'070'000	17'656'058
Direct costs										
Directly assigned staff	115'481	0	152'518	0	115'297	0	217'685	428'008	2'091'237	3'120'226
Compute server costs (incl. sys admin staff)	1'117'645	0	925'649	414'315	606'046	12'781	0	0	159'380	3'235'816
Other costs	0	0	0	0	0	0	0	0	10'575'437	10'575'437
Total	**1'233'126**	**0**	**1'078'167**	**414'315**	**721'343**	**12'781**	**217'685**	**428'008**	**12'826'054**	**16'931'478**

FIDIREVISA
Società di revisione e consulenza

BDO Visura
Alliance partner

Membro della
Camera fiduciaria

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

Lugano, den 20. Januar 2006/GZ/zn

Sehr geehrte Damen und Herren,

auftragsgemäss, haben wir das Financial Reporting (4. Quartal 2005/Jahresabschluss) des CSCS SWISS NATIONAL SUPERCOMPUTING CENTRE für das am 31. Dezember 2005 abgeschlossene Geschäftsjahr geprüft.

Für das Financial Reporting (4. Quartal 2005/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 Financial Reporting (4. Quartal 2005/Jahresabschluss) mit angemessener Sicherheit erkannt werden. Wir prüften die Posten und Angaben des Financial Reporting (4. Quartal 2005/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 Financial Reporting (4. Quartal 2005/Jahresabschluss) als Ganzes. Wir sind der Auffassung, dass unsere Prüfung eine ausreichende Grundlage für unser Urteil bildet.

Wir empfehlen, das vorliegende Financial Reporting (4. Quartal 2005/Jahresabschluss) zu genehmigen.

Mit vorzüglicher Hochachtung
FIDIREVISA SA

G. Zwahlen P. Picco
Leitende Revisoren

Beilagen:
– Financial Reporting (4.Quartal 2005/Jahresabschluss)

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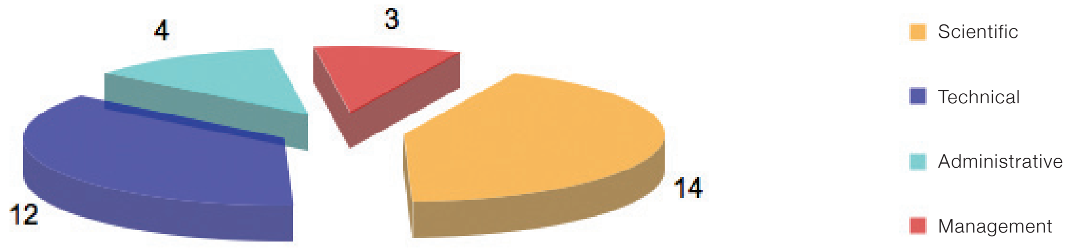
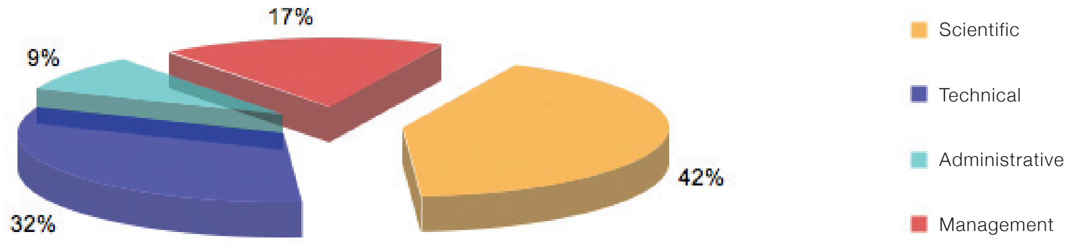
Personnel

Head Count (as of 31st December 2005)



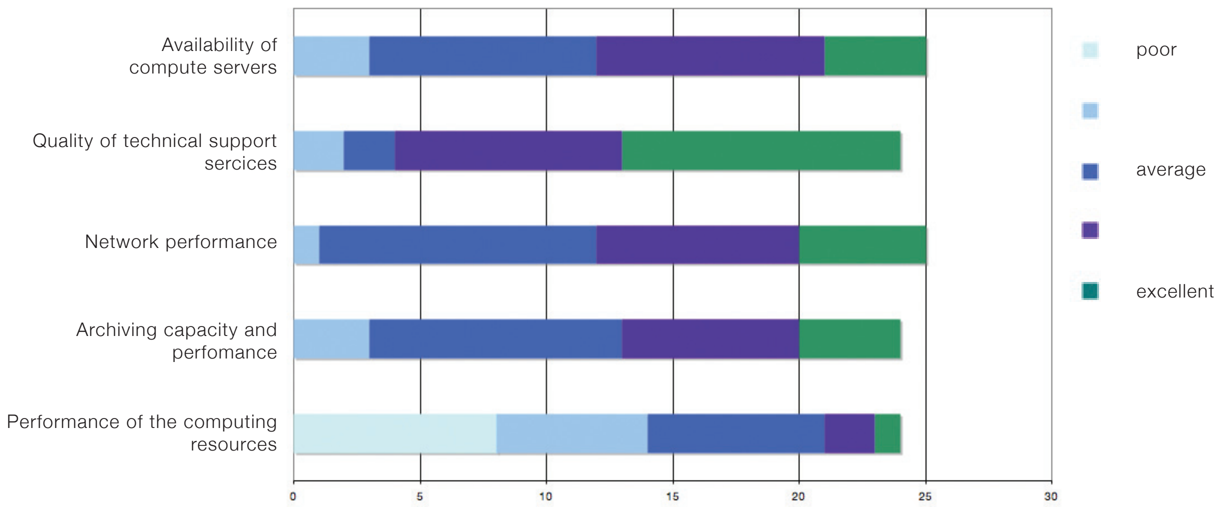
Staffing Costs (total for 2005)



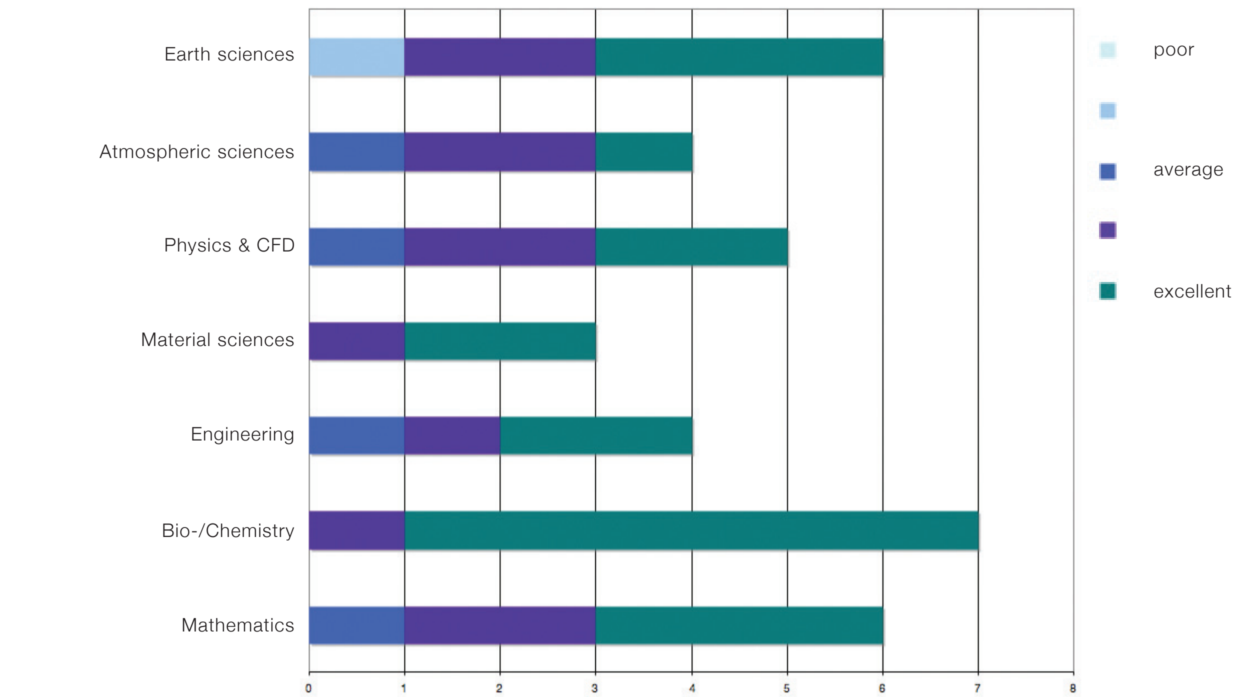
Customer satisfaction (February 2006)

The following customer survey results are based on responses of 57% of the groups that run large projects on CSCS systems.

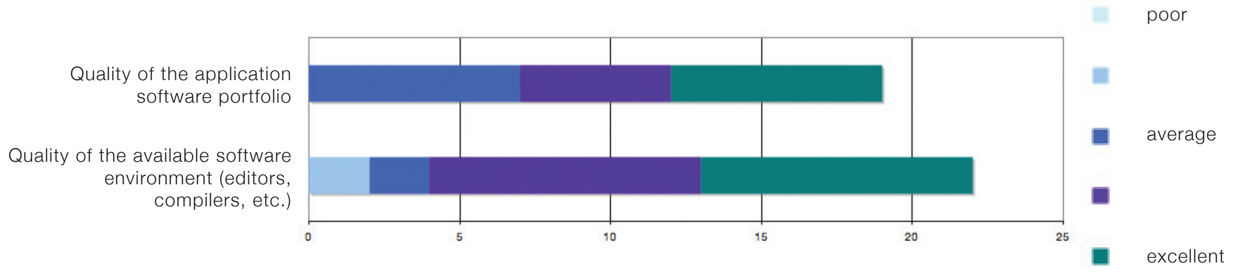
CSCS services portfolio



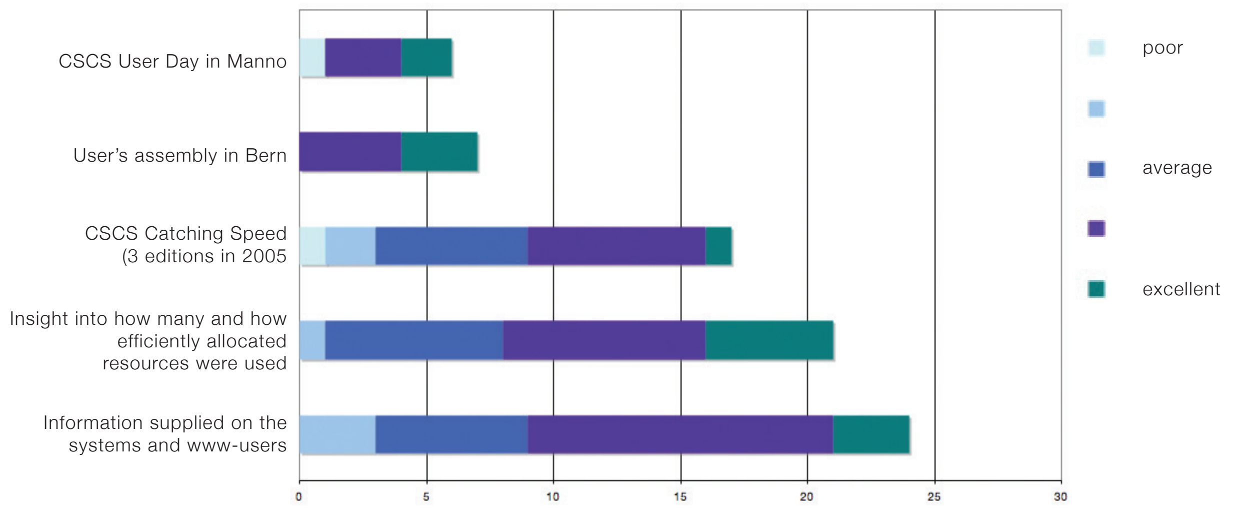
Quality of user support in the following fields



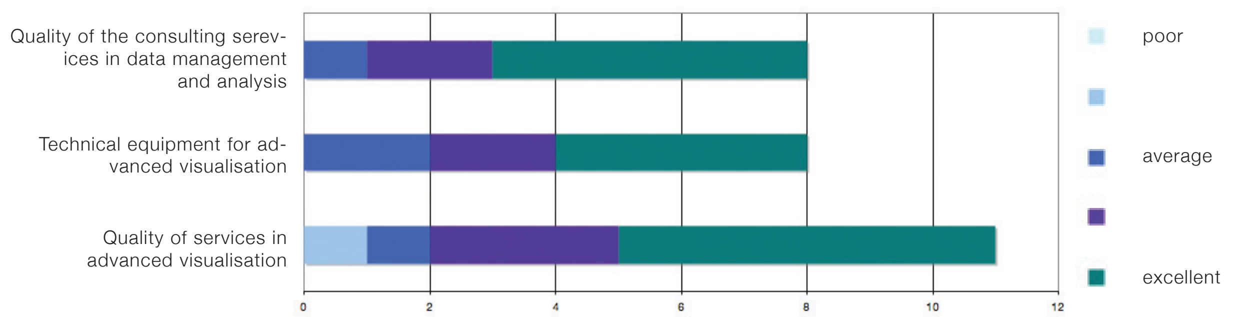
Application and user support



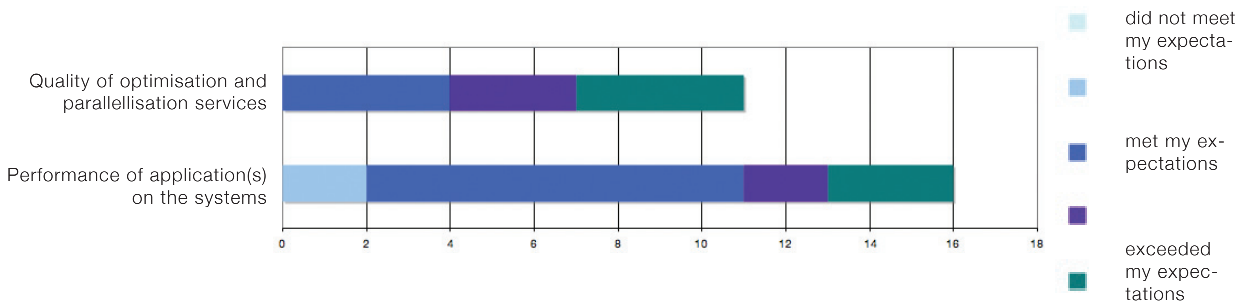
Information services



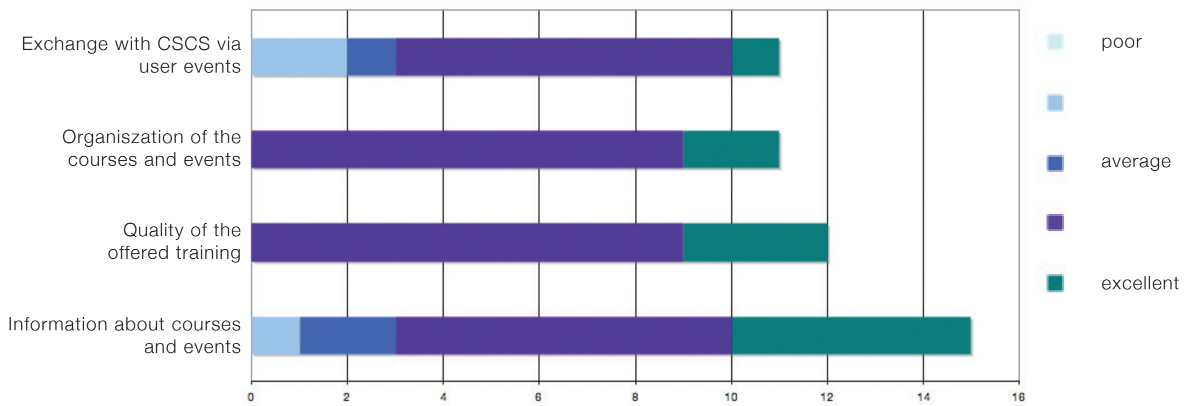
Visualization and data analysis



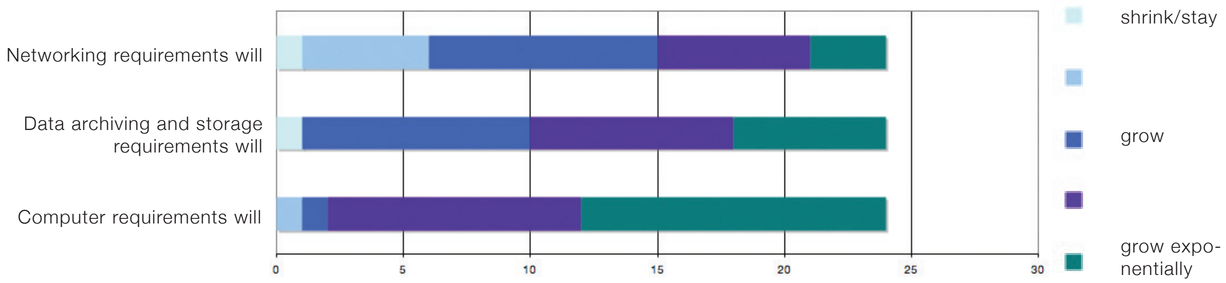
Software support

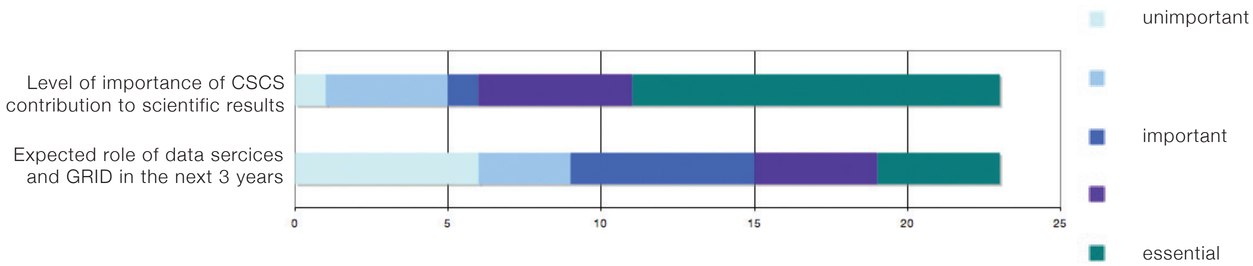


Training courses and events



Future expectations and wishes





Publications

Papers published by collaborators CSCS

Favre J., Foggia Th., Garcin H., Parkinson E. % Braune A.; Simulation of a full Pelton turbine, Return on experience & Handling of large data sets, 23rd CADFEM Users' Meeting 2005

Marmo R., Valle M.; Visualizzazione scientifica: un aiuto per capire, Mondo Digitale, AICA, n. **4**, December 2005, p. 45–58

Valle M.; STM3: a chemistry visualization platform, Zeitschrift für Kristallographie Vol. **220** (2005) Issue 5-6 Pages, 585-588

Valle M., Favre J., Parkinson E., Perrig A. & Farhat M.; Scientific Data Management for Visualization Implementation Experience, Simulation and Visualization 2005 Magdeburg, March 3 – 4, 2005

The Swiss ATLAS Computing Prototype. By S. Gadomski, C. Haeberli, F. Orellana, G.L.Volpato. May 2005. 18pp. ATLAS Note: ATL-SOFT-PUB-2005-003; CERN-ATL-COM-SOFT-2005-007.

Papers published by users of CSCS

Alfredsson M., Dobson D.P., Oganov A.R., Catlow C.R.A., Brodholt J.P., Parker S.C. & Price G.D. (2005); Crystal morphology and surface structures of the orthorhombic $MgSiO_3$ perovskite, Phys. Chem. Minerals **31**, 671-682.

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Arcidiacono S., Walther J.H., Poulikakos D., Passerone D. & Koumoutsakos P.; On the solification of gold nanoparticles in carbon nanotubes, Phys. Rev. Lett., **94**(10):105502, 2005.

Bas D., Bürgi T, Lacour J., Vachon J. & Weber J., Vibrational and electronic circular dichroism of D-TRISPHAT [tris(tetrachlorobenzenediolato)phosphate (V)] anion, Chirality **17**, 143 (2005).

Beniston M., (2005) Warm winter spells in the Swiss Alps: Strong heat waves in a cold season? Geophysical Research Letters, **32**, L01812

Bieri M. & Bürgi T., Adsorption kinetics, orientation and self-assembling of N-acetyl-L-cysteine on gold: a combined ATR-IR, PM-IRRAS and QCM study, Journal of Physical Chemistry, B. **109**, 22476 (2005).

Bieri M. & Bürgi T., Probing enantiospecific interactions between proline and a L-glutathione self-assembled monolayer by modulation excitation ATR-IR spectroscopy, Journal of Physical Chemistry, B **109**, 10243 (2005).

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Bongiorno A. & Pasquarello A., Atomic-scale modelling of kinetic processes during silicon oxidation, Journal of Physics: Condensed Matter **17**, S2051 (2005).

Bongiorno A. & Pasquarello A., O2 oxidation reaction at the Si(100)-SiO2 interface: a first-principles investigation, Journal of Materials Science **40**, 3047 (2005).

Bosse T., Härtel C., Meiburg E. & Kleiser L.; Numerical simulation of finite Reynolds number suspension drops settling under gravity, Phys. Fluids, 17:037101, 2005.

Bosse T., Kleiser L., Favre J. & Meiburg E.; Settling and breakup of suspension drops, Phys. Fluids, **17**:091107, 2005.

Bosse T.; Numerical simulation of disperse two-phase flows: I. Settling and break-up of suspension drops, II. Particle settling in homogeneous turbulence PhD thesis, ETH Zurich, Switzerland, 2005. Diss. ETH No. 15903.

Branduardi D., Gervasio F.L., Cavalli A., Recanatini M. & Parrinello M.; The role of the peripheral anionic site and cation-pi interactions in the ligand penetration of the human AchE gorge, Am. Chem. Soc. **127** (25): 9147-9155 (Jun. 2005)

Buch V., Martonak R. & Parrinello M.; A new molecular-dynamics based approach for molecular crystal structure search, J. Chem. Phys. **123** (5), Art. No 051108 (2005)

Bürgii T.,Combined in situ attenuated total reflection infrared and UV-Vis spectroscopic study of alcohol oxidation over Pd/Al2O3, Journal of Catalysis, **229**, 55 (2005).

Bussi G., Menendez J., Ren J., Canonico & M.Molinari E.; Quantum interferences in the Raman cross section for the radial breathing mode in metallic carbon nanotubes, Phys. Rev. B 71 (4): Art. No. 041404 JAN 2005

Casty C., Handorf D. & Sempf M.; Combined winter climate regimes over the North Atlantic/European sector 1766-2000, Geophys. Res. Lett., **32**, L12801, 2005b.

Casty C., Handorf D., Raible C.C., Luterbacher J., Weisheimer A., Xoplaki E., Gonzalez-Rouco J.F., Dethloff K. & Wanner H.; Recurrent climate winter regimes in reconstructed and modeled 500 hPa geopotential height over the North Atlantic-European sector 1649-1990, Clim. Dyn., **24**, 809-822, 2005a.

Casty C., Wanner H., Luterbacher J., Esper J. & Boehm R.; Temperature and precipitation variability in the European Alps since 1500, Int. J. Climatol., 32, L12801, 2005c.

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