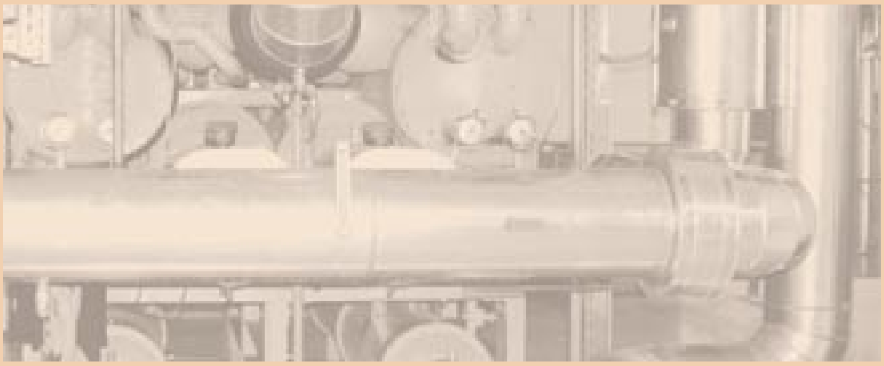
CSCS
Swiss National Supercomputing Centre



Annual Report 2006

CSCS
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Meetings of Steering Board (SB), and Scientific Advisory Board (SAB) in 2006

10.2.2006, SB, CSCS Manno
17.3.2006, SB (Extraordinary), ETH Zurich
17.5.2006, SB, ETH Zurich
4.7. SB (Extraordinary), Bern
21.9.2006, SB/SAB, Bosco Luganese
20.11.2006, SB, ETH Zurich

Content

Dr. Stephan Bieri

Carte Blanche

Costly infrastructure: competition and regulation

Margaret Thatcher had some very intelligent ideas, but not always found the best outlets for them . The case of the British electricity industry demonstrates how important the practical implementation of a theoretical concept is. The deregulation of infrastructure services in the United Kingdom followed – especially in the case of electricity, gas, and water – the same design.

Open access

Deregulation should open a closed market and make it more dynamic. The British government intended to dissolve public monopolies, to debundle vertical market structures, and to introduce the consumer's freedom to choose their provider. The first point meant not only the privatization of ownership – selling the capital of the formerly public-owned utilities – but a novel regulation of the specific market conditions as well. The newly established regulatory agency , under the diligent lead of Prof. Littlechild, had a deep understanding of its mandate that came with the power to reorganize the industry.
Separation of generation, transmission, and distribution, the second point, was successfully fulfilled by restructuring the vertically integrated companies and by opening them for domestic and foreign investors. Over the course of six, seven years, there was efficient competition with better service to clients and significant price cuts. Industries and households were able to reduce or stabilizes their electricity budgets, and new types of consumer contracts were developed. Of course, the mobility of consumers according to the last point stayed relatively modest – only a portion of clients, namely larger firms, did change the provider.
And today? We encounter an internationally oriented, marketing driven industry with large, capital intensive companies; the importance of mergers and acquisition (M&A) grew remarkably. But on the other hand, the specificity of electricity again favoured the rise of regional monopolies. And the capitalistic pressure to make profits partly undermined their investment pattern. Just before stepping down, Prof. Littlechild drew a mixed picture of his term in office, but was able to influence Tony Blair to legislate additional regulation. The first one was a better monitoring of the behaviour of large generators and transmission firms, especially concerning the conditions of free access to power lines. In addition, he mandated the introduction of new quality measures for the industry, including life-cycle cost. Today, the United Kingdom is one of the key driving forces of the EU energy market.

Lessons learned?

Many European electricity and gas regulators took their cues from the British experiment. In Germany, large monopolistic utilities are under intense regulatory scrutiny because of their high price levels and the way they demonstrate their market power towards outsiders. Blackouts are taken as serious indicators for a non-professional grid management. In Switzerland, the opening of the electricity sector is still controversial, partly for fiscal reasons (cantons and communities use electricity prices as indirect tax subject), and partly because of the immobility of the highly decentralised structures. One effect of this situation is a loss of European market share – although Switzerland still has to offer high quality electricity for load management purposes.
Neither “service public” nor “deregulation” are the only solution. In many fields of sophisticated infrastructure, we have to tackle interdependence and openness instead. While consumer needs, technological possibilities, and financial constraints influence a specific concept, only often different approaches and institutional arrangements seem

practical. I think High Performance Computing (HPC) is precisely such a case in point. There are many ways and different options, but providers have to define their way. And, they must be able to implement and to adjust without hesitation.

HPC and Computational Science

In the nineties, CSCS had to develop national "Supercomputing" in the sense of producing economies of scale within a landscape of mainframe computing. The rise of vector machines and – later – the possibilities of massive parallelization (MPP) offered new opportunities. CSCS seized them. But in the meantime, investment costs for components and clusters decreased, and single universities or even faculties have been able to open the door to HPC. Of course, such Capacity Computing may be, over all, very costly in the long term. And in some cases, only vendors profited from it. However, the actual comparative advantage for CSCS as a national provider lies in the field of Capability Computing.

Computational Science is a novel way of conducting scientific work by using the power of computers in a specific way. Developing theories, doing lab tests, and simulating alternative functionalities or properties define an interlinked method of research. No research university, and especially none focusing on Life Science, should miss this track. The integration of adequate HPC is a key element. The question that remains, however, is whether this should be done alone or in a joint effort with others?

In my eyes, technological and financial reasons ask for more co-operations, nationally and internationally. HPC should be understood as a holistic approach, combining computer performance with task driven services and "pulled" R&D. Therefore, minimal scales and specialisation are needed. The development of hardware, software, and HR must be seen as a system. The notion of a "centre" implies at least the following:

- designing a joint architectural concept of capacities with an integrated communication network (grid) and complementary data storage, and
- creating a complementary knowledge base covering imaging, data mining, and the use of metadata.

What to do?

Some people believe that spontaneous collaboration within a network is sufficient. I am not convinced. Of course, user driven clubs (e.g. bioinformatics) are bringing together grid related capacities, more or less cost-effective and technically innovative. The LHC case, an intelligent multi-level network, shows another aspect: the possible externalization of cost from a project to those owning capacities. Bottom-up initiatives are useful, but the long-term allocation of resources must be planned top-down. Universities, regional clusters, nations, and international communities have to design their HPC systems and express their priorities. Exactly as is the case for neutron sources, clinical test facilities or other large research installations.

Here, the analogy to the electricity sector is striking. The grid is a backbone for transmission, but has no intrinsic value as such. Because of its overhead role, open access is essential. Theoretically, a grid can be designed and run by any institution or firm following the architecture mentioned above.

Switzerland is a small, open economy, depending on the global exchange of goods and services. This is also true for the university sector where scientific production is international per se. We cannot change these conditions, but we can strengthen our domestic scientific infrastructure. A national user lab uniting the support of 12 plus 7 universities and 4 research institutes seems to be manageable. But a threefold leadership problem must be solved:

- identifying a strong and sustainable investor, capable of designing the system and ready to collaborate with industrial partners,
- nominating a scientifically sensible, efficient provider with the necessary authority to undertake national load management,
- setting common standards for grid collaboration, specific pooling, and procurement.

Who could manage such a job if not the ETH Domain? The new Performance Mandate of the Domain shows that Federal Government has a clear commitment. But evidently, there is not an unlimited amount of time to realize it.

Activity Report

Dr. Marie-Christine Sawley, CEO

Introduction

Major initiatives in supporting leadership class science

The accomplishments of the CSCS in the past year are in line with the qualitative and quantitative growth of the Centre. The computing infrastructure was extended considerably by putting the Cray XT3 massively-parallel system into production at the beginning of 2006 which was soon followed by a 50% extension of its capacity. In 2006, we also launched a new type of offer called Swiss ALPS (for Advanced Large Projects in Supercomputing). This initiative is aimed at enabling scientific breakthroughs by means of large computational research projects. Four projects (climatology, earth sciences, molecular dynamics and biomaterials) have been granted for a period of two years starting 1st January 2007. We plan to establish strong working relationships with such outstanding research groups by assigning specialised CSCS staff to each of them to identify the computing needs and to help solving technical problems in order to facilitate as much as possible their research work. In this way, we hope to develop outstanding collaborations between each ALPS group and the CSCS in areas of strategic importance such as optimization and parallelization, the handling of very large parallel data and scientific visualization.

During the last quarter of 2006, we proceeded with the installation of the new HPC platform, an IBM Power 5-575 with InfiniBand Interconnect. This new system will reach its full production in the course of 2007, offering significant capacity for applications requiring shared memory combined with a good interconnect network.

Our role and contributions within the community software development have increased considerably in particular with the release of a completely remodeled version of “Molekel”, an open source (GPL) multiplatform molecular visualization program originally developed at CSCS.

Project highlights
The national Grid development in Switzerland has taken a decisive turn thanks to two converging trends: the portfolio of Grid projects (from the Swiss Bio Grid to the Intelligent Scheduler System) are starting to produce good results. In parallel, a major effort has been made with the Swiss Grid Initiative under the form of a partnership between research institutions, a step that will also enable us to participate in the infrastructure projects of the European community and to collaborate with other international partners.

While supporting MeteoSwiss in tuning their new production suite (high resolution, increased frequency of forecast, more stringent requirements), we have made significant progress, and the prospect for the operation of the high resolution model by 2008 looks very positive.

International profiling
On the international scene, we represent our country in the European task force for high-end computing Europe (HET), playing an active role in the development of the research infrastructure. It is essential for us to develop a strong profile in order to assure our scientists the best possible conditions for high-level HPC infrastructure. During 2006, CSCS continued to be involved in the Lincei Initiative, a study financed by the European Science Foundation, for developing and maintaining community codes.

Outlook and forecast
CSCS users are members of the national computational science community, and benefit from the advanced computing resources which we make available through peer reviewing of the proposed projects. Research groups that obtain access to CSCS resources establish a relationship with the Centre CSCS without the need of participating in the funding of the Centre, as is the case for contractual partners. Serving the academic community is our core business, which relies on funds for operation and periodically requires the financing of new investments. It is the responsibility of CSCS, in accordance with its governance, to take the actions for deploying and maintaining the computing infrastructure along with the needed services, and proposed the strategic development thereof. The next performance mandate is being prepared for ensuring the growth of HPC in Switzerland, through infrastructure, buildings, research and user support, and software development. A strong partnership between CSCS as the national service provider, its users and partners will enable a successful, long term strategy.

I wish you pleasant reading.

Marie-Christine Sawley

Fulfilment Status of the CSCS Performance Agreement 2004-2007

Since 2004, CSCS operates on the basis of a global budget and a performance agreement with ETH Zurich, its leading institution. The performance mandate (available on the CSCS web site) defines the goals to be achieved during the 2004-2007 period and the annual global budget granted. The mandate includes CSCS commitment to implement quality assurance measures, including regular controlling and reporting and external peer reviews.

The performance agreement between ETH Zurich and CSCS for 2004-2007 includes nine goals subdivided into three groups that are quoted below:

1. High-Performance Computing & Networking methods and software
   a. CSCS hires additional highly competent staff in innovative fields of scientific computing. It significantly extends its current human resources base in scientific computing.
   b. CSCS participates in at least two national and international collaborations for developing new computing tools for specific research communities.
   c. CSCS supports more than two strategic research groups in an integrated way, enabling them over a period of two years to produce new scientific results of international significance.

2. Operations of complementary HPCN computer architectures
   a. CSCS constantly operates a system that is represented in the upper quarter of the TOP500 list.
   b. CSCS increases its sustained computing capacity by a factor of three over as many years.
   c. CSCS supports at least two major groups in day-to-day work of high criticality.

3. Positioning the centre both nationally and internationally
   a. CSCS is involved in at least three major international collaborations in computational science during the performance period.
   b. CSCS starts and manages at least one national grid initiative during the performance period.
   c. CSCS establishes a programme of courses, workshops, and summer schools with an annual throughput of participants that exceeds CSCS' headcount by more than factor two.

Three years of the 2004-2007 period have elapsed and negotiations for the new performance agreement are about to start. Now is the right time to assess past achievments. All goals stated in the performance agreement (above) are considered, and the comments show that CSCS has achieved all of them already after three years, frequently even surpassing the expectations expressed for the performance period of four years.

Goal 1a: Extending the scientific computing staff
The following table presents the development of CSCS between 2004 and 2006. It shows that the number of employees has more than doubled (in-

	1/2004		12/2006		Change between 04 and 06	
	Headcount	Proportion	Headcount	Proportion	Headcount	Proportion
Administration	2	10%	5	12%	+3	+2%
Technical staff	13	65%	13	32%	0	-33%
Scientific staff	3	15%	18	44%	+15	+29%
Management	2	10%	5	12%	+3	+2”
Total units	21	100%	41	100%	+21	-

Table 1: The table shows clearly how strongly the share of the scientific staff grew during the performance period.

crease of 105%) and underscores a major increase in the scientific staff:

The constant total in the technical staff (13 pesons), however, does not indicate that this part of the staff did not change. Instead, some employees at CSCS, whose work was rated as technical in the beginning of 2004, were re-classified as scientific during the performance period because the scope and the depth of the assigned tasks changed. New, purely technical staff joined CSCS, thus keeping the head-count in the technical unit constant.

Goal 1b: National and international collaborations for new tool developments

The aim is to strengthen the profile of CSCS in scientific software engineering and development. CSCS is involved in a multitude of such projects, especially in the Advanced Large Projects in Supercomputing (ALPS) and in the Grid activities described in later sections of this report. In addition, the further development of the Molekel software should be highlighted. Despite it's large, worldwide user base, Molekel was not further improved following it's initial development at CSCS in the 1990's. In 2004, a survey had indicated the existence of a market for an upgrade of Molekel, and CSCS engaged in a total re-design of this software based on modern, public-domain libraries and added functionalities. The impressive result of this effort (see below) underlines the expertise in the area of visualisation software development at the centre.

Goal 1c: Supporting strategic research groups for obtaining scientific results of international significance

The ALPS programme was introduced at CSCS in 2006 for enabling research projects aiming specifically at scientific breakthroughs by means of large-scale computing. Projects of this type are required to involve a scientific collaboration between the applying research group and CSCS. The first four projects, which were accepted in 2006 and are described in a further section of this Annual Report, clearly show that CSCS has fulfilled this important goal.

Goal 2a: Constant operation of a system in the upper quarter of the TOP500 list

As shown in Figure 1, in the past newly installed systems at CSCS rapidly fell out of the TOP500 list be-

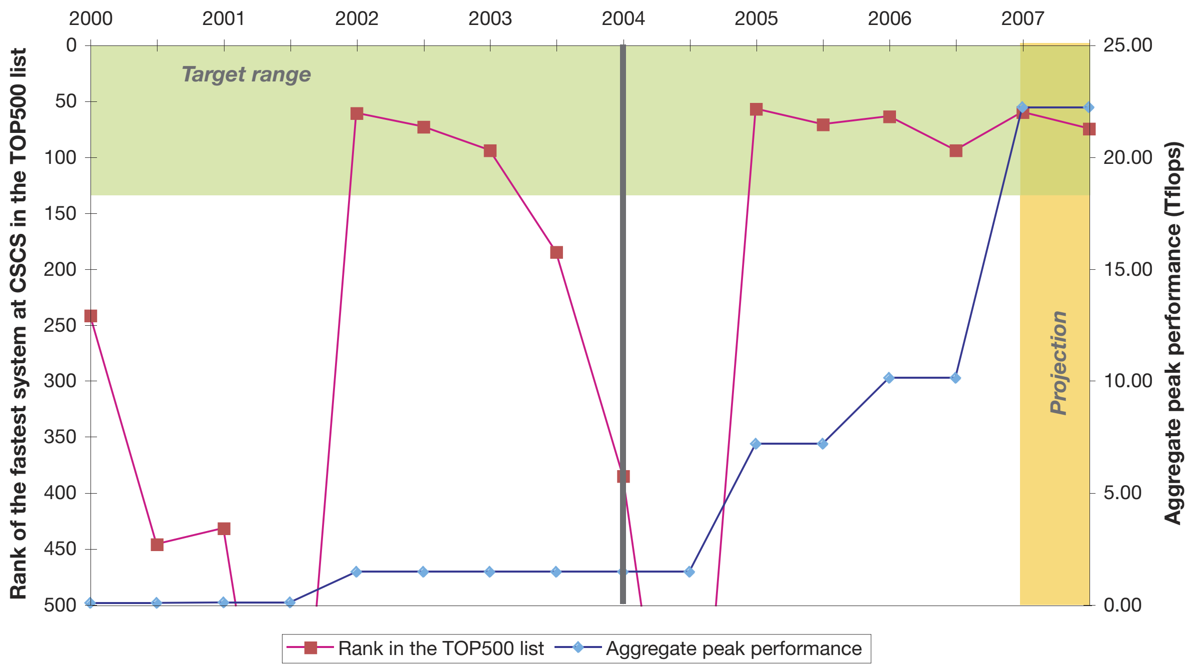


Figure 1: Development of the rank of the most performing system of CSCS in the TOP500 list and of the aggregate peak performance at CSCS

cause of insufficient further developed after installation. Following the introduction of the Cray XT3 in mid-2005, CSCS continued to further develop the performance and capacity of the system according to user needs. A 50% extension was realized in 2006 and dual-core processors will be installed in 2007 to maintain the system performance, according to international standards, within the Top100 range.

Goal 2b: Increasing sustained computing capacity by a factor of three over as many years
At the beginning of 2004, CSCS operated two production systems, a NEC SX-5 vector computer and an IBM SP4 constellation. These systems were replaced with a Cray XT3 massively-parallel system, installed in 2005, and an IBM P5 constellation purchased in 2006. The new IBM P5 was not yet in production by the end of 2006. Hence, Table 2 compares sustained compute capacities for a series of representative codes between the two prior systems and the Cray XT3 system for exactly the same test case, underscoring the impressive performance improvement due to the introduction of the Cray XT3, and demonstrating the fulfillment of goal 2b.

Goal 2c: Supporting at least two major groups in day-to-day work of high criticality
CSCS has two contractual partners for whom it guarantees essential daily IT services: MeteoSwiss and CHIPP, the Swiss Institute for Particle Physics. The collaboration with MeteoSwiss already has a tradition of seven years and comprises the commitment to deliver compute, processing, and storage resources for the daily weather forecasts of Switzerland. The partnership with CHIPP was founded during the current performance period. CSCS has started to build and operate a dedicated cluster infrastructure for the scientific analysis of the data from the new particle accelerator at CERN, called LHC. This infrastructure will be developed further until 2009 and will be maintained and operated by CSCS even beyond that date.

Goal 3a: Involvement in at least three major international collaborations in computational science
As illustrated below, the ALPS programme, has awarded compute and support resources to four research projects. For each of them, the international collaboration potential had to be outlined. Two projects were submitted jointly with external researchers: Prof. Gary Glatzmaier from the University of California, Santa Cruz, belongs to the research team of Prof. Andrew Jackson from ETH Zurich, and Prof. Klaus Schulten from the Universiy of Illinois, Urbana-Champaign, is integrated in the project of Prof. Viola Vogel of ETH Zurich. The two other projects are more loosely connected to a series of international collaborators: The project of Prof. Michele Parrinello includes collaborations with the Universities of Bologna, Milan and Rome, and the University of Pennsylvania. The project of Prof. Christoph Schär in-

Code	aLMo	COBOLTS	Amber	NAMD
Application area	Weather forecasting	Computational fluid dynamics	Molecular dynamics	Molecular dynamics
Benchmark	7km grid operational suite		Human Factor IX protein test case	ApoA1 test case
System beginning of 2004	NEC SX-5	NEC SX-5	IBM SP4	IBM SP4
Total no. of processors	16	16	256	256
Required capacity (no. of CPU x hours)	14	8	1	1.89
System by end 2006	Cray XT3	Cray XT3	Cray XT3	Cray XT3
Total no. of processors	1650	1650	1650	1650
Required capacity (no. of CPU x hours)	100	128	0.25	0.56
Factor of sustained system capacity increase	14.4	6.4	25.8	21.75

Table 2: The table shows how impressively well CSCS succeeded in fulfilling this goal already before the new IBM P5 system went into production.

cludes collaborations with the Max-Planck-Institute of Climatology in Hamburg, the Joint Research Centre of the European Commission ISPRA, the California Institute of Technology, the Swiss Weather Service MeteoSwiss, ECMWF at Reading, the research consortium CLM, and the NCCR climate.

Goal 3b: Starting and managing of at least one national grid initiative

As described below, CSCS has successfully initiated the Swiss Grid Initiative, a national effort in Grid computing. Already in 2004, CSCS started the Swiss BioGrid, an application field oriented knowledge-grid initiative, and partnered with CHIPP for the LHC Computing Grid.

Goal 3c: Establishing a programme of courses, workshops, and summer schools with an annual throughput of participants that exceeds CSCS' headcount by more than a factor of two

The following table summarises the educational efforts during the last three years underlining the growing involvement of CSCS in a variety of educational activities with participations well above target:

Year	events	participants
2004	4	175
2005	8	200
2006	11	515

It should be noted that CSCS organized and hosted in 2006 the international CUG06 conference with more than 170 participants.

Dominik Ulmer

The EGEE real-time monitor represents each institution running a Grid ‹node' as a pulsating colored dot, which alternates between green and red, depending on the load of the system. The lines connecting nodes represent active data transfer operations.

Grid Activities

Grid Computing is addressing the new paradigm of collaborative science, where discoveries are being sought in large national and international collaborations. Grids provide means to share resources among different scientific communities and to facilitate, in this way, scientific contacts and collaboration. It also aims to maximize the overall resource capacity for the benefit of science. Researchers throughout Switzerland have already engaged in several Grid-related projects of national and international scope in which CSCS is directly or indirectly involved. CSCS has been engaged in Grid activities since the beginning of 2004, and its Grid Team has grown to a total of five staff members by the end of 2006. The growth has boosted Grid activities, and CSCS has consolidated its portfolio of projects and markedly extended its activities.

The mandate for the current performance period asked CSCS to establish a Grid initiative of national scope. The Swiss Grid Initiative was thus established and officially launched in September 2006 in Geneva, with the participation of many Swiss institutions and projects. The Initiative has rapidly gained considerable support and is actively evolving and shaping itself into a form most suitable for Switzerland, involving all interested parties. CSCS has spearheaded the effort, acting as the main driving force, organizing the launch in Geneva as well as follow-up events. As agreed within the community involved, the Swiss Grid Initiative will have two main functions:

1. It will offer a contact base for all Swiss Grid projects, including support for all projects, users and administrators.
2. It will coordinate a Swiss National Science Grid Infrastructure that is operated by the participating institutions.

The Swiss Grid Initiative aims to be a solution-oriented, multi-institutional and multi-disciplinary collaborative organization involving all interested parties in Switzerland. It strives to build a research environment using Grid technology and infrastructure that will be suitable for the completion of the production-level research tasks. The collaborative program will include activities in research, technological development, deployment and testing, as well as training and outreach.

In addition, the Swiss Grid Initiative will represent the interests of Swiss academic research institutions and Swiss Grid projects. It aims to become the national promoter for Grid projects and to enable the participation of Switzerland in national, European and world-wide collaborative projects. The largest projects in which CSCS is currently involved are "Enabling Grids for E-science in Europe" (EGEE), the largest EU-funded Grid project, and the "Worldwide Large Hadron Collider Computing Grid" (WLCG). CSCS is working since 2004 with the community of Swiss particle physics researchers, which is organized within the "Swiss Institute for Particle Physics" (CHIPP). This community is strongly involved in the Large Hadron Collider project at CERN, which uses the WLCG for data analysis. CSCS acts as the Swiss regional centre within the WLCG hierarchy.

CSCS is a full member of the EGEE-II project which started in April 2006, and as such receives funding from the EU that enables the operation of the local Grid resource. In this context, CSCS has taken on the role of contributing to the community support inside the EGEE German-Swiss federation (DECH).

CSCS was also co-organiser of the Swiss Grid Crunching Day on December 7th, 2006 in Fribourg, where the use of the EGEE infrastructure for the Swiss community was demonstrated with a complex application developed at the Ecole d'Ingenieurs de Fribourg.

Several events, in 2006, involving the CSCS and concerning the Swiss Bio Grid project are worth mentioning. The Bio Grid project was strengthened considerably, when Dr. Arthur Thomas joined as project manager. The Swiss Bio Grid infrastructure has been consolidated thanks to the involvement of CSCS in leading and assisting the partner sites with installation and testing. Several new projects are now using this infrastructure. The Proteomics Project intends to use the Grid infrastructure to analyse millions of spectral data for identification purposes. Thanks to a software grant from Sybase Corporation, the Avaki Datagrid approach to distribute data could be tested on the Swiss Bio Grid infrastructure.

Proteomics studies analyze mass spectrometry data with the help of specialized software and databases.

CSCS also actively participates in other projects like the Intelligent Scheduling System ISS and the South European Partnership for Advanced Computing SEPAC. Collaborations have been initiated with the Faculty of Informatics of the University of Lugano (USI) and the Institute for Research in Biomedicine (IRB) in Bellinzona.

Peter Kunszt

Software Services

The introduction of the Cray XT3 into production, the arrival of the IBM Power 5 machine, and the preparation for MeteoSwiss high resolution forecasting dominated the activities of the software services group in 2006.

In addition to the continued porting and optimization work on the Cray XT3 which was carried out together with the user and application support group, software services developed the policy and infrastructure for accounting, scheduling and prioritisation on the main Cray XT3 system, Palu. The new scheduling policy has enabled the Cray to act as a true large-scale MPP machine with jobs consuming large processor counts and tackling large-scale scientific problems, whilst maintaining an extremely high utilisation rate on the machine of around 90%.

The expansion of Palu in the Summer of 2006 was accompanied by the launch of the Swiss ALPS scheme, a new type of project designed to target scientific breakthroughs. These projects are to be given large amounts of compute time over a two year period and they will also involve a greater degree of interaction between computer science specialists at CSCS, who will be mainly based in the Software Services group, and the scientists who will be carrying out the research. The initial call for proposals produced four projects which are to be supported, and software services personnel began to work on introducing these projects to the XT3 system at the end of 2006.

As with the introduction of the XT3, software services personnel worked alongside the members of the user and application support group to port software to the new IBM Power 5 system which arrived in the Summer of 2006. This porting work involved the migration of user groups and applications from both the existing IBM Power 4 system and the NEC SX-5, both of which are coming to the end of their useful life.

During 2007, MeteoSwiss will move to a new higher resolution forecasting model with a much more computationally demanding suite, and it was the software services group which has been involved in determining the correct sizing of machine to host this suite as well as providing the software infrastructure to support the 3-hourly forecasting that this new model will require. As a first step, the existing lower resolution model was ported to a single cabinet Cray XT3 system at the end of 2006, and continued progress has been on the higher resolution model which will enter into production in Summer 2007.

Neil Stringfellow

User and Applications Support

As computational sciences and engineering are focusing on progressively more complex systems and phenomena, simulations by their nature require an integrated, multidisciplinary, multi scale and multi-physics approach. When offered the possibility of a new (larger) computational system, scientists strive to extract the maximum throughput and performance for further advancing in their scientific investigation. In addition to this observation, we have seen three trends emerging while supporting the user community over the last year.

More and more applications are now able to benefit from massively parallel systems, mainly by gradually improving their scaling capabilities. For some applications the scaling capacity still remains a challenge and members of the group, along with software support, have been working to help users make this important transition. Porting, debugging, optimization as well as tuning the programming environment have been mainly focused on the Cray XT3, as well as on the IBM Power5 cluster which was undergoing acceptance and being prepared for production. A considerable effort was invested in consolidating and regularly updating the technical documentation made available on the CSCS User web portal.

In the meantime data intensive applications are also gaining momentum, and in several application fields we observe an increasing data transfer rate between the archive and the computing servers. For example, CSCS has been acting as one of the main computational laboratories for the NCCR-Climate community. This community sets new challenging requirements not only related to efficient high-end computing, but also to data archiving and data post-processing. Large data set, spanning several Terabytes, are not only archived, but are also regularly accessed by data analysis and data verification experiments.

The second trend is that a few groups are also developing the concept of job launchers, to be able to maximize their production on a large, shared system. We are moving into the realm of schedulers attached to the user application -an enriched concept of the linear work flow - and we already anticipate that the next generation of such launchers will be able to couple tasks being executed on different systems.

The third trend has been the important turnover of the Large Project community during the last three years. In 2006, we had 44 proposals for Large projects, out of which there were 12 new ones (a record in recent years) while 8 came to an end. Chemistry and material science account for almost 60% of all aggregated computing cycles, followed by Physics and Environmental sciences, both at 16%, and Engineering with 6%. Interestingly, new projects are exhibiting particularly strong multi-disciplinary features, (for example bio-materials and applied mathematics, bio-sciences and mechanical properties), so that categorizing applications in one specific field will become ever more challenging! As a consequence of this growing complexity, the online users support and ticketing system has been streamlined and will continue to be consolidated to face the growing number and complexity of the requests.

The team was re-enforced by the arrival of a new collaborator, Dr. Maria Grazia Giuffreda, who helped the consolidation and completion of the CSCS Computational (Bio-) Chemistry Framework. 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 applications in computational sciences for molecular dynamics, crystallography, chemistry and climatology.

Even if a special section is devoted to the collaboration with MeteoSwiss in this report, it is worth mentioning that a significant effort was also spent by this group for preparing the new pre- and post processing suite for MeteoSwiss's new high resolution operational model.
Marie-Christine Sawley

Technical and operational Services

The main activities of the Technical and Operational Services Section in 2006 have been

- The operation and maintenance of our HPC servers, data management and storage systems, networks, and dedicated pre- and post-processing systems
- The extension of the Cray XT-3 server Palu from 1'100 to 1'664 compute nodes and the upgrade to dual-core processors of the smaller XT-3 server Gele
- The commissioning and test of the new IBM P5 server Terrane with 768 processors, including the first deployment of Infiniband interconnect technology at CSCS
- Improvements to the capacity and performance of CSCS infrastructure.

Since the beginning of 2006, the job scheduling algorithm on our Cray computers adapts the priority of queued jobs according to the amount of allocated resources already used by the corresponding user and his project. This ensures (1) that all projects get a chance to use the resources allocated to them and (2) the machine is utilized to its maximum capacity. We will deploy the same "fair share scheduling algorithm" on the new IBM computer to be put into production in January 2007.

We have deployed a Storage Area Network (SAN) in order to improve the efficiency of our disk storage procurements and to ease the maintenance of our storage systems.

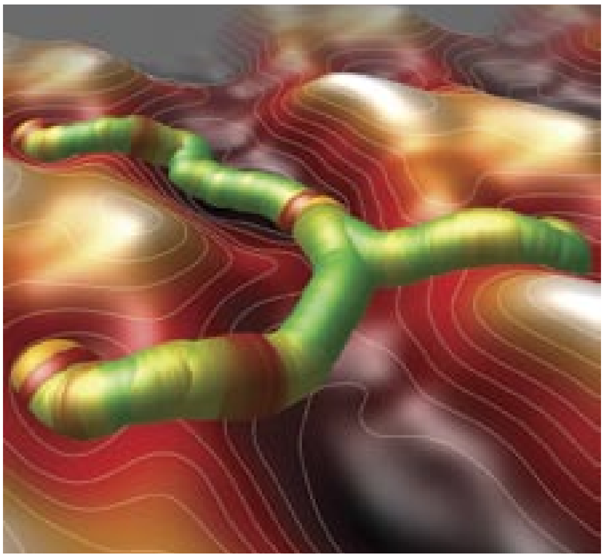
An improved voice and video conferencing equipment allows CSCS to host multi-party teleconferences, thus improving the communication with our users. An improved wireless LAN eases the work of short and medium term CSCS visitors.

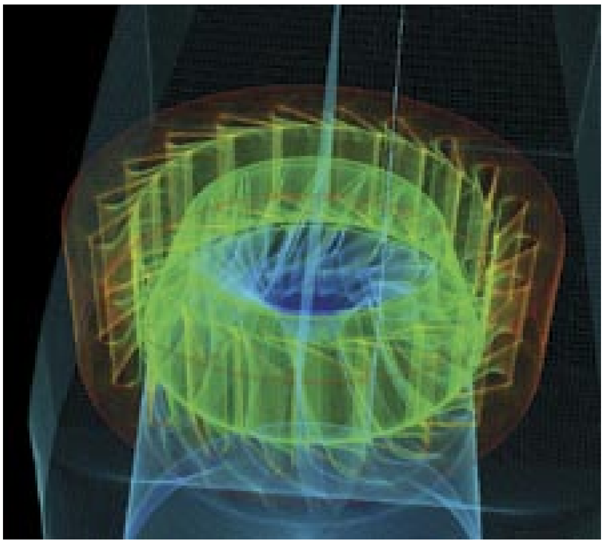
On-going work will allow further enhancements of our services in the first quarter of 2007. An extension of the disk archive and a new server will improve the performance of our disk archive. The performance of our machine room network will be increased to 10Gbit/s. User authentication and authorization for most CSCS systems will be provided through a unique centralized system.

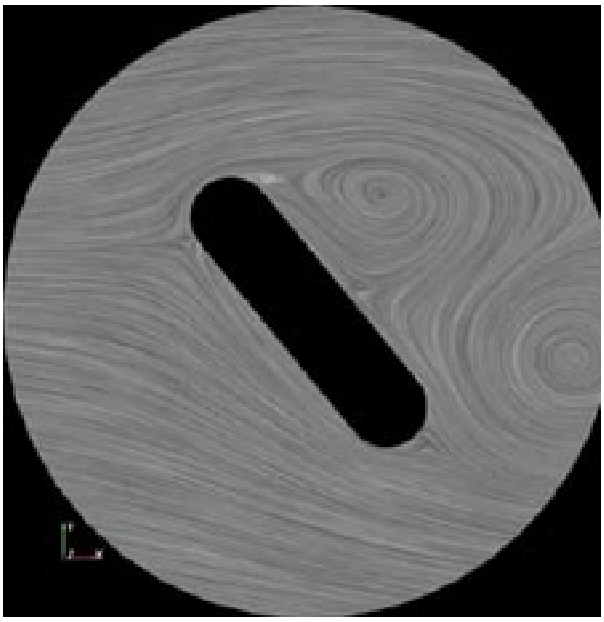
Big and fast computers produce lots of heat. In order to adequately cool the new big systems installed in 2006, we increased the size of our machine room and deployed the infrastructure which allows us to water-cool computer racks. Further improvements of our cooling and ventilation are scheduled at the beginning of 2007 in order to have sufficient cooling capabilities during hot summer days.

Paolo Conti

Panoramic view of the machine room at CSCS.


Paths to the energy minimum of three molecular conformations


A translucent wireframe rendering of a Francis turbine


Turbulent circular jet entering perpendicularly into a laminar boundary layer.

Data management, analysis and visualization

A new Staff Member and Molecular Visualization

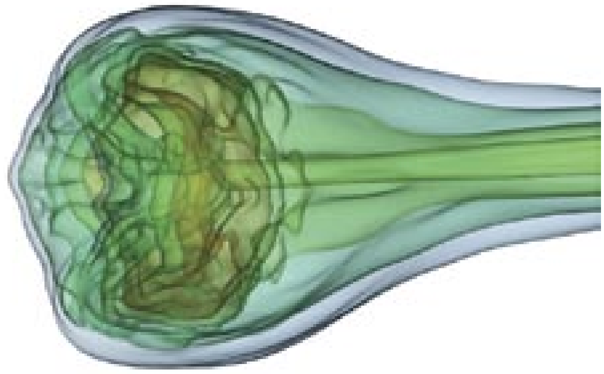
Ugo Varetto joined us in June 2006 to initiate a big re-deployment effort of CSCS's flagship Molecular Visualization application Molekel. Molekel has been linked with the history of CSCS since its creation. The rapid advance of software technology and graphics rendering have been such in the early years of this new century that we felt it was the right time to deploy a modernized version of Molekel. Molekel was released on December 2006 and has already been downloaded by hundreds of sites worldwide. The primary focus for this version has been on user interaction, multiplatform support and integration with open-source libraries. Some basic features such as visualization of residues, and PostScript export have been added as well. The program has been built in a modular way with several components intended to be reused outside of Molekel. Most of the developed components will probably be released as contributions to open-source projects such as VTK, Qt, and OpenBabel. While working on Molekel, the other main molecular visualization packages in the field (VMD, Molden, PyMol, Chimera) and libraries (OpenBabel, BALL) were reviewed, and this helped consolidate our expertise in the visualization of molecular sciences.

USPEX and STM3

The USPEX code (Prof. A. Oganov, ETH Zurich) enables crystal structure prediction at any P-T conditions, given just the chemical composition of a material. USPEX produces a large set of structures, each with a corresponding free energy. Its users are interested in selecting the few lowest-energy structures and in verifying the structural elements that the system uses throughout the run, especially at low energies. We supported these two tasks with the visualization of the structures found in USPEX with our STM3 molecular visualization toolkit where a dedicated set of techniques for crystallography and the capability of directly accessing the USPEX outputs has been developed. The prototyping capabilities of STM3 have also been used to find and develop new scenarios of code usage in USPEX.

Volume Rendering

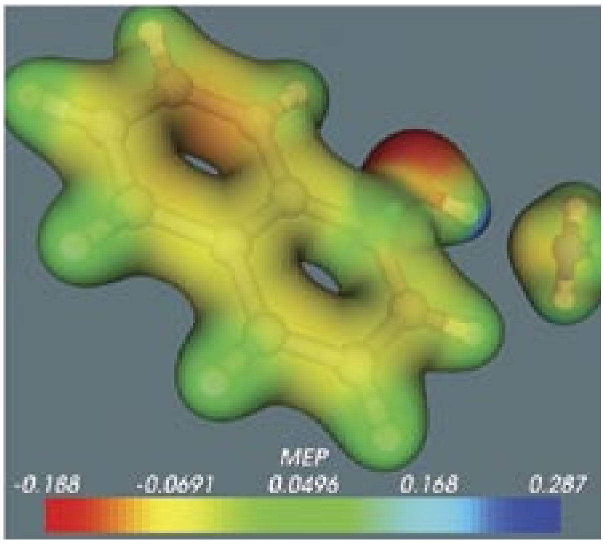
Our activity remained focused on acquiring practical expertise and benchmarking different techniques for parallel and distributed volume rendering, to prepare for the deployment of a visualization cluster to CSCS users. Development of data/material transfer functions for interactive rendering, and pixel compositing APIs form the bulk of our effort.



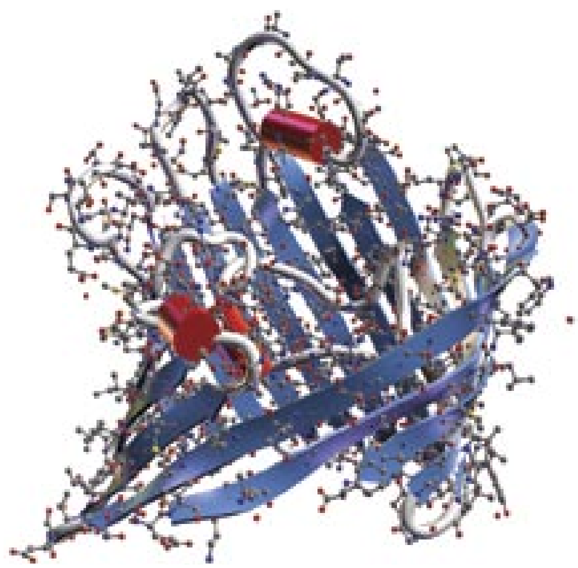
Supersonic hot flow against a high-density cold condensation

Mesh-less Data Handling and Visualization

We have been involved in an ERCOFTAC Special Interest Group on Smooth Particle Hydrodynamics (SPH) and contribute with expertise in Data Analysis, Data Formatting and 3D Graphics for particles. Our software ”sparticles” is a high performance particle rendering package. To achieve high performance, ”sparticles” transfers particles to the graphics card as single points and renders them to screen using GPU shading language programs. ”Sparticles” is intended to be used by researchers in the field of Smoothed Particle Hydrodynamics and Discrete Element Modelling, though it can be used for arbitrary particle based data. CSCS has made 5 releases of ”sparticles” during 2006, supporting features such as the ability to track particles through time with trails, colour and use transparency based on arbitrary scalar parameters to aid visibility and improve file access via support for parallel I/O such as HDF5. In addition to our visualization support, we are actively involved in developing and promoting the use of a ”standard” file format known as H5Part (for HDF5 particle data) to aid both the performance of our users code and the portability of their data between analysis tools. We have also supported the parallel reading and visualization of netCDF files with a ParaView module for several years for mesh-less and mesh-based data.



Molekel: Molecular surface color-coded with electrostatic potential



Porine molecule with residues

The robustness and portability of our data importer has been improved to handle higher dimensional data, more general storage of scalar/vector fields and the splitting of data files between processors or between time steps. Our netCDF code is now used in research centres at several sites around the world.

Time Dependent Data Analysis and Visualization

CSCS has worked extensively on supporting large time dependent datasets and in particular the visualization of unsteady flow. To enable the analysis of time based data, the visualization group has created a series of extensions to the widely used visualization toolkit (VTK) to enable the processing in parallel of time dependent data. The visualization group has produced a particle tracking module for VTK which is capable of tracking millions of particles in terabyte sized datasets and saving these particles for later animation or movie generation. The work on particle tracing complements our experiences in particle visualization to allow us to generate trajectories of particles in huge datasets, store them using parallel I/O and render them at high speed.

2007 Eurographics Parallel Graphics and Visualization Workshop (May 20-21,2007)

We have been chosen to host the event and have spent efforts in promoting the event with sponsors, organizing the technical content of this two-day workshop and chairing the paper review process.

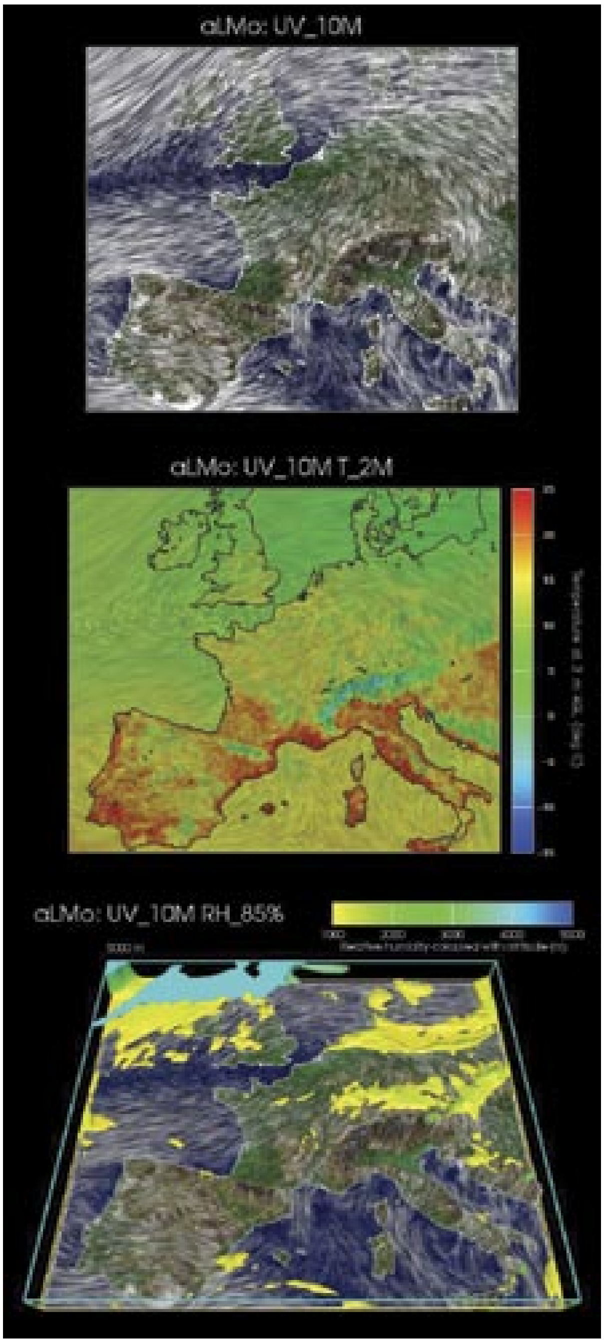
Training activities

Several courses were given by our staff, on "introduction to visualization" and "visual communication principles", "ParaView Software Usage", "Visualization for Chemistry", and "AVS/Express and its usage for the molecular visualization toolkit STM3", taught at ETH Zurich, EPFL-Lausanne, USI Lugano, CINECA and CSR4.

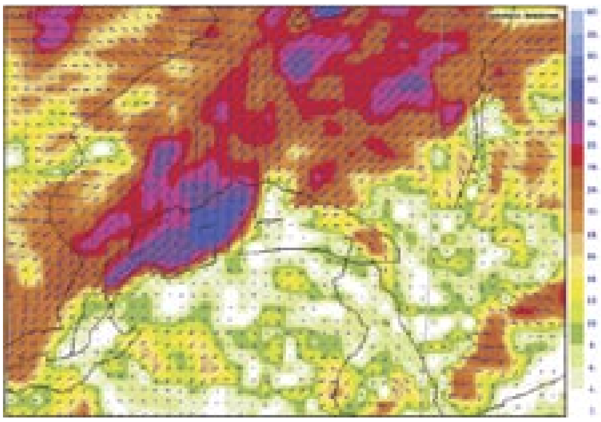
Jean Favre

MeteoSwiss

The Swiss national weather service has been carrying out its production and research computations on numerical weather prediction at CSCS for several years now. Its model -recently renamed COSMO - is developed in the framework of the international consortium of the same name COSMO and calculates twice a day, at a resolution of 7 km the atmospheric evolution for the next 72 hours over a domain covering most of Western Europe. Many internal and external



Wind velocity, temperature and humidity calculated by aLMo.



Example of wind forecast for the region of the lake of Geneva with the new model COSMO at a resolution of 2.2km.It is running regularly with a preoperational status and will become operational beginning of 2008.

MeteoSwiss clients critically depend on the timely production and dissemination of the COSMO output; in particular, mitigation of natural hazards and services like air traffic control are based on meteorological information. As an example, results produced by COSMO are used by other codes 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.

MeteoSwiss is currently in the challenging phase of the development of a new version of COSMO capable of higher resolution at the kilometric scale, targeting a further increase of the quality of the forecasts for the very short range and especially adapted to the complex topography of Switzerland and the Alpine region. CSCS worked with MeteoSwiss to respond to the challenges of the adequate HPCN infrastructure, software environment and HPCN support services. Significant work has been carried out by the software group of CSCS and Cray specialists for optimizing the most demanding part of the COSMO code in order to meet the strict requirements of the model. The new version of COSMO with a resolution of 2.2 km will become operational at the beginning of 2008. The present operational version (with a resolution of 7 km) has been migrated beginning of 2007 on one cabinet of a dual core Cray XT3 of CSCS.

Angelo Mangili

Outreach

2006 was once again an active year for conferences, events and courses at CSCS.

CSCS User Events

Given the large attendance of last years User Assembly Day held in Bern we decided to keep this as a fix event for interacting with our users. The 2006 User Assembly again took place in Bern on May 22nd. For the event 10 members of CSCS travelled to Bern to exchange with our users. The event attracted an important number of participants.

The traditional CSCS User Day was held in the last week of September. Last year we had announced that we were working on remodelling this event. We felt that this was an important place to discuss subjects of general interest to all of our users. We decided to structure the event based on three subjects: Scientific Software development and community codes, Breaking the Teraflop Limit and Data Management and Scientific Visualization. Each subject was enriched by keynote speeches by Prof. J. Hutter from the University of Zurich, Dr. M. Luescher from CERN and Prof. G. Lake from the University of Zurich. A panel session was held on the subject of “Who needs the Petaflop?”. The tra-

Students of the Quantum Dynamics Workshop in September ditional poster sessions were maintained as they provide an excellent opportunity for our users to interact amongst each other as well as with CSCS staff members. Next year's User Day will take place on September 24th and 25th.

Courses and workshops

In 2006 we concentrated on consolidating the growth of courses offered at CSCS as requested by our performance mandate. Having introduced the Cray XT3 platform during 2005 we continued to offer introduction courses to the system in 2006.

Inauguration of the IBM SP5 Dr. Marie-Christine Sawley CSCS, Prof. Dimos Poulikakos ETH Zurich and Thomas Klein IBM (from left to right)

The visualization group was once again very active, proposing multiple courses on and off-site during the year. To cite just a few: Jean Favre gave a Paraview Visualization course in February at EPFL, Mario Valle then proposed a course on Advanced visualization for Chemistry and in September Jean Favre and John Biddiscombe gave a course on Visualization in Fluid Dynamics.

We were pleased to welcome back Rolf Rabenseifner from HLRS to give a course on Parallel Programming that has enjoyed a very good attendance for the past 2 years. In September we had the pleasure of hosting a CUSO workshop on Quantum Dynamics in Chemistry given by Prof. M. Meuwly of the University of Basel.

Conferences and events

In May of 2006 CSCS hosted the annual Cray User Group conference (CUG). This 4 day event was held at the Palazzo Congressi in Lugano and successfully attracted 170 participants. This event is aimed at bringing together Cray users from around the world to exchange on their experiences amongst each other as well as with Cray employees. It offers a regular and unique opportunity for users to give their feedback and raise issues and question with the constructor. CSCS looks forward to hosting more events of this kind in the future.
Upon request by the Steering Board CSCS submitted itself to a Peer Review in July. Prof. Knut Faegri of the University of Oslo chaired the review. The other members of the review team were Dr. William Feiereisen from Los Alamos National Laboratory, Prof. Guy Brasseur from NCAR, Prof. Ernest Feytmans from the Swiss Institute for Bioinformatics, Anwar Osseyran from SARA, Prof.Heinrich Rohrer Nobel Prize winner, Dr. Stefan Heinzel from DKRZ. Mr. Kurt Baltensberger from ETH Board and Prof. Manuel Peitsch from Novartis and member of the CSCS Steering Board accompanied the review providing the peers with requested background information. During the review the peers met with members of CSCS' governing bodies, CSCS users, CSCS staff and contractual partners as well as stakeholders. The report of the review is published on the CSCS website.

CUG 06 Logo

In September we were able to celebrate the inauguration of the new IBM P5 supercomputer named Terrane. The event was attended by users, politicians and decision makers from the ETH domain and industry alike. Introduction courses for this new system will start in spring 2007.

Having hosted the Commission for public building of the cantonal parliament in 2005, we had the honour of hosting the meeting of the Commission for public building of the national parliament in 2006. 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 – was 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.

CSCS also organized and hosted the community workshop on climate and environmental sciences of the LINCEI initiative in December.

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 2007. We hope to welcome you at one of our numerous events throughout the year!

Ladina Gilly

Research Digest

Prof. Andrew Jackson

Interview

with Prof. Andrew Jackson

by David Bradley, Science Base, UK

Prof. Dr Andrew Jackson is a researcher in the Institute of Geophysics at the ETH's Hönggerberg campus. His research focuses on analysing data from ground stations and Earth-orbiting satellites using CSCS facilities to help build a model of geological, electrical and magnetic processes taking place in the Earth's mantle and core.

Why geophysics?

That's a long story. I was always interested in the outdoors as a youngster and became interested in physical geography, the way the landscape is shaped by natural forces. A physics degree and a smattering of geology led to the discovery that geophysics helps us understand the Earth.

How do you study the Earth's interior?

It's a scientific detective story - few direct observations tell us immediately about the interior of the Earth - one usually has to piece together the story and draw conclusions. We can measure the magnetic field on time scales longer than a year and deduce what the field at the surface of the liquid iron core must look like - but even then, it is a smoothed and filtered version of reality. Trying to deduce the conditions in the core that are consistent with this picture, and other evidence, such as the record of the field locked up in the magnetisation of rocks, is a very tricky process; hence the need for CSCS facilities.

Why is fundamental scientific research important?

Its importance is twofold. First, scientific discoveries are just as marvellous achievements as art, music and literature. Secondly, many achievements, such as Internet security, have been built on fundamental research, in this case the mathematical Riemann hypothesis.

How do you measure the electrical conductivity of the earth's mantle?

We can use the rapid variations of the field to deduce properties about the electrical conductivity of the Earth. Compared to reconstructing the magnetic field at the top of the core, in the mantle the problem is much trickier, and the conclusions much less direct. We are gearing up for the 2010 European Space Agency's SWARM mission, which will use three satellites to monitor the Earth's magnetic field with unprecedented accuracy, amongst other things, which will improve our understanding of the mantle.

Are there practical applications for this research?

The oil industry is interested in electric and magnetic fluctuations on the seafloor that might reveal the presence of oil. They do this successfully now, but there is always room for improvement.

What long-term aims do you have for this work?

I would love to understand how heat loss produces the Earth's magnetic field, which has existed for billions of years. Similarly, if we can detect variations in the mantle's electrical conductivity, it may tell us about the temperature structure, and the influence of compositional variations, perhaps the presence of water. These are very heady goals!

In what ways are the CSCS facilities important to your research?

The computational facilities available under the ALPS project will give us the chance to get closer to the correct physical regime of convection and magnetic field generation. Applying lots of processors to a problem has been a major step forward in many spheres. Not only is the hardware important to our work, but we also look forward to making use of the expertise available at CSCS in algorithm development and visualisation.

ALPS

Presentation of the four projects by David Bradley, Science Base UK

In 2006, the Swiss National Supercomputing Centre (CSCS) announced the first awards of the newly launched Swiss ALPS (Advanced Large Projects in Supercomputing). The comprehensive program reserves about half the time on the centres supercomputers for projects with high potential to achieve breakthroughs, both for science and supercomputing techniques, of international significance.
The following four projects were selected:

- Investigating the origin of magnetic fields of the earth and other planets (principal investigator: Andrew Jackson).
- At the molecular level how does cell function and behaviour change under mechanical force (principal investigator: Viola Vogel).
- Investigate climate change on European and Alpine scales and possible future extreme weather events (principal investigator: Christoph Schär).
- Investigate the role of protein interactions of interest in diseases such as Alzheimer and HIV (principal investigator: Michele Parrinello).

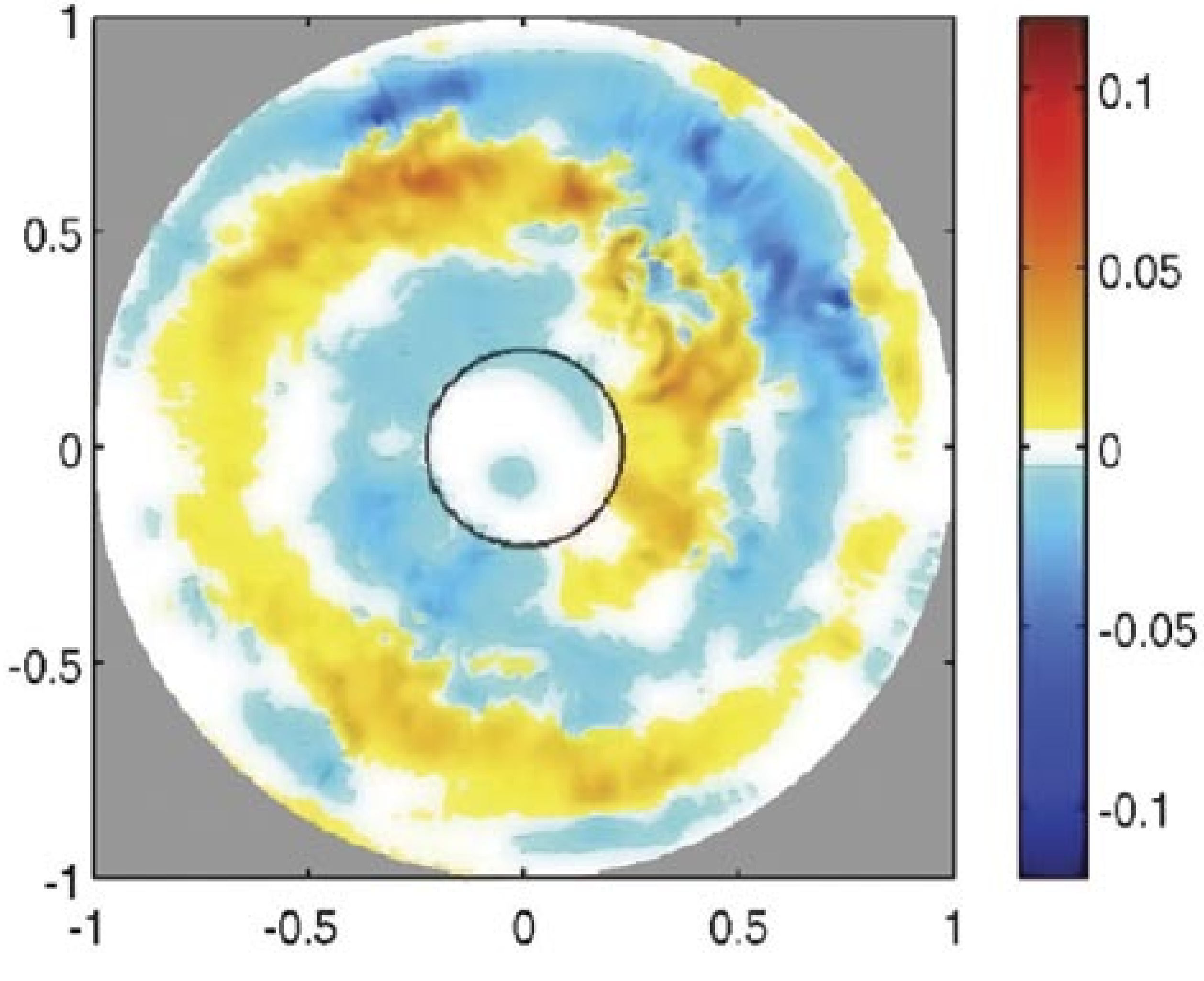
The Swiss ALPS awards are granted for two years at a time, and the work will be carried out on the centre's 1664-processor Cray XT3 and new IBM 768-processor p5-575 systems. It is envisaged that up to 16 million CPU hours will be used to carry out these four projects. Aside from targeting significant breakthroughs, qualifying projects must require a large amount of compute time that cannot be found anywhere else in Switzerland, as well as strong collaboration between CSCS and the research groups.

Dynamic core
(Prof. Andrew Jackson, ETH Zurich, Institute of Geophysics)

The Earth's inner core is a solid mass of iron, but floating above this, thousands of kilometers, beneath our feet is a swirling mass of molten iron and other lighter elements that are constantly stirred by heat rising from the core. The resulting convection currents are in part responsible for the Earth's magnetic field but understanding in depth how these convection currents and the dynamo effects arise requires detailed insider knowledge.

With the help of CSCS computers made available under the ALPS project, Prof. Dr Andrew Jackson of the Institute of Geophysics at ETH's Hönggerberg campus hopes to simulate processes deep within the Earth that can only be observed indirectly. He and his colleagues hope to unearth the secrets of the Earth's magnetic field, which will have implications for terrestrial geology and might offer an explanation for the magnetic pole reversals that have occurred throughout Earth's history. The simulations might also help astronomers understand the magnetic behaviour of other planets in our Solar System and beyond and provide insights as to the origin of the enormous atmospheric bands we see on planets such as Saturn and Jupiter.

Albert Einstein suggested that the origin of the Earths magnetic field was one of the greatest unsolved questions of early 20th century science. Even today, while much has been accomplished, there still remain issues about exactly how the magnetic North-South divide arises in our planet. Part of



Kinematic paradiso - modeling the geodynamo effect (Credit: Dr Jon Rotvig (ETH Zurich) the problem is that the range of timescales involved in core processes is enormous. Some take place over the course of a day as the Earth rotates while others last for thousands or millions of years perhaps as the Earth precesses about its axis. Such a range represents an unprecedented computational challenge, Jackson says, however with 21st Century computing power, the problems could nevertheless be overcome.

Jackson and his colleagues hope to work on several novel calculations that side-step the sticky problem of core viscosity and that make full use of the CSCS Cray XT3 to produce simulations of the geodynamo, the magnetic generator at the Earth's core and the convection bands observed on Jupiter and Saturn.

The collaboration between Jackson's team and CSCS will allow several sophisticated calculations to be carried out. Ultimately, these will answer a range of fundamental questions such as: "How do the banded zonal wind structures seen at the surface of Jupiter and Saturn originate?" and, "What are the underlying mechanisms responsible for magnetic reversals on Earth?"

Jackson explains that the team is in a unique position in Switzerland to address such questions as the partnership brings together his team's codes and geophysical expertise with CSCS optimization, parallelization and visualization and computational resources. He suggests that the results that will emerge from this project will represent a major leap forward in our understanding of the behaviour of planets.

Simulating proteins

(Prof. Michele Parrinello, ETH Zurich, Computational Sciences)

Chemical communications between proteins are at the heart of the multitude of processes continually taking place in every cell in our bodies. They are essential to cellular control, gene regulation, and the transfer of chemical signals. When those lines of communication are broken, however, the result can be disease and ill health, as specific proteins stop working, clump together into tangled masses, or allow bacteria and viruses to invade.

A team at ETH led by Michele Parrinello is now using the CSCS supercomputing facilities to help them unlock the protein interactions of interest in diseases such as Alzheimer's and HIV.

"Modelling these interactions at a full atomistic level would help greatly in understanding the fine details of how they progress and in designing new drugs," explains Parrinello. Such work will be complementary to the growing number of detailed protein structures obtained through X-ray crystallographic techniques, nuclear magnetic resonance spectroscopy, mass spectrometry and other analytical methods. The simulations will have one crucial difference from these experimental results in that the analytical approaches investigate proteins in isolation whereas the computer will simulate interacting proteins.

Unfortunately, computer simulations of protein-protein interactions have remained out of reach of biomedical researchers until recently. Parrinello, whose group has been at the cutting edge of such developments, hopes to change all that by investing a large computer time allocation in protein modelling so that several fundamental processes of medical importance might be revealed in detail.

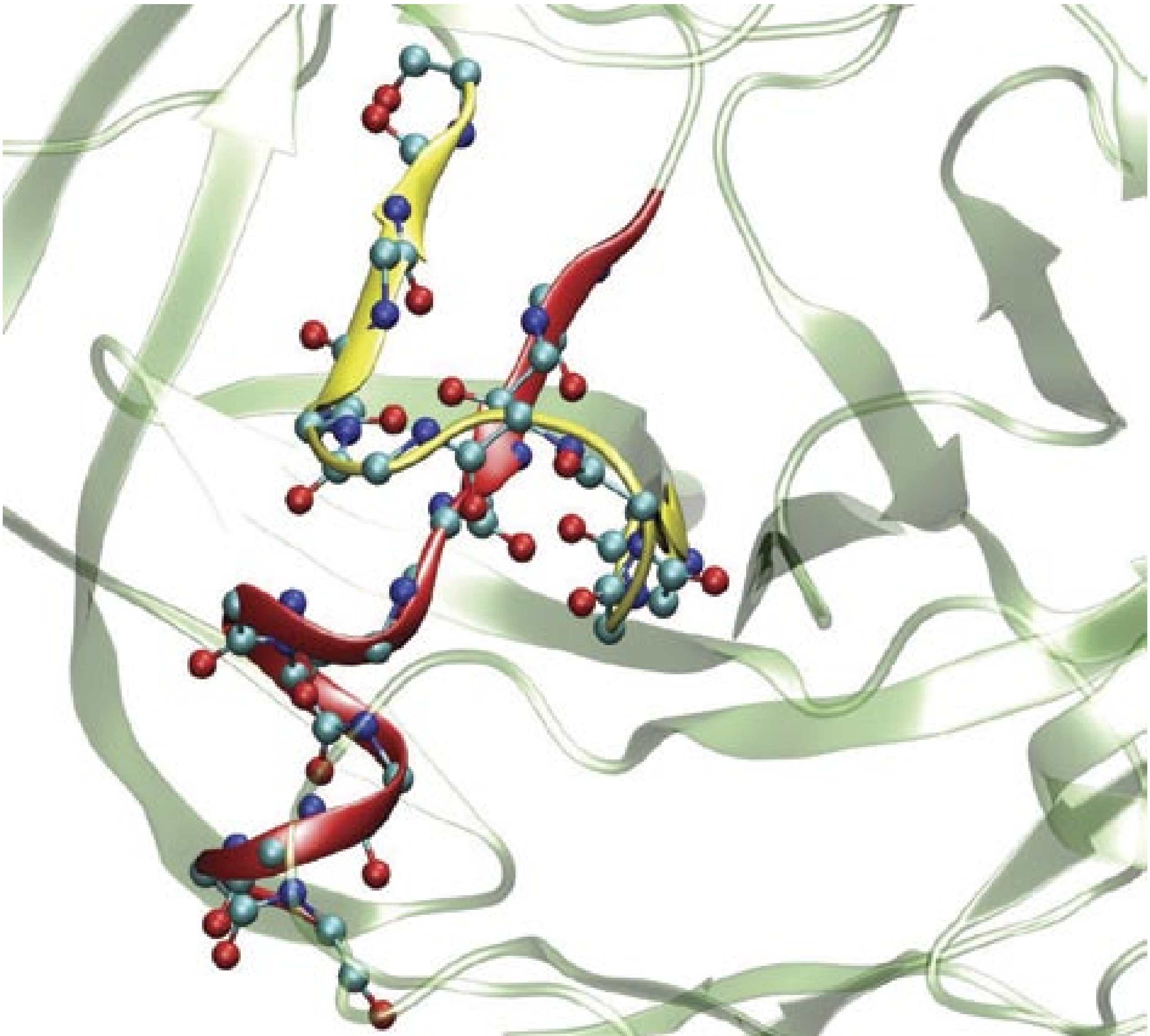
One area of interest that the simulations will shed light on, is the way in which fibrous tangles of proteins, known as amyloid fibrils, aggregate in the brains of Alzheimer's sufferers. The tangles interfere with brain cells, blocking signals and destroying neurons, leading ultimately to the characteristic dementia associated with this disease. Simulating the tangles may offer new clues as to how they arise and the very long-term possibly suggest new targets for therapy.

The researchers also plan to model the regulation of two enzymes, cyclin-dependent kinases (CDK2 and CDK5), involved inextricably in normal cell replication and the errant multiplication of cells seen in cancer. Again a clearer picture of how these proteins malfunction could lead to novel therapies. Similarly, modeling how the protease enzymes of the AIDS virus, HIV, fold into their active form could help in the design of new drug molecules to inhibit these enzymes and so block viral replication.

The team anticipates their simulations, once underway, will represent the state-of-the-art in these areas of research. The simulations will exploit a new algorithmic technique that circumvents the intrinsic problems associated with conventional statistical simulation of proteins. The method, known as metadynamics, provides a way to simplify the movements of the proteins being studied. This allows much more data to be processed than with conventional methods so any simulation can operate on a much grander scale than earlier protein simulations. That said, Parrinello explains that the HIV protease system with its approximately 50,000 atoms will require about 1.3 million CPU hours on the CSCS Cray super computer and the kinase simulation bout 1.1 million. The smaller amyloid system need just 0.7 million CPU hours.

"Metadynamics represents a major step forward with respect to straightforward atomistic simulations when time scale is a problem," explains Parrinello. Indeed, the approach has already proved its worth in simulations of other systems, such as the docking of a drug molecule with a simple digestive enzyme. The simulation took less than a tenth the time required for a conventional algorithm, he says.

Using the new technique of metadynamics, the researchers anticipate that their approach will eventually provide biomedicine with the clearest picture yet of the proteins involved in these diseases, which could eventually lead to new therapeutic agents for tackling them. Parrinello suggests that the techniques he and his colleagues will develop will also have wider applications across the protein simulation field, allowing scientists ultimately to piece together a complete map of all the interactions between proteins taking place in our bodies.



An HIV protein folding (Image courtesy of Massimiliano Bonomi, ETH Zürich)

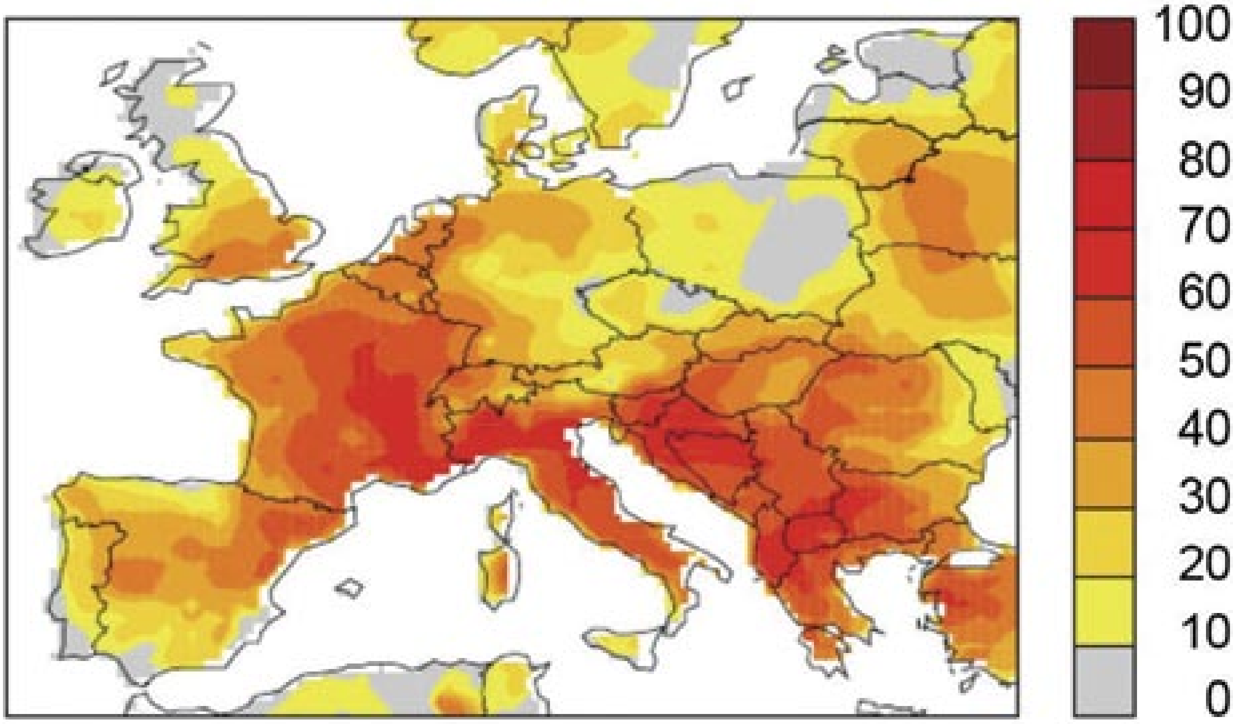
Warming water cycle

(Prof. Christoph Schär, ETH Zurich, Institute for Athmospheric and Climate Science)

Climate change predictions are uncertain, but all computer models of global warming project that summer temperatures in Europe will rise considerably. Most models also exhibit pronounced increases in the year-to-year variability of summer temperatures. So will the frequency of heat waves like those that swept across the Continent in 2003 increase? Using simulations carried out with CSCS resources, Christoph Schär and his group at ETH Zurich hope to finds answers and explain the role of climate change on the European summer climate and water cycle.

Understanding why summer variability might increase has not been clear until recently. Recently, the team published their findings in the journal Nature (Sonia Seneviratne et al, 2006, vol 443, 205-209), pinpoints the underlying reasons why central and eastern Europe will become more variable and suffer repeated heat waves as global warming progresses. The prime mover is apparently due to the special relationship between the continental land mass and the atmosphere itself. In particular, Seneviratne and colleagues have found that changes in temperature will lead to changes in the amount of moisture evaporating from surface soils. This in turn affects the temperature of the region. Moreover, as the region's climate changes, this feedback loop will be affected still further as the type of vegetation that the land supports changes.

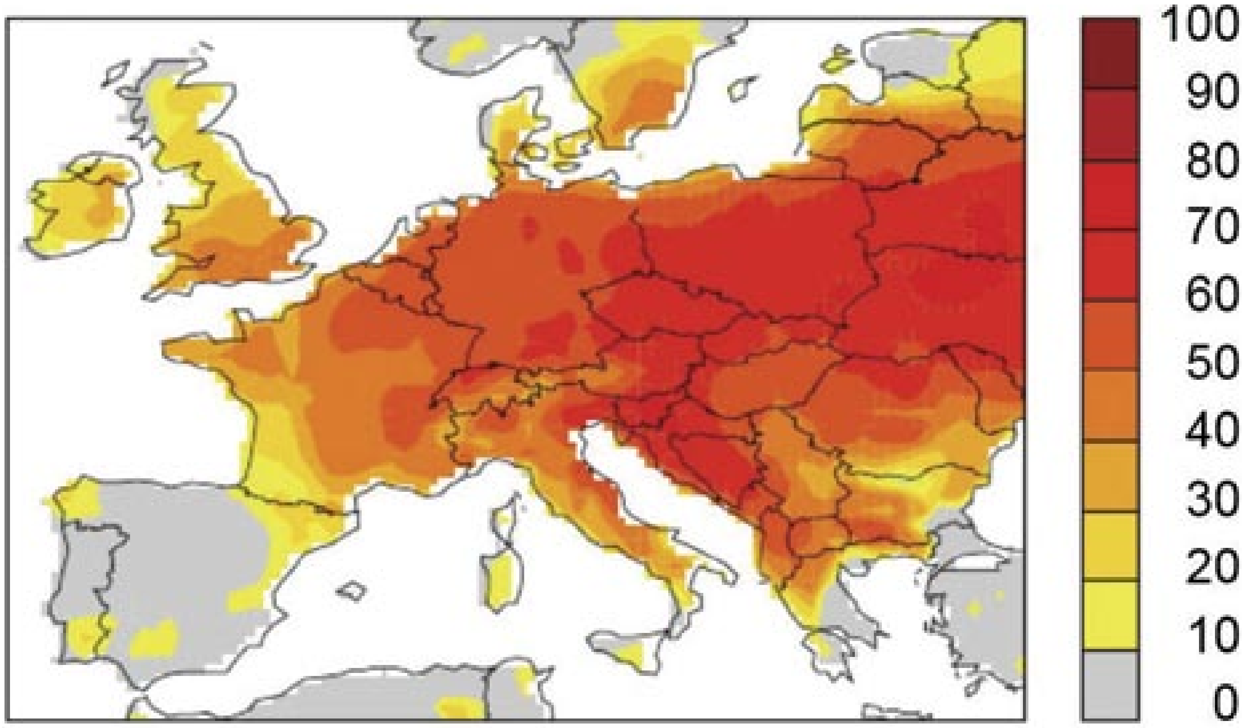
There are numerous feedback loops that may come into play more prominently as temperatures rise, involving moisture, surface reflectivity, and plant growth. However, these feedback loops operating between the land and the atmosphere are rather complex. This ensures that any specific predictions made for a particular region will not necessarily follow the predictions unless all feedback systems are taken into account in the simulations.

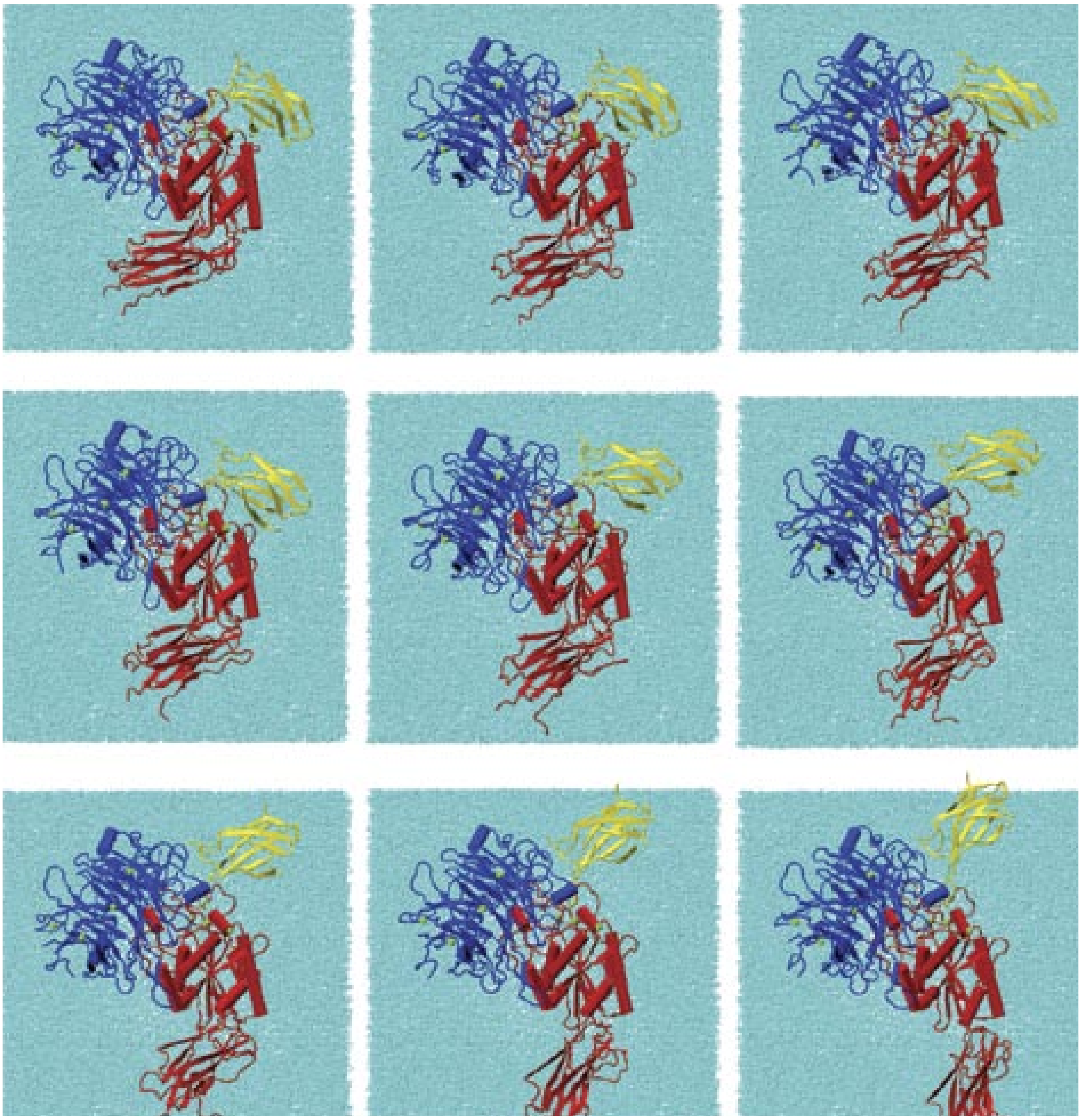


The two panels highlight the increasing importance of land-atmosphere coupling in response to climate change. The two panels show the fraction (in %) of year-to-year climate variations that is due to land-atmosphere coupling, for the current climate (panel on page 32) and future climate (panel on p.33). The increasing role of land-atmosphere coupling is evident particularly in Eastern Europe.

The researchers explain that the effect of the interactions between the land and the atmosphere is particularly strong in central and eastern Europe. This arises because the upward trend in global temperatures will most likely lead to a northwards shift of climate zones in the northern hemisphere. Such a shift will imply that a transition from dry to wet climates will occur further and further north as temperatures rise rather than as at present where the north-south divide actually occurs at more southerly latitudes.

These transition zones of temperateness are especially sensitive to feedback processes between soil and air, the researchers explain. However, a clearer understanding of how they operate could ultimately contribute to improved seasonal forecasting and so help us to cope with the consequences of climate change.





Hinge opening of the integrin headpiece takes just 6 billionths of a second

The bacterial finger trap
(Prof, Viola Vogel, ETH Zurich, Laboratory for Biologically Oriented Materials)

Understanding how bacteria keep their grip on surfaces could lead to new ways of preventing them from sticking to body tissues and causing disease, according to research underway at ETH Zurich. Viola Vogel and her colleagues in the Laboratory for Biologically Oriented Materials are looking at how cells behave at the molecular level when they are pulled upon by fluid flow. One particular aspect of this work has focused on the sticky hair-like protrusions on the surface of bacteria such as Escherichia coli with the aim of figuring out how this bacterium copes with changing fluid flow conditions in the body.

E coli's protrusions, more properly known as fimbriae, have a sticky protein, known as FimH, at their tips that allow the bacteria to attach themselves to sugars on the surface of cells. ”We need computational tools to visualize at high structural resolution how mechanical forces can activate this unusual receptor-ligand bond,” explains Vogel. The team is using a CSCS supercomputer to create a computational model based on known protein crystal structures or the crystal structures of receptor-ligand complexes. The model simulates how the known structure, immersed in a box filled with water molecules, deforms if stretched mechanically. This approach is used by Vogel’s graduate student Lina Nilsson to investigate how the proteins can be switched by force from a low to strong binding of sugars on tissue surfaces in their natural environments.

The team discovered that, unexpectedly, the bond between FimH and a sugar molecule gets stronger when a tensile force is applied. It is almost as if the bacterium holds on tighter when a force is applied that would otherwise pull it from the surface. Vogel and her colleagues describe the unusual ”catch bond” that forms between protein and sugar as acting like a ”finger trap”. The harder one pulls to extricate a finger the tighter the trap grips it.

This cellular finger trap allows bacterial cells to maintain their hold on cells and so allow it time to multiply and cause an infection. The fimbriae proteins also play a key role in allowing E. coli to stay attached to mucus membranes, such as those lining the nose, urinary tract, and intestines.

Vogel explains that the fimbriae are composed of interlocking helical segments of protein domains just seven nanometers wide. Under tension, the helices can be uncoiled to many times their initial length, perhaps as water runs down inside the esophagus or urine exits the bladder. The helices uncoil one by one like stretched springs and maintaining the bond between bacterium and sugar-coated surface. When the force drops, as might occur on internal surfaces when the fluid flow stops, the fimbriae recoil to maintain the overall tension. ”The fimbriae uncoil and coil to dampen sudden changes in forces caused by rough and rapidly changing flow conditions,” Vogel explains, ”This maintains the optimal force needed to keep the finger trap-like FimH anchor from breaking loose.”

Manu Forero, graduate student working with Vogel at ETH Zurich, found that uncoiling and recoiling of the fimbrial protein helices actually balance each other at an intermediate force level. This corresponds to the force at which the sticky protein tip forms the most stable bond with the surface. In other words, the bacterial fimbriae have evolved to endow the microbe with the most effective way of clinging on to cells under harsh flow conditions.

The researchers, who have collaborated on this work with colleagues at the University of Washington, USA, suggest that this mechanism might one day be exploited in developing news ways to fight bacteria that persist even in the harsh fluid environments of the human urinary tract or gut. Such a biological nanodevice might even find biotechnological or nanotechnological applications, the researchers add.

List of Large User Projects 2006

Name	Organiszation	Project Title
Aemmer D.	ETH Zürich	Computational Science and Engineering in Nanoelectronic
Arbenz P.	ETH Zürich	Multi-level Micro-Finite Element Analysis for Human Bone Structure
Baiker A.	ETH Zürich	Hydrogenation reactions in heterogeneous enantioselective catalysis and homogeneous catalysis in supercritical CO_2
Bakowies D.	ETH Zürich	Atomizations energies from ab-inition calculations without empirical corrections
Besson O.	Uni Neuchâtel	Numerical solution of Navier Stokes equation in shallow domains
Brönimann S.	ETH Zürich	Climate and Stratospheric Ozone during the 20th century
Bürgi Th.	Uni Neuchâtel	Structure and enantiospecificity of chiral nanoparticles and interfaces
Cooper W.A.	EPF Lausanne	Computation of stellarator coils, equilibrium, stability and transport
Deubel D.	ETH Zürich	Quantum Chemical Studies of Transition Metal Anticancer Drugs
Folini D.	EMPA	Inverse modeling to monitor source regions of air pollutants
Gervasio F.	ETH Zürich	Charge transfer and oxidative damage to DNA
Hasenfratz P.	Uni Bern	Full QCD with 2 + 1 light chiral fermions
Hauser A.	Uni Genève	Photophysics and photochemistry of transition metal compounds: Theoretical Approaches
Helm L.	EPF Lausanne	Magnetic interactions in extended systems
Hutter J.	Uni Zürich	Development and application of ab-initio molecular dynamics methods
Joos F.	Uni Bern	Modelling CARBOn Cycle CLIMate Feedbacks (CARBOCLIM)
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
Krajewski F.	ETH Zürich	Ab-initio simulation of the nucleation of silicon with a novel linear scaling electronic structure method
Läuchli A.	EPF Lausanne	Computational Studies of Strongly Correlated Electron System
Leriche E.	EPF Lausanne	Direct numerical simulation ot the buoyancy-driven turbulence in a cavity: the DNSBDTC project
Lüscher M.	CERN	Numerical lattice gauge theory
Maddocks J.	EPF Lausanne	Large-scale atomistic molecular dynamics simulations of DNA minicircles
Martonak R.	ETH Zürich	Crystal structure prediction from computer simulations
Meuwly M.	Uni Basel	Electronic Structure Calculations for Chemical Reactions involving Transition Metals
Oganov A.	ETH Zürich	Computational mineral physics and cristallography
Pasquarello A.	EPF Lausanne	Disordered network-forming materials

Name	Organization	Project Title
Passerone D.	Uni Zürich	Computational investigation of relevant photochemically active molecular switches
Poulikakos D.	ETH Zürich	Biothermofluidics for Cerebrospinal fluid diagnostic and control-development of a knowledge base Explosive vaporization phenomena in microenclosures
Raible Ch.	Uni Bern	Modelling and Reconstruction of North Atlantic Climate System Variability (MONALISA)
Raitieri P.	ETH Zürich	Computational study of molecular nano-machines
Röthlisberger U.	EPF Lausanne	Mixed quantum mechanics / molecular mechanics study of systems of biological interest
Schär Ch.	ETH Zürich	Modelling weather and climate on european and alpine scales
Schwierz C.	ETH Zürich	aLMO reanalysis and hindcast for the Alpine Region
Sennhauser U.	EMPA	Reliabilty and degradation physics of ultrathin dielectrics (Nanoxide)
Sljivancanin Z.	EPF Lausanne	Solid Surfaces and Interfaces
Van Lenthe H.	ETH Zürich	What genetic loci regulate bone strength?
Van Swygenhoven H.	PSI	The atomistic modeling of size effects in plasticity
Vogel P.	EPF Lausanne	Developing High-resolution Models How Mechanical force Changes Protein Function
Wild M.	ETH Zürich	Global Climate Change: Modelling Climate Dynamics on Decadal Time Scales

Facts & Figures

Income & expenditure flow (1.1.2005-31.12.2005)

Expenditures		Income	
Investments	**8’064.17**	**Basic Budget**	**16’207.00**
		Contribution ETH Zurich	12’207.00
Materials, Goods & Services	**0.00**	Contribution ETH-Board	4’000.00
Personnel	**5’468.91**		
Payroll	3’993.11		
Employer’s contributions	507.42		
Other	968.38	**Third-party contributions**	**1’004.34**
		MeteoSwiss	585.89
Other material expenses	**5’411.67**	EGEE	181.81
Floor space	173.51	European Science Foundation	173.60
Maintenance	237.51	Other third-party	63.04
Energy & media	898.57		
Administrative expenses	119.30		
Hardware, software, services	3’571.15		
Services & remunerations	413.07		
Other	-1.44		
Expenses total	**18’999.91**	**Income total**	**17’211.34**
Balance			**-1’788.56**

– All figures are given in kCHF.

– The balance is rolled over to the 2007 budget.

Cost Distribution

Cost element	Q1	Q2	Q3	Q4	Total
Costs of goods & services	**-**	**-**	**-**	**-**	**-**
Salaries	*949.60*	*914.83*	*995.48*	*1’133.20*	*3’993.11*
Contribution social insurances	*128.63*	*110.91*	*118.63*	*149.26*	*507.42*
Other personnel costs	*207.03*	*278’77*	*217.63*	*264.96*	*968.38*
Total costs of personnel	**1’285.26**	**1’304.50**	**1’331.74**	**1’547.42**	**5’468.91**
Costs of administration and building infrastructure	*352.10*	*334.15*	*371.29*	*371.35*	*1’428.89*
Costs of hardware, software, IT-services	*491.54*	*832.91*	*985.03*	*1’261.67*	*3’571.15*
Other services & remunerations	*22.24*	*78.64*	*45.48*	*266.72*	*413.07*
Other costs	*1.28*	*0.90*	*1.31*	*-4.93*	*-1.44*
Depreciation of investments	*778.44*	*891.54*	*1’629.36*	*1’433.70*	*4’733.04*
Total costs of materials	**1’645.60**	**2’138.13**	**3’032.47**	**3’328.51**	**10’144.71**
Extraordinary costs	**-**	**-**	**-**	**43.90**	**43.90**
Internal payments to ETH Zurich	**-**	**1.19**	**-**	**0.86**	**2.05**
Total costs	**2’930.86**	**3’443.82**	**4’364.20**	**4’920.69**	**15’659.57**

– All figures are given in kCHF.

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	Millions of produced CPU hours	Average Utilization (%)	Annual direct costs in 2005 (kCHF)
NEC SX-5/16	NEC custom	16	1	N/A	N/A	64	2000	128.00	125.80	-	0.08	62.75%	1'268
IBM pSeries 690 Turbo	Power-4 1.3GHz	256	8	Double Colony	400	768	2002	1,380.00	736.60	-	1.47	65.74%	992
Cray XT3	AMD Opteron 2.6 GHz	1354	1664	Cray XT3	7600 (per router) 2'000'000 (total)	3'300	2005	8'652.80	7'182	94	10.47	88.25%	4'805
IBM P5 p575	Power-5 1.5 GHz	768	48	Infiniband 4X DDR	1'000	1'650	2006	4'608.00		-	0.93*	55.79%*	668*

* Time period from 1st October until 31st December 2006

Usage Statistics

Usage by research fields

	Chemistry	Atmospheric Sciences	Material Sciences	Physics	Other	Internal
NEC	1.32%	55.18%	4.12%	11.52%	26.96%	0.89%
IBM SP-4	68.18%	15.46%	6.82%	3.82%	3.03%	2.70%
Cray XT3	28.81%	7.45%	35.30%	21.21%	5.37%	1.86%
IBM P5	65.74%	0.02%	28.27%	2.56%	1.54%	1.86%

Usage by customer

	ETH Lausanne	ETH Zürich	PSI	Uni Basel	Uni Bern	Meteo Schweiz	Others
NEC	13.14%	44.44%	0.00%	0.00%	0.00%	38.46%	3.96%
IBM SP-4	8.32%	52.28%	2.45%	2.25%	17.22%	0.00%	17.48%
Cray XT3	9.21%	40.89%	20.97%	0.40%	7.07%	4.67%	16.79%
IBM P5	16.91%%	65.86%	0.00%	0.00%	0.02%	0.00%	17.21%

Cost analysis

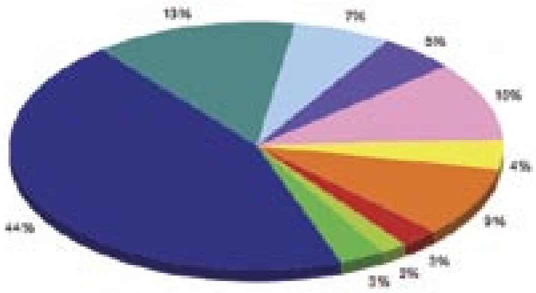
Cost Coverage Calculation per Customer (all figures in kCHF)

Customer	ETH Lausanne	ETH Zurich	PSI	EMPA	Uni Basel	Uni Bern	CERN	Uni Genève	Uni Neuchâtel	Uni Zurich	Meteo Schweiz	CHIPP	CSCS	TOTAL
Income	**3'906**	**9'497**	**1'993**	**810**	**0**	**0**	**0**	**0**	**0**	**0**	**586**	**0**	**419**	**17'211**
Distribution direct costs														
Personnel	91	375	87	1	2	31	25	46	4	31	271	56	14	1'033
Building	10	47	6	2	1	11	1	4	2	4	9	0	2	98
Energy	34	152	34	3	2	24	9	13	3	14	24	0	6	320
IT expenses and maintenance	246	1'062	72	48	20	164	15	59	23	53	460	0	38	2'260
IT depreciation	424	1'849	833	0	16	281	243	77	34	289	186	0	82	4'314
Total direct costs	**805**	**3'487**	**1'032**	**53**	**42**	**511**	**294**	**198**	**65**	**391**	**950**	**56**	**142**	**8'025**
Distribution of indirect costs	820	3'557	942	51	42	496	268	264	64	362	623		145	7'634
Total costs	**1'625**	**7'044**	**1'974**	**104**	**84**	**1'007**	**562**	**462**	**129**	**753**	**1'573**	**56**	**287**	**15'660**

Cost Coverage Calculation per Research Field (all figures in kCHF)

Research field	Chemistry	Engineering	Atmospheric Sciences	Material Sciences	Physics	Mathematics	Biology	Other research	Grid	CSCS	Total
Income	**0**	**0**	**586**	**0**	**0**	**0**	**0**	**0**	**182**	**16'443**	**17'211**
Distribution direct costs											
Personnel	620	272	366	235	259	4	11	4	227	14	2'010
Building	45	7	21	9	13	0	1	0	0	2	98
Energy	127	16	47	45	69	1	5	2	0	6	320
IT expenses and maintenance	665	329	793	147	263	3	16	6	0	38	2'260
IT depreciation	1'369	80	296	756	1'563	34	103	33	0	80	4'314
Total direct costs	**2'826**	**704**	**1'523**	**1'192**	**2'166**	**42**	**136**	**45**	**227**	**140**	**9'001**
Distribution of indirect costs	2'382	354	955	1'005	1'659	33	110	37	0	123	6'658
Total costs	**5'208**	**1'058**	**2'478**	**2'197**	**3'825**	**75**	**246**	**82**	**227**	**263**	**15'660**

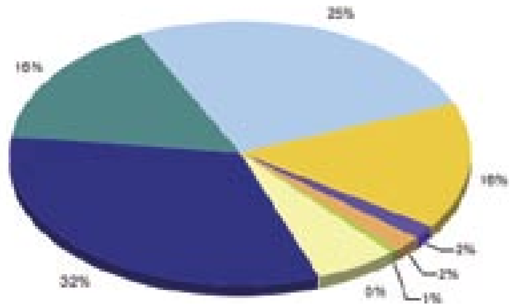
Cost of machines per institution based on direct costs during reporting period



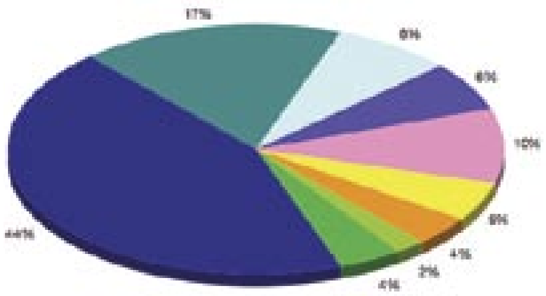
- ETH Zurich
- PSI
- Uni Bern
- Uni Zurich
- ETH Lausanne
- CERN
- MeteoSchweiz
- Uni Genève
- CSCS
- Other universities

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

- Chemistry
- Physics
- Material Sciences
- Atmospheric Sciences
- Biology
- Internal
- Mathematics
- Engineering



Usage distribution based on produced CPU hours per institution during the reporting period

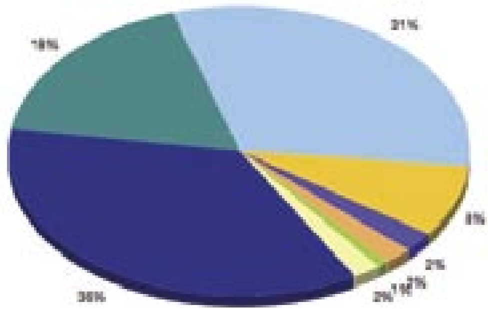


- ETH Zurich
- PSI
- Uni Bern
- Uni Zurich
- ETH Lausanne
- CERN
- MeteoSchweiz
- CSCS
- Other universities

the field "others" includes broaching, testing and benchmarking of XT3

Usage distribution based on produced CPU hours per discipline during the reporting period

- Chemistry
- Physics
- Material Sciences
- Atmospheric Sciences
- Biology
- Internal
- Mathematics
- Engineering



FIDIREVISA

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

Lugano, den 19. Januar 2007/GZ/ZN

Sehr geehrte Damen und Herren,

auftragsgemäss, haben wir das Financial Reporting (4. Quartal 2006/Jahresabschluss) des CSCS SWISS NATIONAL SUPERCOMPUTING CENTRE für das am 31. Dezember 2006 abgeschlossene Geschäftsjahr geprüft.

Für das Financial Reporting (4. Quartal 2006/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 2006/Jahresabschluss) mit angemessener Sicherheit erkannt werden. Wir prüften die Posten und Angaben des Financial Reporting (4. Quartal 2006/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 2006/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 2006/Jahresabschluss) zu genehmigen.

Mit vorzüglicher Hochachtung
F I D I R E V I S A SA

G. Zwahlen
Leitender Revisor

i.V. N. Zanetti

Beilagen:
– Financial Reporting (4.Quartal 2006/Jahresabschluss)

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Associazione dei
Comuni Svizzeri

Membro della
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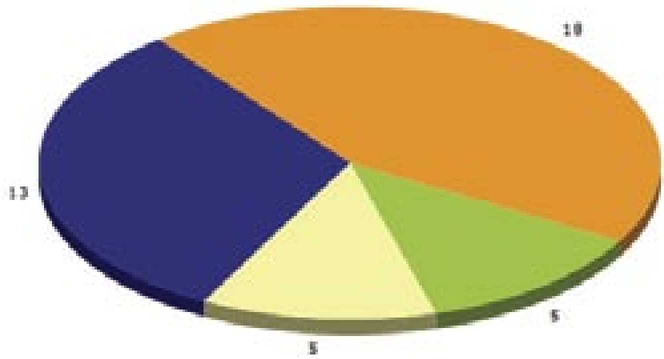
Impact factor for papers listed in the 2005 Annual Report

Publication	Impact factor	Principal investigator	Application field
Oganov A.R., Martonák R., Laio A., Raiteri P. & Parrinello M. (2005); Anisotropy of Earth's D" layer and stacking faults in the $MgSiO_3$ post-perovskite phase, Nature **438**, 1142-1144.	29.273	A. R. Oganov	Multidisciplinary Sciences
Stocker T.F. & Raible C.C.; Water cycle shifts gear, Nature, **343**, 830-833, 2005.	29.273	C. C. Raible	Multidisciplinary Sciences
Martonak R., Donadio D., Oganov A.R. & Parrinello M. (2005); Crytal structure transformations in SiO_2 from classical and ab initio metadynamics. Nature Materials **5(8)**, 423-626, August 2006.	15.941	A. R. Oganov	Chemistry / Molecular Dynamics
Oganov A.R. & Ono S. (2006); The high pressure phase of alumina and implications for Earth's D" layer, Proc. Natl. Acad. Sci. **102**, 10828-10831.	10.231	A. R. Oganov	Multidisciplinary Sciences
Zimmerli U., Gonnet P., Walther J.H. & Koumoutsakos P.; Curvature inducted L-defects in water conduction in carbon nanotube, Nano Letters, **5(6)**, 1017-1022, 2005.	9.847	P. Koumoutsakos	Chemistry /Nano Sciences
Hauser A., Enacescu C., Lawson Daku L.M., Vargas A. & Amstutz N.; Low-temperature lifetimes of metastable high-spin states in spin-crossover and in low-spin compounds: the rule and exceptions to the rule, Coord. Chem. Rev. **250(13-14)**, 1642-1652, July 2006.	9.779	A. Hauser	Chemistry
Bonnehommeau S., Guillon T., Lawson Daku L.M., Demont P., Sanchez Costa J.-F., Molnar G. & Boussekscu A; Photoswithching the Dielectric Constant of the Spin Crossover Complex $[Fe(L)(CN)_2].H_2O$, Angew. Chem. Int. Ed.;**45(10)**, 1625-1629, 2006.	9.596	A. Hauser	Chemistry
Raiteri P., Martonák R. & Parrinello M.: Exploring polymorphism: the case of benzene. - Angew. Chem. Int. Ed. 2005, **44**(24), 3769-3773	9.596	M. Parrinello	Chemistry
Beltran C., Edwards N.R., Haurie A., Vial J.-P. & Zachary D.S.; Oracle-based optimization applied to climate model calibration, Environmental Modelling and Assessment **11(1)**: 31-43, February 2006.	8.654	C. C. Raible	Atmospheric Sciences
Drouet L., Edwards N.R. & Haurie A.; Coupling climate and economic models in a cost-benefit framework: A convex optimization approach. Environmental Modelling and Applications **96(3)**: 035507, January 27, 2006.	8.654	C. C. Raible	Atmospheric Sciences
Arcidiacono S., Walther J.H., Poulikakos D., Passerone D. & Koumoutsakos P.; On the solidification of gold nanopartcles in carbon nanotubes, Phys. Rev. Lett., **94(10)**: 105502, 2005.	7.489	D. Poulikakos & P. Koumoutsakos	Physics
Gervasio F.L., Laio A. & Parrinello M.; Charge Localization in DNA Fibers, Phys. Rev. Lett. **94(15)**, 158103, 2005.	7.489	M. Parrinello	Physics
Ghose S., Krisch M., Oganov A.R., Beraud A., Bossak A., Gulve R., Seelaboyina R., Yang H. & Saxena S.K. (2005): Lattice Dynamics of MgO at High Pressure: Theory and Experiment; Phys. Rev. Lett. **96(3)**, 035507	7.489	A. R. Oganov	Physics
Giaccomazzi L., Umari P. & Pasquarello A.; Medium-range structural properties of vitreous germania obtained through first-principles analysis of virational spectra, Phis. Rev. Lett. **95**, 075505, 2005.	7.489	A. Pasquarello	Physics
Giustino F. & Pasquarello A.; Infraed spectra at surfaces and interfaces from first principles: Spatial evolution across the Si(100)-SiO_2 interface, Physi. Rev. Lett. **95**, 187402, 2005.	7.489	A. Pasquarello	Physics
Hornekaer L., Šljivancanin Ž., Xu W., Otero R., Rauls E., Laegsgaard E., Hammer B. & Besenbacher F.; Metastable structures and recombination pathways for atomic hydrogen on the graphite (0001) surface, Phys. Rev. Lett. **96(15)**, 156104, April 2006.	7.489	Ž. Šljivancanin	Physics
Läuchli A., Domenge J.C., Lhuillier C., Sindzingre P. & Troyer M.; Two Step Restoration of SU(2) Symmetry in a Frustrated Quantum Magnet, Phys. Rev. Lett **95**, 1372086, 2005.	7.489	A. Läuchli	Physics
Umari P. & Pasquarello A.; Fraction of boroxol rings in vitreous boron oxide from a first-principles analysis of Raman and NMR spectra; Phys. Rev. Lett. **95**, 137401, 2005.	7.489	A. Pasquarello	Physics

Source: ISI Web of Knowledge [SM]

Personnel

Head Count (as of 31st December 2006)



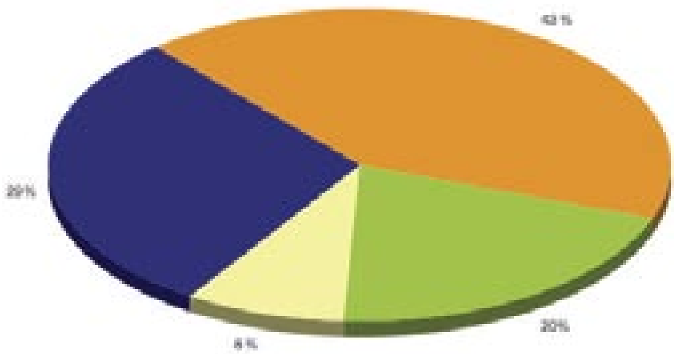
Management

Admministrative

Technical

Scientific

Staffing Costs (total for 2006)



Publications

Papers published by users of CSCS

Adams D.J. & Oganov A.R. (2006); Ab initio molecular dynamics study of CaSiO3 perovskite at P-T conditions of Earth's lower mantle. Phys. Re B73, art. 184106.

Altermatt P.P., Schenk A., Schmithüsen B. & G. Heiser; A Simulation Model for the Density of States and for Incomplete Ionization in Crystalline Silicon. II. Investigation of Si:as and Si:b and Usage in Device Simulation, Journal of Applied Physics, vol. 100, no. 11, pp. 113715, Dec

Altermatt P.P., Schenk A. & Heiser G.; A Simulation Model for the Density of States and for Incomplete Ionization in Crystalline Silicon. I. Establishing the Model in Si:P, Journal of Applied Physics, vol. 100, no. 11, pp. 113714, Dec 2006

Andreussi O., Donadio D., Parrinello M. & Zewail A.H.; Non-equilibrium dynamics and structure of interfacial ice, Chem. Phys. lett. 426 (1-3), 115-119, (2006)

Arbenz P., van Lenthe G. H., Mennel U., Müller R. & Sala M.; "A Scalable Multi-level Preconditioner for Matrix-Free Micro-Finite Element Analysis of Human Bone Structures". Technical Report 543, Institute of Computational Science, ETH Zürich, December 2006.

Arbenz P., van Lenthe G.H., Mennel U., Müller R. & Sala M.; Multi-level µ-finite element analysis for human bone structures. In: Workshop on state-of-the-art in scientific and parallel computing. Umeå, Sweden; accepted, 2006.

Baettig M., Wild M. & Imboden D.; 2006: A climate change index ˆ where climate change may be most prominent in the 21st century. Geophys. Res. Lett., (in press).

Barducci A., Chelli R. Procacci P., Schettino V., Gervasio F.L., Parrinello M.;Metadynamics simulation of prion protein: □-structure stability and the early stages of misfolding, J. Am. Chem. Soc. 128 (8), 2705-2720 (2006)

Behzadi B., Vargas A., Ferri D., Ernst K. H. & Baiker A.; Cinchonidine adsorption on gold and gold-containing bimetallic platinum metal surfaces: An attenuated total reflection infrared and density functional theory study. J. Phys. Chem. B, 110 (2006) 17082.

Bieri M. & Bürgi T.; Enantiodiscrimination between an N-acetyl-L-cysteine SAM and proline: An in situ spectroscopic and computational study,. ChemPhysChem ,7, 514 (2006).

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Boldyreva E.V., Ahsbahs H., Chernyshev V.V., Ivashevskaya S.N. & Oganov A.R. (2006); Effect of hydrostatic pressure on the crystal structure of sodium oxalate: X-ray diffraction study and ab initio simulations. Z. Krist. 221, 186-197.

Bonalumi N., Vargas A., Ferri D. & Baiker A.; Theoretical and spectroscopic study of the effect of ring substitution on the adsorption of anisole on platinum. J. Phys. Chem. B, 110 (2006) 9956.

Bongiorno A., Pasquarello A., Hybertsen M. S. & Feldman L. C.; Ion scattering simulations of the Si(100)-SiO2 interface, Physical Review B 74, 075316 (2006).

Bouffanais R., Deville M.O., Fischer P., Leriche E. & Weill D.; Large-Eddy Simulation of the Lid-Driven Cubic Cavity Flow by the Spectral Element Method Journal of Scientific Computing, DOI: 10.1007/s10915-005-9039-7, Vol. 27 (1-3), pp.151-162, 2006.

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Brugger S.C. & Schenk A.; New One-Particle Monte Carlo Method for Nanoscale Device Simulation, Technical Proceedings of the 2006 NSTI Nanotechnology Conference and Trade Show, Boston, MA, USA, vol. 1, pp. 673-676, May 2006

Brugger S.C. Schenk A. & Fichtner W.;Boltzmann Equation, Monte Carlo Simulations, Transport Models, and Noise: A Bridging Formalism Based on Exact Moments of the Inverse Scattering Operator,SIAM Journal of Applied Mathematics SIAP, vol. 66, no. 4, pp. 1209-1226, Mar 2006

Buch V., Martonak R. & Parrinello M.; Exploration of NVE classical trajectories as a tool for molecular crystal structure prediction, with tests on ice polymorphs, J. Chem. Phys. 124 (20), 204705 (2006)

Bucher D., Guidoni L., Raugei S., DalPeraro M., Rothlisberger U., Carloni P. & Klein M.; Polarization and Charge Transfer in the KcsA Potassium Channel, Biophys.Chem. 124, 292-301 (2006)

Bussi G., Gervasio F.L., Laio A. & Parrinello M.; The free energy landscape for beta hairpin folding from combined parallel tempering and metadynamics", J. Am. Chem. Soc., 128: 13435-13441, 2006

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Calanca P., Roesch A., Jasper K.. & Wild M.; 2006: Global warming and the summertime evapotranspiration regime of the Alpine region. Clim. Change, 79, 65-78.

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Invited talks and seminars

Biddiscombe J., Favre J., Valle M., HPC User Forum, ETH-Zurich, 1st June 2006, Parallel Visualization Projects at CSCS.

Favre J. , Paraview Visualization Software, two-day training at EPF-Lausanne, February 2006.

Favre J., Biddiscombe J., Foggia T., 1st International SPHERIC SPH Workshop, May 2006, Rome – Particle Data Management and Visualization.

Kunszt P.; ”Grid and Distributed Computing practice”, Presentation at the 3ème cycle romand d›informatique GRID and P2P Computing (Crans-Montana, du 6 au 10 mars 2006).

Kunszt P.; ”The Swiss Grid Initiative”, Invited talk at the Nordic Grid Neighbourhood Conference in Helsinki, on June 1st.

Kunszt P.; as lecturer on ”National Grid Infrastructures”, EGEE Summer School Budapest (July 3-8)

Kunszt P.; Invited talk about the ”Swiss Grid needs for the ARC Middleware” at the ARC Design Week Hungary, Sept. 4th.

Sawley M.-C., SOS 10, March 6th -8th , 2006, Maui, 10th Workshop on ”Distributed Supercomputing”, Capability Machines Panel.

Sawley M.-C., Irish Centre for High End Computing, (ICHEC), October 20th, 2006, Dublin, “Towards a coherent HPC Ecosystem, a national debate”.

Sawley M.-C., SC06, November 16th, 2006, Oak Ridge National Lab booth “Supporting Science on National Capability Computing Systems”.

Stringfellow, N. & Ulmer, D.: ”Introducing a Cray XT3 massively-parallel computer at CSCS”, Lawrence Berkeley National Lab, Berkeley, CA, 1.März 2006

Ulmer D., ”Grand Challenge Applications on the Cray XT3”, Supercomputing 06, Tampa, Fl, 14.-17. November 2006

Ulmer, D.: ”Petaflops Computing”, Cray Technical Workshop, Oxford, 10-12. Oktober 2006

Conference papers and posters

Biddiscombe J., Swiss Numerics Colloquium 2006, EPFL, High-speed particle rendering using point sprites.

Biddiscombe J. & Stringfellow N.; CUG 2006, May 8-11 2006, CrayViz: A Tool for Visualizing Job Status and Routing in 3D on the Cray XT3.

Favre J. , Walder R., Folini D., Swiss Numerics Colloquium 06: AMR Simulations and Visualizations in Astrophysics.

Favre J., Parkinson E., Swiss Numerics Colloquium 06: Parallel visualization applied to tera-scale rotor-stator simulations in water turbines.

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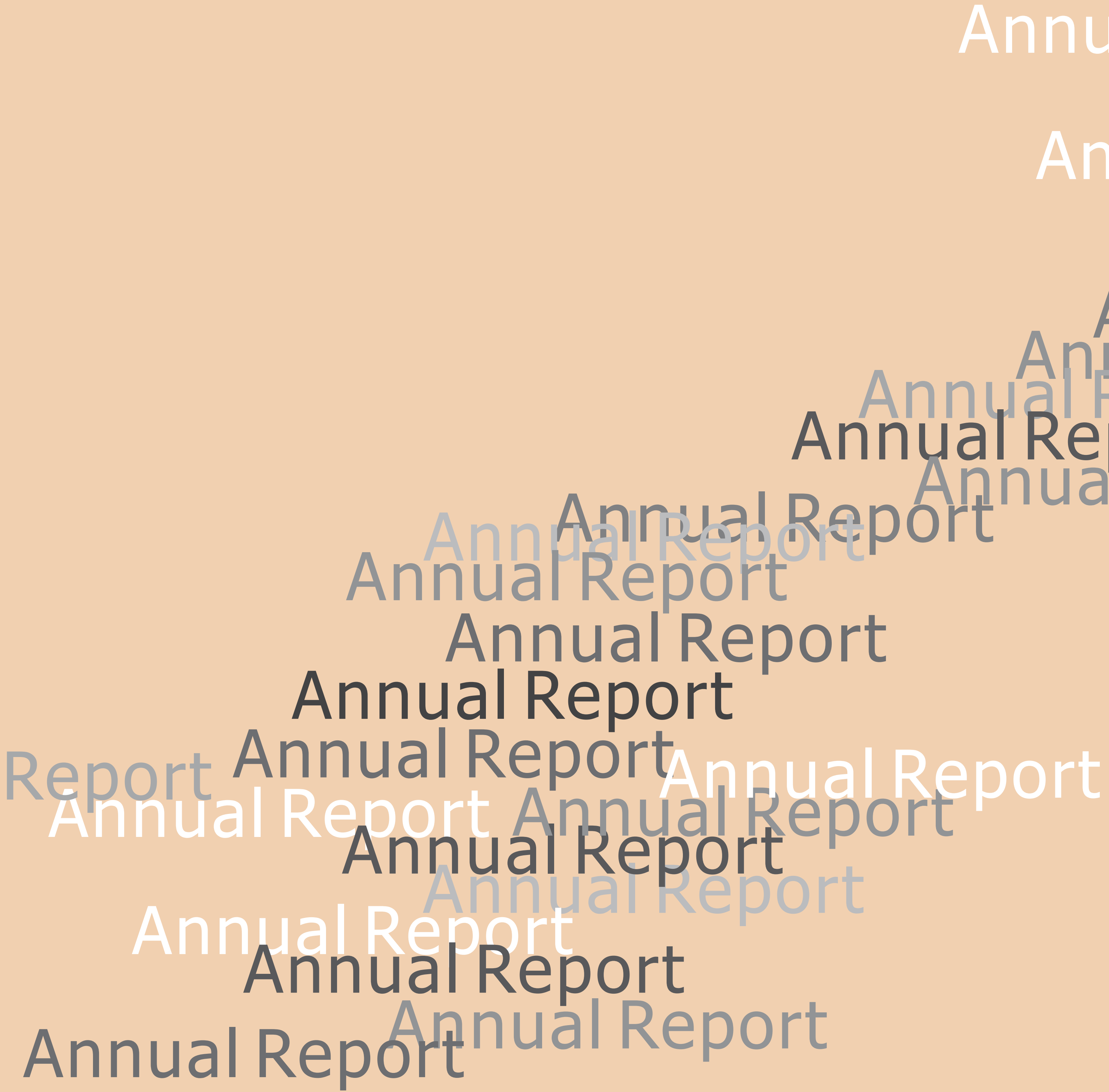
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