

## Annual Report 2007

Meetings of Steering Board (SB), and Scientific Advisory Board (SAB) in 2007

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#### **Carte Blanche**

Computational science becomes more and more important as a scientific tool and is the third leg besides theory and experiments. Simulation of processes or problems in nature with different scales such as climate models or material behaviour needs huge computational power. Computer codes for myriads of processors working simultaneously on a given problem have to be developed to make full use of the available technology. In addition, the hardware expands in size and power, and the cooling of supercomputers becomes a challenging issue. During 2007, a national strategy for High Performance Computing and Networking (HPCN) was developed by a team of the ETH Domain led by Prof. Giorgio Margaritondo. The recommendations of this group clearly define CSCS as the location of the national top-end machine in Switzerland with access for all university groups, but also recommends investments in nodes at the universities and, most importantly, investments in people for education of students and development of codes. ETH Management together with CSCS will prepare a message to the Swiss Parliament for the necessary investments.

After more than four years in office, Marie-Christine Sawley left CSCS at the end of the year to move to the ETH Institute of Particle Physics (IPP) to take part in the challenging computing tasks at the Large Hadron Collider (LHC) of CERN. Already at CSCS she enabled the planning and installation of a Tier2 Computing Centre for all Swiss university groups working at LHC. Under her directorship CSCS acquired the Cray XT3 machine as the first European high performance computing institution, in collaboration and co-financing with the Paul Scherrer Institute (PSI). She redirected CSCS to be more service oriented to users and made a great effort to embed CSCS in the 6th and 7th European framework program. In March Marco Baggiolini joined CSCS as a co-director and will stay in charge until a new director is found.



Prof. R. Eichler, President ETH Zurich

To operate complex infrastructure like hardware and system software, competent people are needed. This type of manpower is traditionally not funded by research organisations like Swiss National Science Foundation and can only be provided by a national centre. To make optimum use of sophisticated computing resources for the users the institute needs in addition top class scientists to help the users in the adaptation of their problems for the available hardware and software. These scientists need also an understanding of advanced hardware and infrastructure, and in an ideal case provide the vision together with the vendors for the next generation computing architecture. The management of ETH is committed to improve the scientific links of CSCS with academia at universities and industry in general and with ETH and USI in particular.

I would like to thank all staff of CSCS for their constant effort to provide a well maintained computing infrastructure for the benefit of scientists and engineers from Swiss universities and research institutes.

Prof. Ralph Eichler President ETH Zurich

## Activity Report



Prof. Marco Baggiolini, acting Director

#### Introduction

The history of CSCS reflects the impressive and rapid development of supercomputing. The Federal Institute of Technology (ETH Zurich) installed the first national supercomputer in Manno in 1992, an impressively large machine performing 5 billion operations per second, which could now be outperformed by a laptop. Today CSCS supercomputers reach 26,500 billion operations per second. The 15th year in CSCS history was particularly eventful. It reinforced the change from vectorial to massively parallel architectures yielding higher performance and enabling the centre to support a wider variety of scientific applications. The change started in 2005 with the installation of a Cray XT3 computer (co-financed by CSCS and the Paul Scherrer Institute) and was followed in 2007 by the upgrading of the Cray XT3 with dual core processors and the installation of a Cray XT4, used by MeteoSwiss for weather forecast simulations.

#### The year of the national HPCN strategy

Aware of the increasing importance of supercomputing for scientific progress, the ETH Board led the elaboration of a national strategy for ensuring the timely participation of Swiss research to the ongoing international developments toward petascale computing. The strategy report was presented to the Secretary of State for Education and Research in July 2007. In keeping with the Message of the Swiss Government, the strategy assigns to CSCS the task to develop, install and host a petaflop computer within three to four years. CSCS will also assure optimum access to increased computing power to research groups from Swiss academic institutions with the aim of maintaining their international competitiveness in areas of research and development where our country is traditionally strong. More than fifty research group leaders working in Switzerland in fields as diverse as chemistry, physics, material sciences, climatology, geology, biology, genetics, experimental medicine, astronomy, mathematics, computer sciences have expressed their full support to the national strategy. Basic and applied research in many areas of life and natural sciences is moving out of the laboratory and increasingly relies on modelling and simulation. Massively parallel computing is the relevant instrument, petaflop (eventually exaflop) computing is the future. Switzerland cannot miss the opportunity to maintain its leadership in science.

#### Preparing for the future

At CSCS, petaflop computing was on the horizon already in 2005, when the first massively parallel computer was installed for a more efficient support of an increasingly sophisticated and diversified community of users. In 2007, CSCS thus decided that preparing for a timely realisation of petaflop computing was its most urgent goal. The alternative would have been status quo, which is seldom reasonable in science and always wrong for supercomputing. To be ready to act when political and financial decisions will be made, several preparatory steps were taken at CSCS in 2007. Two possible plans for strategy implementation were elaborated, allowing for different rates of delivery of financial support.

- For a better service to Swiss science, CSCS renewed its organisational structure and strengthened high performance computing a fundamental support service for users of petascale systems by hiring several additional international experts.
- Plans were elaborated for strengthening the data analysis & visualisation unit in order to cope with increasing data output and complexity.
- A project team with members from CSCS, ETH Zurich and ETH Board was formed to work on the planning of a new building for CSCS, capable of hosting petascale machines.
- Several locations for the new CSCS building in the region of Lugano, in short distance from the university, are being evaluated.

 Collaborations with foreign supercomputing centres and with industry were set up for developing a petascale prototype and preparing the procurement of a full-scale system.

#### New resource allocation policy

Again in 2007, the procedure for allocating compute resources to users was modified in anticipation of the petascale developments. Requests for computing time are now subjected to a technical review performed at CSCS to find out whether the computational aspects are adequately planned, and whether the project truly needs access to largescale parallel supercomputing facilities. A separate assessment by external experts then addresses the scientific value and the feasibility of projects. If the request is considered valid, CSCS grants the necessary compute resources and ensures technical assistance during the whole duration of the project.

Professor Marco Baggiolini Acting Director of CSCS

#### **Preparing for Petaflops - The Years Ahead**

Since commencing work under global budget in 2004, CSCS has developed as the driving force for supercomputing in Switzerland. The momentum, Swiss computational science has gained since, is expressed in the submission of a national strategy for high-performance computing to the Swiss parliament in 2007. The ultimate goal of the strategy is to lead the country into the era of petaflop computing, i.e. to make a supercomputer available to research, which is able to deliver a million times a billion computations per second. CSCS will have a central role in the implementation of the strategy, which explicitly mandates the centre to concentrate on the highest end of computing only. During the next years, it therefore has to prepare the ground for a successful - effective and efficient - realisation of the national HPC strategy, once its financing has been approved by parliament.

The strategic importance of the petaflop goal of the HPC strategy becomes visible when put in context with the TOP500 trends (see Figure 1). In 1992, the trend of CSCS' performance plotted just below position 50 of the list. However, over the following 15 years, the performance of the centre developed slower than its international competitors: the trend curves of CSCS and position 50 diverge. According to these trends, CSCS would reach the petaflops goal by 2015, whereas position 50 would reach it already 2 years earlier. HPC is an essential tool for computational research, which has become the third leg of science besides theory and experiment. Therefore, the availability of sufficient HPC capacities is a competitive factor for the research capabilities of the country, capabilities vital to Switzerland as a knowledge-based society. The HPC strategy consequently proposes not only to make up for the lost competitiveness of Switzerland compared to position 50, but to accelerate the development further and to achieve a petaflop of computational power already in 2011.

The overall goals of CSCS for 2008-2011 can therefore be formulated as follows:

Provide the technical conditions for hosting a petascale system by the end of the performance period Petascale supercomputers will be very large installation, consuming megawatts of electrical power. CSCS and ETH Zürich are together planning a new building for CSCS, which will be able to host such an installation. CSCS will prepare itself for operating such a system by working closely with HPC manufacturers in order to get early access to petaflop technologies. In particular, data facilities for storing, managing and analysing the huge amount of data to be expected from these simulations will be developed.

#### Prepare and adapt the application codes for using petascale systems and organise CSCS services to support petascale applications

Being able to operate a petaflop computer is not enough – CSCS must support its research community so it is able to use the vast amount of compute power provided by the system. CSCS therefore will focus on parallel software engineering capacities which will support very large research projects in scaling to hundreds of thousands of processors expected for a petascale system. This will include the investigation of innovative ways to exploit and develop parallel algorithms.

### Contribute substantially to the creation of a national network of competence in HPC

A petaflop computer cannot be an isolated installation; it must be set within the framework of a national HPC ecosystem and in a network of competence between HPC experts. Building relationships between CSCS and other institutions for collaboration and exchange of know-how will be vital for the success of the petaflop enterprise.

Can we model climate change during the next hundred years and how will we cope with its consequences? Can we simulate the way a virus manipulates the genome of a cell in order to develop new drugs and cures? Can we develop new sources of energy, which will allow us to develop better living conditions of all humans on the planet and at the same time conserve earth's resources? Petascale computers will help Swiss researchers in finding answers to these and other urgent questions, and CSCS is ready to prepare this new era of computational research in Switzerland.

Dominik Ulmer

#### **Quantum Leap in Weather Forecasting**

The increasing number of extreme weather conditions observed in recent years has a strong impact on the alpine region. Switzerland's mountainous relief can lead to surprisingly distributed weather patterns: there can be sun on one side of a mountain pass, whilst the opposite valley is drenched in rain. Such phenomena can only be anticipated with the help of high-resolution weather forecasts.

Due to the growing number of disasters caused by bad weather the Federal Office of Meteorology and

Climatology (MeteoSwiss) has developed a weather forecast of higher precision and frequency. This new forecasting suite will work on the basis of a 2-kilometre grid as opposed to the 7-kilometre grid that is currently in use. In order to deal with the leap in compute power triggered by the new forecasting suite, CSCS, has given MeteoSwiss access to the Cray XT massively parallel computer architectures. This change in compute platform is a complex process that requires the migration of data, the porting and optimisation of the compute codes and of course the validation and verification of the results obtained, which is crucial for weather forecasting.

As of January 2008 this new high-resolution forecast will go into production with 8 daily simulation runs lasting 25 minutes each, up from the former 2 daily low-resolution simulation runs of 60 minutes. This increase in number of runs and resolution along with the shortening of the run-time leads to a 10-fold increase in required compute power. This challenge was met by CSCS with the newly installed Cray XT4 that was inaugurated on September 17th. All large computers at CSCS are given the name of a Swiss mountain. The Cray XT4 used by Meteo-Swiss was named "Buin". With its 448 dual-core



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

processors it provides a compute power of 5 trillion (10<sup>12</sup>) computations per second.

During the validation period, CSCS experts demonstrated the ability of the Cray XT systems to provide the stability and reliability required for the new highresolution forecasting suite. During the entire validation period lasting several months the machine delivered its services with the reliability of a Swiss clock.

The new supercomputer "Buin", with its elegant Swiss cross design, will also be made available to researchers from the Swiss universities and federal institutes of technology for scientific simulation projects in fields such as chemistry, physics, nanoscience, material sciences, fluid dynamics and, of course, climate research.

In January 2008, thanks to the joint effort of MeteoSwiss and CSCS on the meteorology of the alpine region, Switzerland will become the first country in Europe to benefit from a high-resolution weather forecast.

Neil Stringfellow

#### **Technical Services**

As every year, the Technical Services Section concentrated its efforts on the operation of our HPC platforms and surrounding infrastructure that serves our users.

In April the Cray XT3 system "Palu" was upgraded to dual-core processors. The 18 cabinet machine now offers 1664 dual core compute CPUs. In August "Palu" was joined by the newly purchased Crax XT4 "Buin" with 880 AMD Opteron cores at 2.6GHz that reaches a peak performance of 4.5 Tflops. This machine was purchased to cover the increased computational needs of MeteoSwiss



Cray XT 4, called Buin. allows next generation weather forecasting.



Grid size comparaison: Subjective single grid element comparaison between COSMO-7 and COSMO-2 in the Swiss Valais region near Martigny. Using a grid size of 6.6 km the chance to miss an entire valley is often quite high, even at 2.2 km this example would require finer grid resolution below 1 km.

when it moved to a high-resolution operational weather forecast at the beginning of 2008. Instead of computing twice a day on a 7km grid as it has done so far MeteoSwiss will now be computing every three hours on 2.2km grid. By allowing scientific users to run in between these compute cycles we are able to fill the machine around the clock.

Having passed acceptance at the end of 2006, the IBM P5 was brought into full production in January 2007. It offers 768 processors connected by dual plane Infiniband. A "fair share scheduling algorithm" was implemented on this platform in the first quarter. This system ensures that all projects should be able to use the allocated resources and the machine is utilized to its maximum capacity.

In August we were able to bring the new archive server and new tape drives into full production. After some initial teething problems this server is now able to handle the current workload and can be further expanded to accommodate further increases. Anticipating an increase in data traffic of 80% each year, we currently expect this server to cover the growth of the next two years.

December saw the installation of the first phase of the LCG cluster "Phoenix" that required a minimum bandwidth of 600Mbit, which will lead to an upgrade of the Internet link to 10Gbit in the 1Q2008. This cluster will continue to grow over the next three years in order to sustain the needs of the Swiss Institute of Particle Physics (CHIPP) community.

Inside the machine room we increased the network capacity to 10Gbit/s and continued to deploy the central user authorisation and authentication system. This system should service all CSCS servers by early 2008.



Machine room at CSCS

The project for a centre-wide parallel file system, that was initiated in the 3Q of this year will be one of the main focuses for 2008 and will bring a vast improvement for our users.

#### Davide Tacchella

#### **National and International Collaborations**

#### European Projects

The largest EU project for the establishment of a distributed Grid infrastructure is called Enabling Grids for e-Science in Europe (EGEE-II). CSCS supports the Swiss community of researchers interested in making use of this infrastructure, mainly the Swiss Institute of Particle Physics (CHIPP) whose members are very strongly involved in the latest of CERN's experiments, the Large Hadron Collider LHC. The LHC data is analysed on the Worldwide LHC Computing Grid WLCG. CSCS is the WLCG Swiss Tier 2 centre, operating a recently acquired SUN cluster with over 400 CPU cores and 200 terabytes of storage.

In 2007, CSCS joined a consortium of European supercomputing centres called Partnership for Advanced Computing in Europe PRACE, whose aim is to establish a competitive European supercomputing service for science. The consortium launched an EU-funded project with the same name, starting on January 1st 2008.

#### National Projects

The Swiss Bio Grid project, led by CSCS, was brought

to a successful conclusion in 2007. The project has demonstrated the advantages of Grid and distributed computing in the domain of life sciences. The experience gained through the Swiss Bio Grid by CSCS and its partners is one of the cornerstones of the new Swiss National Grid Association SwiNG, co-founded by CSCS. It counts 18 academic member institutions (from the ETH domain, cantonal universities and universities of applied sciences). One of the projects on the Swiss Bio Grid (the proteomics pipeline project of the Swiss Institute of Bioinformatics SIB in Geneva) will be continued within the framework of SwiNG. CSCS also participated in the South European Partnership for Advanced Computing SEPAC project

(with the University of Zürich, ETH Zürich and a consortium of Italian universities and HP) and the Intelligent Scheduling System ISS project (with the EPFL, the Ecole d'Ingenieurs de Fribourg and partners from Germany).

Peter Kunszt

#### ESPHI (European Smoothed Particle Hydrodynamics Initiative)

#### Visualisation and Analysis of SPH Data

Smoothed particle hydrodynamics (SPH) is a meshfree method for simulation which was originally developed in the field of Astrophysics, but has recently been applied to areas as diverse as solid mechanics, molecular dynamics, biomechanics and fluid dynamics. Within the field of CFD, SPH has the potential to become the method of choice in the next generation of software for a range of applications - primarily because it does away with the need for volumetric meshes, which are time consuming to create and difficult to manage and adapt to flow physics. SPH offers the ability to handle very complex solid shapes using boundary representations alone, and also the capacity to handle mixed-fluids and fluidstructure interactions within a unified approach.

Analysis and visualisation of SPH data is challenging, the mesh-free nature of the data means that there is no connectivity information between data points, and therefore no direct means of displaying a continuum representation of the computed fields. Customized tools which are capable of interpolating between particles are required to validate simulation results. Within the ESPHI project we are developing tools for the probing of field values, integration of numerical quantities over surfaces and fast and interactive visualisation of data within a framework which permits the analysis of both meshed and mesh-free simulations.

John Biddiscombe

#### COST Action D37

The European Science Foundation COST (Cooperation in the field of Scientific and Technical Research) is one of the longest-running instruments supporting co-operation among scientists and researchers across Europe. CSCS contributes to various working groups of the COST's action D37 (Grid Computing in Chemistry).

One of the outcomes from COST involvement is the collaboration with the OpenBabel team and CESGA (The Supercomputing Centre of Galicia) to add support for new file formats into Molekel and OpenBabel. In this way the outcomes of this project will be of benefit for the whole open-source community.



COST Action D37

#### Data Management, Analysis and Visualisation

#### Parallel Visualisation Cluster and Remote Visualisation

2007 is the first year CSCS offers a remote visualisation service. We operate an HP cluster of 32 CPUs and 32 GPUs, available for remote login and visualisation with 10 external links. Any installed visualisation tool can access data produced on the CSCS supercomputers, use hardware accelerated graphics rendering and copy – to the desktops of remote users – the full frame buffers. The application is application-independent, allows the use of multiple graphics nodes providing parallel visualisation, enables collaboration via broadcast of the frame buffers, and has been well accepted by our most demanding users.

The parallel cluster has allowed us to benchmark several load balancing and parallel rendering methods; two very large user projects at CSCS provided motivation. For the ETH Zurich Institute of Biomechanics and Institute of Computational Science, we provided a data I/O interface and filtering to allow parallel processing of very large unstructured meshes (simulations by Prof. Arbenz and Prof. van Lenthe). Our current record was established with the visualisation of a mesh of 410 million hexahedral cells. On the structured grid side, 3D cartesian meshes of size 800^3 are the final target for the project of Prof. Jackson (ETH-Zurich Institute of Geophysics). We dedicated a large amount of resources to this project to enable parallelism, Direct Volume Rendering, and many spherical space (and time-space) averaging routines. The visualisation cluster received a much needed increase of memory at the end of the summer to accommodate the needs of such large projects. With a total memory of 192 Gbytes, we are now able to easily handle parallel visualisation jobs of "moderate size". We expect increased usage in 2008 thanks to the global parallel file system currently being installed.

#### Visualisation tools and toolkits

STM4: the evolving molecular visualisation toolkit The STM3 molecular visualisation toolkit has undergone a major restructuring to better support new user requests for new and advanced visualisation techniques. STM4, the new version, has at its core an expanded Data Model to better describe molecular structures and a new set of visualisation modules created to support specific user projects.

STM4's main strengths are its quick prototyping capability, which permits a tight interaction with the users to elicit their real needs, and the ability to use standard visualisation techniques intermixed with the more standard chemistry visualisation. Those capabilities make STM4 a tool that does not overlap



Molekel

with other visualisation tools, like Molekel, which is more end-user oriented.

Besides the STM4 visualisation support to chemistry related research users, the toolkit is the base for specific visualisation projects allowing them to concentrate on the development of project-specific functionalities. For example a crystal structure classification and analysis tool for Prof. Oganov's USPEX tool has been implemented.

#### Molekel

Several versions of Molekel have been released in 2007, resulting in several thousand worldwide downloads. The focus for the new versions has been on responding to users' feedback to fix issues and add new features. Several enhancements to data input, interaction and rendering have been implemented, including:

- Better support for quantum chemistry formats
- Option to blend vibrational modes
- Depth order independent rendering of transparent surfaces
- Anti-aliasing
- Display of radiation spectra
- Support of programmable shaders

The work on Molekel and the collaboration with users has helped us enhance our skills in molecular visualisation and advanced (GPU-based) rendering techniques which will be used in future versions of Molekel and other programs developed in the Visualisation Group.

#### **CSCSVolView**

We continued to work on providing a prototyping tool for Direct Volume Rendering (DVR), using VTK component classes. More data interfaces were added, with a time-collection animation feature. DVR can be of particular interest for users with very large structured data, because it by-passes the need to generate geometry (often a big bottleneck in memory with very large overhead for transient data). DVR based on ray-tracing is embarrassingly parallel and when multi-threaded, it can take advantage of the multi-core architectures found in newer platforms. We anticipate a growing usage of DVR at CSCS.

#### pv-meshless

The parallel rendering and analysis tool ParaView is used extensively at CSCS by the visualisation group and also by its users. It is a powerful software package designed for the visualisation and analysis of large data sets from many fields of science, but lacks support for particle based simulation results. We have extended the ParaView package by adding a set of new rendering modes which permit the fast visualisation of particle data and have integrated a number of modules for the analysis of point based data sets.



Molekel



CSCS VolView



pv-meshless: Visualisation of particle data with ParaView

#### Transient Data Support

CSCS has collaborated with researchers in the USA at Kitware Inc. and Sandia National Laboratories to improve the handling of time based data within the Open Source Visualisation Tooklit (VTK) and the rendering software ParaView which is based upon it. New mechanisms have been added to the pipeline architecture to allow the arbitrary (random access) retrieval of pieces of data from any time step. This has enabled the creation of complex new visualisation modules (such as particle tracing in unsteady flows) which were not possible prior to this work. We are now using these new modules to further develop analysis tools for unsteady data which will be available to CSCS users.

Jean Favre and Ugo Varetto

#### Outreach

#### CSCS User Events

Due to the changes in the academic calendar this year's User Day took place a bit later than usual on October 5th and 6th in Manno. It was split into presentations by Professors John Maddocks (EPFL), Sonia Seneviratne (ETH Zurich), Stefan Gödecker (University of Basel), Andrew Jackson (ETH Zurich), Rolf Walder (ETH Zurich) and Jürg Hutter (University of Zurich).

Topics of general interest such as the Swiss National HPC strategy, CSCS hardware and software roadmap and information about the changes in the resource allocation process were covered by members of CSCS. For the first time there was also a special interest group (SIG) session that allowed users from similar areas of interest to meet and discuss specific concerns they may have and give feedback to CSCS. This initiative met with great enthusiasm and CSCS received useful feedback and input from its user community. We will certainly maintain and develop the SIGs as an important part of future User Days. For the event CSCS also published the first edition of its User Information brochure.

#### Courses and workshops

During 2007 CSCS organized a number of courses for its user community. Having put the new IBM P5 into production at the start of the year introduction courses were offered to familiarize users with the new machine. Given the success in recent years we also invited Mr. Rolf Rabenseifner of HLRS to teach



his summer school on parallel programming. We will be maintaining this course in 2008.

During the year CSCS also hosted the COST D37 and the EGEE/SBG workshops and the ESF meeting

In 2008 we will be extending our current selection courses to cover further areas of interest to our users.

#### Conferences and events

Having hosted the Cray User Group conference in 2006 CSCS had the honour of hosting the EGPGV (EuroGraphics Symposium on Parallel Graphics and Visualisation) in May.

In September we inaugurated our XT4 Buin that will allow the Federal Office of Meteorology and Climatology to be the first country in Europe to run a high resolution operational forecasting suite. This was a critical step in improving the precision of forecasts – especially for extreme events such as floods and high winds.



In addition to the official events CSCS also gets numerous visits from companies, schools and universities.

All in all it was a busy and interesting year and we look forward to celebrating the 15th anniversary of CSCS on January 30th 2008.

Ladina Gilly



#### Infrastructure

2007 was another busy year for the Facility Management unit that saw the completion of the work started in 2005 to upgrade and extend the infrastructure of CSCS.

Given the rise in the average summer temperatures in Ticino over the past years the condensation towers that were servicing the two existing cooling machines reached the limit of their capacity. In order to overcome this issue four new cooling towers were added in May. Two of these service the existing cooling machine, whereas the other two service the newly acquired cooling machine that was brought into production in October.

In order to increase the available electrical power a 4th transformer was installed and the entire existing switchboards upgraded to current standards. In the last quarter of the year we also saw the first dynamic UPS machine come into service at CSCS. This offers a capacity of 770KW and will service most computers in the machine room from 2008.

An additional precooling unit was installed to improve the airflow around the Cray XT3. Two new water-cooling circuits were installed to serve the SUN cluster for CHIPP – the Swiss Institute of Particle Physics.

2007 was also the year in which the NEC SX5 was switched off after 6 years of production and in May the SP4 gave way to the new IBM P5 that had already gone into production in January.

Ladina Gilly



## Research Digest



Prof. Dr. Ivo Sbalzarini

#### Interview

with Prof. Dr. Ivo Sbalzarini by David Bradley, Science Base, UK

Dr. Ivo Sbalzarini is an Assistant Professor in the Institute of Computational Science at ETH Zürich. He heads the Computational Biophysics Lab, which develops and uses methods from computational science (data analysis, modelling, and simulation) to gain an understanding of the working mechanisms of living systems.

#### What does computational biophysics involve?

Unfortunately there is no unique and concise definition of biophysics, it does, however, mean that we use the laws of physics to gain a mechanistic understanding of the functioning of living systems. This assumes that the same physical principles are valid for living matter as for dead matter. Computational biophysics tries to do exactly this by developing and applying methods from computational science and computer science. With all its modern assays and complex data formats (images, videos, high-throughput screens) biology can thus be viewed as an important technology driver.

#### What is your focus?

We are developing and applying methods from image processing, sensitivity (robustness) analysis, and large-scale parallel computer simulations of biological systems. The synergy is obvious: image processing tools are needed in order to extract quantitative information from the primary data, then a model can be formulated and simulated (requiring supercomputing). Sensitivity analysis is the overarching loop that allows us to assess model performance and quantify simulation uncertainties. This is a very active field of research in computational science at the moment.

#### Why is it important?

In order to understand the connection between genotype and phenotype, we must consider the spatial organisation and compartmentalisation of the living systems, as well as the correct physics of the interactions. This involves the automated (unbiased) processing of large amounts of experimental data. Computer simulations allow control and observation of all variables, which is not possible in classical experiments. Due to the complexity of biological systems, new computational methods for data analysis and large-scale simulations are needed, requiring supercomputing resources.

#### What is the CSCS role in the research?

CSCS provides the computer resources that we need for our simulations of diffusion processes in complex geometries, of the electromagnetic fields in the human head and brain, and of the molecular dynamics of lipids and proteins. In addition, we participated in the development of a portable and transparent software library for supercomputer simulations. This library currently forms the software basis underlying all our simulation programs and enabling state-of-the-art parallel efficiency and scaling.

#### Do other researchers use your tools?

All our software tools are open source and implemented in user-friendly packages (with manuals and graphical user interfaces). They are being downloaded and used by many labs and researchers around the globe. In addition, we have numerous collaborations with groups in biology, both at ETH as well as outside ETH, which ensures that the tools are useful and usable and not just 'nice theories with no application'.

#### What are the big problems in biophysics?

On the application side: explaining how the genetic code and its sequence predetermine the physicochemical functions of a living system all the way up to high-level social behaviour and interactions. Which parts of the phenotype are genetically determined and which parts are not? Where do self-organisation phenomena and environmental influences play a role?

On the computational methods side: spanning the 13 orders of magnitude from the atomic scale to the whole organism or ecosystem using multiscale computational methods. Developing such computational algorithms and the corresponding software and middleware tools is one of the current challenges in our field.

#### What's your biggest achievement in your current role?

Definitely the building of my current research group of 4 PhD students and 2 postdocs. I was extremely fortunate to find such a highly talented and motivated group, working with them is extremely inspiring and a pleasure every day.

#### **Presentation of Three Large User Projects**

by David Bradley, Science Base, UK

We propose here a special insight into the work of three scientists, who carried out their research using computing resources from CSCS. The reader can find the list of all the 2007 projects on page 30.

#### MONALISA II

#### paints a picture of climate change

(Prof. Christoph C. Raible, Climate and Environmental Physics, Physics Institute, University of Bern, Switzerland)

The power of CSCS computing resources is being brought to bear on the enormous problem of climate change in the work of Christoph Raible of the University of Bern working on the MONALISA II project (Modelling and Reconstruction of the North Atlantic-Climate System Variability). "In order to assess ongoing and potential future climate change with confidence it is necessary to put such changes in a long-term perspective," Raible explains. However, instrumental records are limited and the only other information available is proxy data such as tree rings or documentary data. To improve our understanding of the processes that cause climate variability models of atmosphere-ocean general circulation are needed.

The researchers have focused on the Maunder Minimum (MM), a period of low solar activity that occurred between 1645 and 1715, the probably coldest period that is known as the Little Ice Age. It provides researchers with a useful baseline for assessing the effects of atmospheric circulation and



Simulated climate change could explain stormy differences across the ages

the hydrological cycle at a time when the climate was only affected by natural factors, e.g., solar activity and volcanoes.

By building on an early proxy-based study by others, the researchers have simulated the climate during the MM to tease out natural forcing signals, such as solar activity and volcanic eruptions, which emerge as clearly affecting temperature and partly rainfall across the hemispheres. On more local scales, however, these natural phenomena are masked by internal atmosphere-ocean variability. However, it is these regional results that have the widest implications in the search for suitable locations to reconstruct historical climate change and so improve predictive models. "Our ensemble simulations of the MM deliver a beneficial test bed," explains Raible, "which could improve the understanding of what is recorded in proxy data."

Other researchers have demonstrated using proxy data that storminess in Northern Europe was much worse around the MM but an independent proxy reconstruction of sea level pressure across the North Atlantic suggests otherwise, that on average Northern Europe suffered weaker winds. In order to understand this seeming contradiction, Raible's team has compared the proxy results with their MM simulations.

The findings of Raible and colleagues suggest that cyclonic weather systems associated with strong winds were shifted south, so that there were indeed fewer storms over Northern Europe. The team has also compared MM simulations with today's weather systems. The results show that even in areas, where the number of cyclones decreased, like Northern Europe, the intensity of cyclones at the extremes nevertheless rises in winter.

Moreover, Raible and colleagues have developed a hypothesis to explain this underlying intensification process. They suggest that the North-South temperature gradient plays a key role in intensifying the extremes of cyclonic weather systems as well as affecting pressure in the North Atlantic when comparing the MM with today. "Our modelling results help to overcome the apparent contradiction showing that a decrease of the number of storms in northern Europe is accompanied by an intensity increase," says Raible. He concedes that these results are based on a single model and that the difference is only statistically significant between MM versus today.

Nevertheless, bringing together proxy data and modelling results will help to overcome the disadvantages of each and emphasise their advantages. "Carefully interpreting such simulations could help to deepen the understanding of wind and hydrological sensitive proxy data and to put them into a dynamical context" adds Raible, "The strength of modelling studies also lies in providing mechanisms explaining changes in proxy data."

Raible points out that global efforts to simulate climatic conditions during the last millennium are now becoming significantly more robust thanks to such work and the steadily growing proxy data from other parts of the world such as South America and the Mediterranean Basin.

#### **Exotic matters**

(Prof. Andreas Läuchli, Institute for Numerical Research in the Physics of Materials, EPF Lausanne, Switzerland)

Andreas Läuchli of EPFL in Lausanne, Switzerland uses CSCS computer power in his quest to understand some of the most exotic phases of matter.

Gas, liquid, and solid are the well-known phases of matter, and among them are electrical insulators, semiconductors and metals. However, the discovery of quantum mechanics adds a whole new range of exotic species to the materials menagerie because of the weird and wonderful effects of quantum fluctuations.

For example, about twenty years ago researchers at IBM Rüschlikon discovered the enigmatic high-temperature superconductors. In this material phase matter can conduct electricity with no loss of energy and can exclude a magnetic field are another state of matter. There also exist quantum magnets in which quantum effects destroy magnetic order. Another phase of matter known as a Bose-Einstein condensate exists as an ultra-cold cloud of atoms that lock on to each others behaviour and move as one.

Then there are controversial supersolid phases of the unreactive gas helium, which are both solid and superfluid simultaneously and under certain conditions have no viscosity and can flow uphill. Finally, there are speculative anyonic quantum phases of matter that have topological order and may one day to a viable quantum computer for solving enormous problems such as precisely modeling fluid flow, stock markets, and even the weather and climate.

"The common origin of these diverse novel phases of matter, the strong quantum fluctuations, pose a substantial challenge to numerical simulations," explains Läuchli. He points out that approximate methods, such as classical molecular dynamics, are not powerful enough to help us understand matter at this level. They do not, for instance, predict the supersolid phase. Similarly, standard approximate quantum chemistry calculations that use the Nobel Prize winning density functional theory or the socalled Hartree-Fock method cannot explain the exotic properties of a quantum spin liquid or topological order. "Unbiased full-quantum simulations are necessary to observe these intriguing states of matter," says Läuchli.

Läuchli adds that with the discovery of novel quantum states, there is a need to develop powerful new algorithms to carry out unbiased simulations of the quantum interactions and fluctuations from which these states emerge. "In the last decade, we have seen important breakthroughs and tremendous improvements in algorithms by many orders of magnitude," he adds, and he and his colleagues have been instrumental in many of these achievements.

A consortium, of which Läuchli's team is a member. is utilising CSCS facilities to run efficient algorithms that can model large quantum systems with incredible accuracy. "We are now on the verge of a scientific breakthrough," he enthuses, "This will enable the direct comparison of full quantum mechanical simulations with experimental measurements and provide an important tool to scientists characterising and designing new materials with strong quantum effects. In May 2007, the team published significant results on a simulation of an ultracold atomic gas in the prestigious journal Physical Review Letters (PRL 98, 180601). In this work they investigated how an atomic gas in the superfluid phase can be guenched into an entirely different phase, a Mott insulator, a material that theoretically should conduct electricity but experimentally is an insulator.

The experimental results discussed by Läuchli and colleagues suggest that this change of phase oc-

curs in a rather surprising way. However, the computational models provide an explanation based on quantum interactions between quasiparticles.

Some quantum magnets become Bose-Einstein condensates under certain conditions, explains Läuchli. In so-called frustrated magnets that have lots of competing interactions within, the kinetic energy of their particles is suppressed. In this situation correlated hopping can take place in which particles move more easily when they have neighbours of the same type than when they are alone. Läuchli's work shows that this correlated hopping gives rise to a very large supersolid phase, where crystalline order and superfluidity coexist. "These results are very exciting, since magnetic materials with large correlated hopping exist," says Läuchli, "and so it might be possible in the future to experimentally address this supersolid phase, which is currently hotly debated in helium-4 experiments and not yet fully understood."



Phase diagram reveals the peculiar landscape of super fluids and supersolids

#### Sensing model behaviour at the interface

(Prof. Dr. Martin Kröger, Departement of Materias, ETH Zurich, Switzerland)

Molecular modelling on CSCS computers could help scientists at ETH Zurich build new types of twofaced molecules, known as amphiphiles, that can bridge the gap between synthetic materials, including polymers, and biological systems. The resulting functional materials could provide a dynamic interface between sensors and living tissues for research and medical diagnostics applications.

Two-faced amphiphiles include a vast range of materials that have a water-loving (hydrophilic) end and a water repellent end (hydrophobic). The simple soap molecule which can dissolve in both water and oil is perhaps the best known example of an everyday amphiphile, but there are many others, that are used in chemical and biochemical research. Many amphiphiles have interesting behaviour segregating themselves and undergoing processes of self-assembly to form sophisticated arrangements of molecules. ETH's Martin Kröger and his colleagues Nikos Karayiannis and Manuel Laso of the Polytechnic University of Madrid, Spain are investigating the potential of phospholipid and polypeptide amphiphiles.

They have focused on three amphiphilic molecules, the toxic peptides alpha-conotoxin AuIB, bucandin, and phospholipase. By using molecular dynamics simulations, Kröger and his team have revealed in atom-by-atom detail the behaviour of these three peptides. Their structural, conformational and dynamic features were extracted by averaging over three different molecular dynamics trajectories for simulation times that ranged from 0.5 microseconds for alpha-conotoxin to 1.2 microseconds for phospolipase A2.

By investigating these complex molecules in water and a liquid crystalline environment, the team could tease out the details of the behaviour of such molecules, which involve between 50,000 and 200,000 atoms at the interface site. Such extensive atomistic molecular dynamics simulations would, explains Kröger, "serve as excellent starting models for successive coarse-graining in a systematic manner that will eventually lead to chemically simple representations of the studied systems."

"The particle trajectories recorded during the computations contain a wealth of so far hidden information which will be explored later by post-processing," says Kröger, "using recently developed multiscale modelling strategies." He adds that an important ingredient is the analysis of fluctuations on the microscale for those few structural variables which have the potential to dominate the material-relevant dynamics of the whole microscopic system. "To this end, the group will make use of its leading expertise in developing and implementing coarse-grained models and new constitutive relationships for complex materials," he adds.

Their work exploits the very recent experimental observation that liquid crystal phases, which exist in nature and not just in digital watches, can be used to probe the structure of phospholipid interfaces at the nanometre scale. They can therefore be used as a powerful and practical tool for investigating the molecular characteristics of such systems and so help researchers design and use sensors for biological molecules.

Such a sensor would work by utilising the principle that as a biological molecule of interest binds to a substrate in the biological tissue, an attached liquid crystal molecule would distort. The resulting defects would propagate to large visible length scales and so magnify a single tiny molecular event and make it visible.

"The length and time scales of the simulated phenomena are traceable only through the application of the NAMD software in a dedicated large cluster of supercomputers over an extended period of time," explains Kröger, "The Large Project initiative at CSCS allows the team to realize this ambitious, but also very demanding, modelling project."

He adds that the results of these modelling studies will be complete by the end of the present LP project. Without access to the computational resources of CSCS the microsecond molecular dynamics simulations would not be.





Toxic molecules could be used to build medical sensors

#### List of Large User Projects 2007

Name	Organissation	Project Title
Arbenz P.	ETH Zürich	Multi-level Micro-Finite Element Analysis for Human Bone
		Structure
Baiker A.	ETH Zürich	Hydrogenation reactions in heterogeneous enantioselective ca-
		talysis and homogeneous catalysis in supercritical $\mathrm{CO}_{_2}$
Bakowies D.	ETH Zürich	Atomisations energies from ab-initio calculations without empir- ical corrections
Behler J.	ETH Zürich	A Neutral-Network Representation of High-Dimensional ab-ini-
		Climate and Strategrapheric Orang during the 00th contury
Bronimann S.		Chimate and Stratospheric Ozone during the zoth century
Bruneval F.	ETH Zurich	Crystal structure prediction from computer simulations
Burgi Th.	Uni Neuchatei	Structure and enantiospecificity of chiral nanoparticles and in-
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
Ensing B.	ETH Zürich	Multiscale modelling of proton conducting polymeric mem-
		branes
Fichtner W.	ETH Zürich	Computational Science and Engineering in Nanoelectronics
Folini D.	EMPA	Inverse modelling to monitor source regions of air pollutants
Fouchet L.	ETH Zürich	Dust in protoplannetary disks
Gervasio F.	ETH Zürich	Charge transfer and oxidative damage to DNA
Gödecker S.	Uni Basel	Atomistic simulations and electronic structure
Hasenfratz P.	Uni Bern	Full QCD with 2 + 1 light chiral fermions
Hauser A.	Uni Genève	Photophysics and photochemistry of transition metal com-
		pounds: Theoretical Approaches
Helm L.	EPF Lausanne	Magnetic interactions in extended systems
Hutter J.	Uni Zürich	Development and application of ab-initio molecular dynamics methods
lanuzzi M.	PSI	Transport properties and microstructural changes in uranium dioxide
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 optimisation of real world
		problems using evolutionary algorithms multiscale modelling, simulations and optimisation of complex systems
Krack M.	ETH Zürich	Nitrogen reduction on pyrite surfaces
Kraiewski F.	ETH Zürich	Ab-initio simulation of the nucleation of silicon with a novel lin-
		ear scaling electronic structure method
Kröger M.	ETH Zürich	Computer-Aided Design of Nanostructured Interfaces for Biological Sensors
Läuchli A.	EPF Lausanne	- Computational Studies of Strongly Correlated Electron System

Name	Organisation	Project Title
Lehning M.	WSL-SLF	Wind field simulations and snow drift modelling over steep terrain
Leyland P.	EPF Lausanne	Large scale compressible flow for aerothermodynamic studies
Lodziana Z.	EMPA	Computational investigation of complex hydrides for hydrogen storage
Lüscher M.	CERN	Numerical lattice gauge theory
Maddocks J.	EPF Lausanne	Large-scale atomistic molecular dynamics simulations of DNA minicircles
Mareda J.	Uni Genève	Molecular Modelling of Artificial Multifunctional Pores and their Catalytic Properties
Martonak R.	ETH Zürich	Crystal structure prediction from computer simulations
Meuwly M.	Uni Basel	Electronic Structure Calculations for Chemical Reactions involv- ing Transition Metals
Oganov A.	ETH Zürich	Computational Crystallography: crystal structure prediction and simulation of planetary materials
Parlange M.	EPF Lausanne	Large-eddy-simulation studies of atmospheric boundary layer flow over complex terrain
Parrinello M.	ETH Zürich	Ab-initio study of proton diffusion in water-methanol solutions
Parrinello M.	ETH Zürich	Ab initio simulations of phase change materials
Pasquarello A.	EPF Lausanne	Atomic-Scale Modelling at Semiconductor-Oxide Interfaces
Passerone D.	Uni Zürich	Computational investigation of relevant photochemically active molecular switches
Passerone D.	EMPA	Atomistic simulation of surface-supported molecular nanostruc- tures and of quaicrystal surfaces
Poulikakos D.	EMPA	Biothermofluidics for Cerebrospinal fluid diagnostic and con- trol-development of a knowledge base Explosive vaporisation 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 sys- tems of biological interest
Sbalzarini I.	ETH Zürich	Simulations of biological systems and development of a paralli- sation framework
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
Seneviratne S.	ETH Zürich	Land-climate interactions: Modelling and analysis
Sennhauser U.	EMPA	Reliability and degradation physics of ultrathin dielectrics (Nanoxide)
Sljivancanin Z.	EPF Lausanne	Solid Surfaces and Interfaces

Name	Organisation	Project Title
Van Lenthe H.	ETH Zürich	What genetic loci regulate bone strength?
Van Mier J.	ETH Zürich	Investigation of 3D Size Effects in Concrete Using Lattice Models
Van Swygenhoven H.	PSI	The atomistic modelling of size effects in plasticity
Vogel P.	EPF Lausanne	Developing High-resolution Models How Mechanical force Changes
		Protein Function
Walder R.	ETH Zürich	Stellar Cosmic Engines in Galaxies

#### List of Advanced Large Projects in Supercomputing (ALPS) 2007

Name	Organisation	Project Title
Jackson A.	ETH Zürich	Convection and Magnetic Field Gneration in Earth and Other Planets
Vogel V.	ETH Zürich	Towards Simulating a Cell Adhesion Site at Angstrom Resolution
Schär Ch.	ETH Zürich	Climate Change and the Hydrological Cycle from Global to European/
		Alpine Scales
Parrinello M.	ETH Zürich	Modelling Protein-Protein Interactions at the Atomic Level

## Facts & Figures

Expenditures		Income	
Investments	6'652'332.28	Basic Budget	11'214'000.00
		Contribution ETH Zurich	8'214'000.00
Materials, Goods & Services	694'281.83	Contribution ETH-Board	3'000'000.00
Personnel	5'477'803.31		
Payroll	4'280'541.25		
Employer's contributions	583'016.60		
Other	614'245.46	Third-party contributions	1'248'744.93
		MeteoSwiss	1'018'968.25
Other material expenses	7'229'236.54	Co-Investmt. Cray Upgrade PSI	127'371.05
Floor space	181'724.38	Contrib. Uni ZH+PSI for CHIPP	77'918.90
Maintenance	2'747'004.43	CHIPP Cluster	-250'000.00
Energy & media	1'196'580.92	Installation costs (internal transfer ETH Zürich)	
Administrative expenses	79'269.24		
Hardware, software, services	2'224'355.96	KTI Project 7338.2 ESPP-ES	186'404.00
Services & remunerations	791'567.50	Other third-party	88'082.73
Other	8'734.11		
Extraordinary incom/expenditures	-985'496.69		
Extraordinary income	-1'379.69		
Internal transfer	-984'117.00		
CHIPP cluster			
Expenses total	19'068'157.27	Income total	12'462'744.93
Balance			-6'605'412.34

- The balance is rolled over to the 2008 budget.

#### Balance current year

Balance according to CSCS funds	998'567.19
Rollover 2007	3'884'407.57
Final balance	-2'885'840.38
Expenses outside of Globalbudget	-3'719'571.96

#### **Cost Distribution**

Cost element	Q1	Q2	Q3	Q4	Total
Costs of goods & services	-	337.85	289.51	66.93	694.29
Salaries	1'115.45	1'093.45	1'053.00	1'018.64	4'280.54
Contribution social insurances	195.57	131.61	125.35	130.48	583.01
Other personnel costs	167.67	156.33	105.60	184.64	614.24
Total costs of personnel	1'478.69	1'381.39	1'283.96	1'333.76	5'477.80
Costs of administration					
and building infrastructure	462.04	983.37	1'565.46	1'193.70	4'204.58
Costs of hardware,					
software, IT-services	686.67	478.67	464.48	594.54	2'224.36
Other services &					
remunerations	86.12	66.58	328.35	310.52	791.57
Other costs	0.14	1.81	0.83	5.95	8.73
Depreciation of investments	1'450.41	1'513.92	1'833.89	1'872.43	6'670.65
Total costs of materials	2'685.38	3'044.36	4'193.01	3'977.14	13'899.89
Extraordinary costs	0.00	0.78	0.00	3.26	4.04
Internal payments to ETH Zurich	0.00	-484.12	0.00	-500.00	-984.12
Total costs	4'164.08	4'280.25	5'766.48	4'881.09	19'091.89

- All figures are given in kCHF.

#### **Cost Analysis**

Breakdown of costs per customer

Customer	ETHZ	PSI	Meteo CH	EPFL	Uni Zurich	CERN	Uni Bern	CSCS	EMPA	Uni Genf	Uni Basel	CHIPP	Other	TOTAL
Income federal base funding	5'999	1'379	0	2'703	0	0	0	0	561	0	0	0	572	11'214
Income third party funds	0	127	1'019	0	0	0	0	24	0	0	0	78	0	1'249
Distribution direct costs														
IT Depreciation Total	3'740	892	591	427	302	90	111	29	143	165	68	83	30	6'671
Technical services	3'740	892	281	427	302	90	111	29	143	165	68	0	30	6'278
User & appl. services	о	0	0	0	0	0	0	0	0	0	0	0	0	0
Data analysis services	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Scient. support services	о	0	0	0	0	0	0	0	0	0	0	83	0	83
Software development services	о	0	0	0	0	0	0	0	0	0	0	0	0	0
MeteoSchweiz	о	0	310	0	0	0	0	0	0	0	0	0	0	310
Personnel Total	1'213	231	203	112	78	70	33	733	24	86	49	217	5	3'055
Technical services	638	152	48	73	51	15	19	5	24	28	12	0	5	1'071
User & appl. services	140	14	156	14	14	0	0	101	0	14	14	0	0	467
Data analysis services	275	50	0	25	13	0	0	125	0	0	13	0	0	501
Scient. support services	о	0	0	0	0	54	0	109	0	43	11	217	0	435
Software development services	160	15	0	0	0	0	15	393	0	0	0	0	0	582
MeteoSchweiz	о	0	0	0	0	0	0	0	0	0	0	0	0	0
IT expenses and mainte- nance Total	1'164	275	264	132	93	58	34	92	44	75	28	121	9	2'389
Technical services	1'143	273	86	130	92	28	34	9	44	50	21	0	9	1'918
User & appl. services	6	0.5	7	0.5	0.5	0	0	4	0	0.5	0.5	0	0	20
Data analysis services	9	2	0	1	0.5	0	0	4	0	0	0.5	0	0	17
Scient. support services	о	0	0	0	0	30	0	60	0	24	6	121	0	242
Software development services	5.5	0.5	0	0	0	0	0.5	13.5	0	0	0	0	0	20
MeteoSchweiz	о	0	172	0	0	0	0	0	0	0	0	0	0	172
Building and energy Total	0	0	0	0	0	0	0	0	0	0	0	876	0	876
Total direct costs	6'117	1'399	1'058	671	473	218	178	854	211	326	145	1'297	45	12'990
Cost coverage	-117	108	-40	2'032	-473	-218	-178	-829	350	-326	-145	-1'219	527	-527
Overhead Total														7'082
CSCS														-1
Administration														1'489
Corporate communication														86
Building and energy														4'332
Technical services														670
Scientific support services														505
Total costs														20'072
- Budget-/3rd party funds transfers														-980
Total costs 2007														19'092

All figures are given in kCHF, deviations may occur, they are due to round ups/downs

Breakdown of costs per resarch field

Research field	Chemistry	Physics	Atmospheric Sciences	Material Sciences	Engineering	Biology	Grid	CSCS	Other	TOTAL
IT Depreciation Total	2'440	1'907	1'044	700	278	161	83	30	26	6'671
Technical services	2'440	1'907	734	700	278	161	0	30	26	6'278
User & appl. services	о	0	0	0	0	0	0	0	0	о
Data analysis services	о	0	0	0	0	0	0	0	0	о
Scient. support services	о	0	0	0	0	0	83	0	0	83
Software development services	о	0	0	0	0	0	0	0	0	о
MeteoSchweiz	о	0	310	0	0	0	0	0	0	310
Personnel Total	666	452	453	213	156	71	380	658	4	3'055
Technical services	416	325	125	119	47	28	0	5	4	1'071
User & appl. services	125	0	156	31	0	31	0	125	0	467
Data analysis services	125	113	13	63	94	13	0	81	0	501
Scient. support services	о	0	0	0	0	0	380	54	0	435
Software development services	о	15	160	0	15	0	0	393	0	582
MeteoSchweiz	о	0	0	0	0	0	0	0	0	о
IT expenses and mainte- nance Total	755	587	409	217	89	51	212	61	8	2'389
Technical services	746	583	224	214	85	49	0	9	8	1'918
User & appl. services	5	0	7	1	0	1	0	5	0	20
Data analysis services	4	4	0.5	2	3	0.5	0	3	0	17
Scient. support services	о	0	0	0	0	0	212	30	0	242
Software development services	о	0.5	6	0	0.5	0	0	14	0	20
MeteoSchweiz	0	0	172	0	0	0	0	0	0	172
Building and energy Total	0	0	0	0	0	0	876	0	0	876
Total direct costs	3'862	2'946	1'906	1'131	523	284	1'550	750	38	12'990
Overhead Total										7'082
CSCS										-1
Administration										1'489
Corporate communication										86
Building and energy										4'332
Technical services										670
Scientific support services										505
Total costs										20'072
- Budget-/Thrid party funds transfers										-980
Total costs 2007								-		19'092

All figures are given in kCHF, deviations may occur, they are due to round ups/downs

**Compute Infrastructure** 

J Type	No. of Processors	No. of Nodes	Inter- connect type	Interconnect bandwidth (MB/s)	Total memory size (GB)	Year of installation	Peak Performance (Tflop/s)	LINPACK Performance (Tflop/s)	TOP500 position Nov. 07	Millions of produced CPU hours	Average Utilisation (%)	Annual direct costs in 2006 (kCHF)
33	28	1664	Cray XT3	7600 (per router) 2'000'000 (total)	3'328	2005	17	0,014	84	20,96	86,21	4'761
7	68	48	Infiniband 4X DDR	1,000	1'650	2006	4.6		I	5,04	75,00	1'910
ö	96	448	Cray XT4	7600(per router)	896	2007	4.7		ı	1,80*	45,54*	1'178

# **Usage Statistics**

Usage by research fields

	Chemistry	Atmospheric Sciences	Material Sciences	Physics	Other	Internal
IBM P5	60.90%	0.76%	20.85%	9.83%	7.09%	0.56%
IBM P4*	67.85%	18.04%	7.36%	%0	5.7%	1.05%
Cray XT3 (PALU)	28.95%	15.08%	7.83%	40.06%	7.66%	0.43%
Cray XT3 (GELE)	47.60%	29.24%	0.00%	17.51%	5.1%	0.55%
Cray XT4*	16.92%	65.66%	12.42%	0.00%	2.14%	2.86%
NEC SX5*	0.00%	41.21%	0.97%	15.67%	40.68%	1.46%

# Usage by customer

	ETH Zürich	ISd	Meteo Schweiz	ETH Lausanne	Uni Zürich	EMPA	Others
IBM P5	64.48%	3.02%	0.00%	10.99%	7.69%	3.76%	10.06%
IBM P4*	56.28%	2.55%	0.00%	7.6%	0.40%	3.02%	30.15%
Cray XT3 (PALU)	58.06%	19.01%	6.04%	5.3%	3.91%	1.29%	6.39%
Cray XT3 (GELE)	49.14%	17.27%	14.23%	0.86%	2.87%	14.85%	0.78%
Cray XT4*	51.87	0.00%	43.90%	0.00%	0.00%	%00.0	4.32%
NEC SX5*	49.26%	0.00%	32.94%	15.06%	0.00%	1.28%	1.46%

IEC SX5: Time Perion from 1st January to 28th February 2007 BM P4: Time Period from 1st January to 19th May 2007 3ray XT4: Time period from 1st July to 31st December 2007

#### CPU Usage per Research Field in 2007



CPU Usage per Institution in 2007



#### Distribution of Costs per Institution 2004-2007



#### Distribution of Costs per Research Field 2004-2007



### PhysicsChemistry

Others

Engineering

Atmospheric Sciences

Material Sciences

OthersCSCS

Uni Bern

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#### CPU Usage per Institution 2004-2007











#### Chemistry



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

Lugano, den 19. Februar 2008/GZ/ZN

Sehr geehrte Damen und Herren

auftragsgemäss, haben wir das Financial Reporting (4. Quartal 2007/Jahresabschluss) des CSCS SWISS NATIONAL SUPERCOMPUTING CENTRE für das am 31. Dezember 2007 abgeschlossene Geschäftsjahr geprüft.

Für das Financial Reporting (4. Quartal 2007/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 2007/Jahresabschluss) mit angemessener Sicherheit erkannt werden. Wir prüften die Posten und Angaben des Financial Reporting (4. Quartal 2007/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 2007/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 2007/Jahresabschluss) zu genehmigen.

Mit vorzüglicher Hochachtung FI)D,IREVISA SA

G. Zwahlen Leitender Revisor

ppa. N. Zanetti

Beilagen:

- Financial Reporting (4. Quartal 2007/Jahresabschluss)

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#### Journal Impact Factor for Papers Listed in the 2006 Annual Report

Publication	Impact factor	Principal investigator	Application field
Martonak R., Donadio D., Oganov AR.&Parrinello M.; Crystal structure transformations in SiO2 from classical and ab initio metadynamics,NATURE MATERIALS5, 623-626 (2006)	19.194	M. Parrinello	Material Sciences
GervasioF.L.,Boero M.&Parrinello M.; Double proton coupled charge transfer in DNA, ANGEWANDTE CHEMIE-INTERNATIONAL EDITION 45 (34), 5606-5609 (2006)	10.232	M. Parrinello	Chemistry
Barducci A., Chelli R., Procacci P., Schettino V., Gervasio FL.&ParrinelloM.Metadynamics simulation of prion protein: beta-structure stability and the early stages of misfolding, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 128 (8) , 2705-2710 (2006)	7.696	M. Parrinello	Chemistry
Bussi G., GervasioF.L.,Laio A.&Parrinello M.; Free-energy landscape for beta hairpin folding from combined parallel tempering and metadynamics, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 128 (41), 13435-13441, (2006)	7.696	M. Parrinello	Chemistry
Diezi S., Ferri D., Vargas A., Mallat T. &Baiker A.; The origin of chemo- and enantioselectivity in the hydrogenation of diketones on platinum, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 128 (12), 4048-4057, (2006)	7.696	A. Baiker	Chemistry
Gautier C. &Burgi T.; Chiral N-isobutyryl-cysteine protected gold nanoparticles: Preparation, size selection, and optical activity in the UV-vis and infrared, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 128 (34),11079-11087 (2006	7.696	T. Bürgi	Chemistry
Markovic D., Varela-Alvarez A., Sordo J.A. & Vogel P.; Mechanism of the diphenyldisulfone-catalyzed isomerization of alkenes. Origin of the chemoselectivity: Experimental and quantum chemistry studies.JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 128 (24), 7782-7795 (2006)	7.696	P. Vogel	Chemistry
Mercier S.R.,Boyarkin OV., Kamariotis A., GuglielmiM.,Tavernelli I., Cascella M., Rothlisberger U. & Rizzo TR.; Microsolvation effects on the excited-state dynamics of protonatedtryptophan, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 128 (51), 16938-16943 ( 2006)	7.696	U. Röthlisberger	Chemistry
Park J.M.,Laio A., lannuzzi M.&Parrinello M.; Dissociation mechanism of acetic acid in water, JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 128 (35), 11318-11319 (2006)	7.696	M. Parrinello	Chemistry
Behler J.&Parrinello M.; Generalized neural-network representation of high- dimensional potential-energy surfaces, PHYSICAL REVIEW LETTERS 98 (14), 146401 (2007)	7.072	M. Parrinello	Chemistry
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Ghose S., Krisch M., OganovA.R.,Beraud A., Bossak A., Gulve R., Seelaboyina R., Yang H.&Saxena SK.; Lattice dynamics of MgO at high pressure: Theory and experiment, PHYSICAL REVIEW LETTERS 96 (3),035507 (2006)	7.072	A. Oganov	Chemistry
Giustino F.&PasquarelloA.MixedWannier-Bloch functions for electrons and phonons in periodic systems, PHYSICAL REVIEW LETTERS 96 (21), 216403 (2006)	7.072	A. Pasquarello	Physics
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Godet J.&Pasquarello A.; Proton diffusion mechanism in amorphous SiO2, PHYSICAL REVIEW LETTERS 97 (15), 155901 (2006)	7.072	A. Pasquarello	Physics
Greber T., Sljivancanin Z., Schillinger R., Wilder J. & Hammer B.; Chiral recognition of organic molecules by atomic kinks on surfaces, PHYSICAL REVIEW LETTERS96 (5), 056103 (2006)	7.072	Z. Sljivancanin	Physics
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Publication	Impact factor	Principal investigator	Application field
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Làuchli A., Mila F.&Penc K; Quadrupolar phases of the S = 1 bilinear- biquadraticheisenberg model on the triangular lattice , PHYSICAL REVIEW LETTERS 97, 087205 (2006)	7.072	A.M. Läuchli	Physics
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Source: ISI Web of Knowledge SM

#### Personnel

#### Average FTE per Unit for 2007



Staffing costs (total for 2007)



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#### Invited talks and seminars

Valle M; Chemistry Visualization Tools in an Integrated Discovery Cycle, Oct. 2007, EGEE 07, Budapest, Hungary.

Valle M; "Beyond Ball-and-Stick - Representation and Perception in Chemistry Visualisation", April 2007, University of Manchester, UK.

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