Annual Report 2009

CSCS
Swiss National Supercomputing Centre
Annual Report 2009
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The Challenging High Peaks of Monte Rosa

On September 18th, 2009 it was my great pleasure and honor to address a distinguished audience at CSCS on the occasion of the official inauguration of Monte Rosa, the new Swiss national Supercomputer at CSCS, together with the President of ETH Board, Fritz Schiesser and the President of ETH Zurich, Ralph Eichler.

Exactly one week later, ETH Zurich inaugurated another Monte Rosa, a high tech alpine lodge, at an altitude of 2'883m above sea level and surrounded by the highest peaks of the Swiss Alps. The analogy between both Monte Rosas, the supercomputer and the high tech lodge, is absolutely striking. Both are cutting edge technology, both deliver highest performance for lowest CO₂ emission and both are made to stimulate us to push the limits of our achievements to the extreme. With the Monte Rosa supercomputer, Switzerland made a leapfrog jump on the supercomputing scale and gained a top five position among the fastest supercomputers in Europe. With Monte Rosa, Switzerland joined what we call the Petascale Race.

Some people claim that the race towards petascale computing started at the beginning of this millennium when Japan surprised the world with the Earth Simulator, a machine so powerful that it matched the combined processing power of the 20 fastest US-based supercomputers at the time. The US was so alarmed that the supercomputing Guru Jack Dongarra dubbed the Earth Simulator “Computenik” comparing it with the Russian Sputnik that caused a lot of commotion in the US during the aerospace race.

Six months later, in order to keep its leadership in supercomputing, the US government granted IBM a DARPA contract of about $300 million to develop a machine that would be ten times faster than the Japanese “Computenik”. About two years later, the
US machine overtook the Earth Simulator’s number one position in the supercomputing Top500 list. In the fall of 2007, the world was again surprised by a newcomer: the Indian Tata installed a cluster with a Linpack performance of 118 TFlops, reaching the 4th place on the Top500 list. This was the first system from outside the US, Europe, or Japan to ever enter the top 5 list. Just one year later, a Chinese machine from the Shanghai Supercomputer Centre appeared amongst the top 10 of the world’s fastest supercomputers. In June 2009, Germany and Saudi Arabia were amongst the top 15 and Switzerland and France held the only other European systems ranked amongst the top 25. Although China was able to join the top 5 elite in November 2009, the Top500 list is still dominated by US-based machines with the Jaguar system at the Oak Ridge National Laboratory leading the list.

It is now the turn of Russia to compare the US achievements in supercomputing with Sputnik. In July 2009 Russian President, Dmitry Medvedev, urged a dramatic change in Russia’s use of high-performance computing and warned that without it Russian products would not remain competitive. Catching up will not be easy. Jaguar already delivers a Linpack performance of 1.75 Petaflops and the NCSA’s Blue Waters machine, expected to be ready by early 2011, will be capable of delivering a peak performance of about 10 Petaflops. And hardly one year later, the Lawrence Livermore National Laboratory will fire up Sequoia, an IBM Blue Gene machine, that will have 1.6 million Power-Processors and 1.6 Petabytes of main memory connected with switching optical communication technology leading to a peak performance of more than 20 Petaflops and thus poised for the number one position in the Top500 list.

So why the race towards Petascale computing? The US, Japan, Europe and even India, China and Russia have identified HPC as an innovation accelerator. Powerful supercomputers help reduce “time-to-insight” and “time-to-solution” for both discovery and invention. Therefore, the slogan of the US Council on Competitiveness is “Out-compete to Out-compete”. One possible way to show the competitive advantage offered by being on the Top500 list is to measure the time gap between supercomputers with equal performance on the list. A scientist who computes his models on No. 500, although still having access to a large supercomputer, actually lags 6 to 8 years behind the scientist who has the privilege to use the supercomputer leading the Top500 list. This timelag is 10 years greater if the scientist uses only a modern PC instead.

This is also why the DOE program INCITE, aiming at “driving America’s leadership in science and innovation, economic prosperity, energy security and global competitiveness”, is stimulating the development and support of large scale HPC applications. Approximately 1.3 billion supercomputer processor-hours will be awarded to academia and industry in 2010. An increase to 100 billion processor hours in 2014 and nearly 1 trillion processor-hours in 2020 is projected. INCITE is also providing American companies with access to unprecedented computing power and resources that will enable them to tackle some of the most challenging problems in basic sciences through advanced simulation and modelling, thus reducing time-to-market and shrinking prototyping costs.

With rising competition from the US, Japan, China and India, it is more important than ever for Europe to focus on innovation. With countries such as China producing more scientists and engineers every year than we have in all of Europe it is critical that we innovate twice as fast. Supernodes hosting Petascale computing, storage, networking resources and Petascale software applications will act as super-magnets attracting high tech multinationals, innovative companies and talented students.
and researchers. But it takes more than this alone to attract scientists and high tech companies. Advanced communication technologies, education, support for innovation, legal frameworks, government policy and vision, and also availability infrastructure and resources such as electrical power play important roles in establishing high tech super-nodes.

While the race to Petascale and even Exascale computing is accelerating, sustainability still poses a major threat. In fact, all three dimensions of sustainability: economic, social and environmental, must urgently be addressed in order to keep up with the high pace of technology developments and related investment costs. The number of large users in HPC is still small. There is a large group of potential users for whom the entry barrier is simply too high. Leveraging investments in HPC requires addressing this group of potential users.

Environmental sustainability is another challenge to be dealt with as power consumption becomes a major economic and environmental threat to reaching the next stage of supercomputing. If scaled up to Petascale and Exascale systems, current architectures, built on thousands of commodity processors of steadily increasing speed, would require megawatts of energy at the cost of millions of Euros which we simply cannot afford. In one of the most painful examples yet of the "headline risk" posed by the high energy use of supercomputers, the UK Meteorological centre in Devon was cited in July 2009 as one of the UK’s worst polluters. The combination of a relatively poor carbon profile and a mission to study climate change had captured the attention of the British press, prompting negative publicity in the UK media. The high energy consumption of supercomputers is not only an environmental problem but a cost issue as well. On average, a compute server has higher energy than depreciation costs today. Virtualisation, software parallelisation and optimising of applications will play a major role in improving sustainability.

Finally, the promise of Petascale computing to offer computational sciences the potential to achieve unprecedented levels of accuracy and fidelity in simulation and modelling will only be realised by applying an extreme degree of parallelism both at application and hardware levels. Physical limitations of miniaturisation, heat dissipation and power consumption have accelerated the trend towards the use of multicore processors, adoption of architectural diversity and implementation of tighter system integration instead of increasing clock speed. Improvement of performance of large-scale scientific applications on Petascale platforms is a complex task requiring a tight coordination between engineers, computer scientists and researchers in highly disparate areas. Extensive performance evaluations must be conducted in order to provide the supercomputer engineers, computational scientists and application developers with critical information about how algorithms and numerical methods perform across various platforms, how to configure the platform of choice and how to adapt the software to optimise scalability and performance. Coping with the trade-offs of tens to hundreds of thousands of processors and memory components and related computing paradigms will play a crucial role in the successful deployment of Petascale computing.

To summarise, HPC has been embraced as an accelerator for innovation and a key factor in maintaining competitiveness. Petascale simulations yield qualitatively superior insight and methods in multiple scientific, industrial, economic and social areas. Petascale helps shrink “time-to-discovery” and “time-to-invention”. Therefore we must “Out-compute to Out-compete”. The challenges of endeavors like Monte Rosa are to increase the number of industrial and scientific HPC users, to introduce HPC through supply chains and to eliminate barriers.
holding back HPC usage, as well as to improve the sustainability of the operation by increasing scalability and reducing power consumption. The so-called HP2C (High-Performance and High-Productivity Computing) project launched in 2009 by Professor Thomas Schulthess will enable CSCS to meet these challenges. With HP2C, CSCS will be able to support several high-impact scientific applications that scale and run efficiently on leadership sustainable computing platforms whilst establishing a network of domain sciences.

It is my great pleasure to congratulate the Director of CSCS, Professor Thomas Schulthess, for the successful launching of the HP2C project and the centre’s achievements under his leadership. Special congratulations also go to Professor Marco Baggiolini, Dominik Ulmer and Ladina Gilly for their persistence and dedication to CSCS and to all CSCS employees for their successful achievements in the last years despite the difficult times behind us. On behalf of the Advisory Board, I wish CSCS and ETH Zurich much success in the continuation of the implementation of The Swiss National Strategic Plan and in fulfilling their critical mission: to support high impact science and the knowledge economy in Switzerland.

Anwar Osseyran
Chair of CSCS Advisory Board
Interview
with Prof. Petros Koumoutsakos
by David Bradley, Science Base, UK

The research of Petros Koumoutsakos of ETH Zurich involves modelling, simulation and optimisation of problems in engineering and the life sciences. His approach has an emphasis on an integrated development of methods, software/hardware and applications. His projects use multiscale modelling and simulation, high performance computing, and uncertainty quantification to address problems in medicine, aerospace, and energy.

What specific projects are you currently involved in?

We are developing particle methods for the simulations of physical systems exhibiting multiple spatial and temporal scales. Specific projects include: Quantitative modelling of tumour-induced angiogenesis (blood vessel growth), the propulsion mechanisms of individual swimming organisms and swarms, rapid destruction of aircraft wakes, and energy-aware high-performance computing.

What do such studies reveal about the world around us and natural phenomena?

We learn about fundamental natural processes and we develop a quantitative language to describe the world around us and our way of interacting with it.

What practical applications does this work have?

Better understanding of physical processes leads to better designs and better diagnosis. For example, our work on tumour angiogenesis is being used to examine the effects of different therapeutic drugs on tumour vasculature while the work on swimming is being used in designing more effective swimming robotic devices. One new technological project we are particularly excited about is the use of heat from supercomputers for cooling/heating of buildings.

How do you mesh observational data with computational work done at CSCS?

Observational data are essential to validate computational models and they can be incorporated in the modelling using data assimilation and uncertainty quantification techniques.

How important is it to be able to use CSCS resources in this work?

It is absolutely critical to have access to the CSCS resources. We need computing resources of CSCS as much as a surgeon needs a scalpel or a carpenter needs a saw.

How do you ensure that your simulations match experimental results?

By performing extensive validation tests using the available experimental data. Furthermore, it is important to collaborate with experimentalists who are willing to conduct experiments guided by the results of
the simulations. This is not a trivial task and an added degree of complexity emerges when we have to match experiments and simulations to real world data.

**What is meant by multiphysics?**

The majority of physical systems and engineering devices involve various processes and physical phenomena that have been traditionally studied within different disciplines. Today, thanks mainly to advances in computing, there is a trend to study systems and devices taking more and more into account all the interacting phenomena. In turn, multiphysics problems imply the development and cross-fertilisation of computational tools that can be useful across disciplines.

**What can you tell us about reverse engineering swimming devices?**

Reverse engineering is the process in which you specify an objective function and then you modify the parameters of the model problem accordingly so as to minimise this objective. In swimming, optimising body shapes for energy efficiency or for speed may lead to different types of swimming forms. In a sense shape optimisation is another way of implementing the well-known statement that “form follows function”.

**What is a nanosyringe?**

This is a nanoscale device that can be used to transport materials with molecular level accuracy across a cell membrane. Simulations provide us with a way to examine different scenarios of such devices as it may be difficult to observe them in action experimentally.

**How might your research help in developing new cancer therapies?**

Our tumour research involves imaging and simulation components. Our imaging work is actually presently used to quantify the effects of various treatments on the morphology of the tumour vasculature. Our work on modelling and simulations is at a very primitive state but our hope is to provide tools that can be used for perturbation studies of the various factors that enter the process of tumour development.

**What are multiscale particle methods used for?**

Particles are computational elements used to represent the evolution of various physical systems. The particle properties (e.g. locations) evolve according to interaction rules that model different systems (e.g. the interaction between charged molecules in chemistry, or agents in traffic modelling) or approximate differential operators that describe physical laws such as the conservation of mass and momentum.

Particle methods have unique multiscale characteristics as they can model physical phenomena ranging from atomistic scales (as in Molecular Dynamics), to scales pertinent to flows past aircrafts (as in Vortex Particle Methods) and even to scales pertinent for astrophysics (as in Smoothed Particle Hydrodynamics). I am not aware of any other computational framework that has such capabilities. These characteristics can be exploited in developing particle methods that use efficiently modern HPC architectures. Particle methods provide an effective framework and a common language that can facilitate multiscale and multiphysics simulations.
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 2009 projects on page 18.

**Nanovectors for Drug Delivery in Oncology: a Combined Modelling/Experimental Study**  
Prof. Andrea Danani, SUPSI, Lugano, Switzerland

A computational study of branching, tree-like polymer molecules could help researchers develop new carriers for small sections of genetic information, known as oligonucleotides, in gene therapy for inherited illnesses, such as cystic fibrosis and Huntingdon's disorder, as well as for killing cancer cells.

Andrea Danani of SUPSI in Switzerland explains how gene therapy has gained significant attention over the past two decades as a potential method for treating genetic disorders. It also offers an alternative method to traditional chemotherapy in the fight against cancer. He points out that research efforts are currently focused on designing effective carriers, so-called vectors, which can deliver therapeutic oligonucleotides direct to the cell nucleus.

The oligonucleotides are active genetic agents that are incorporated into the patient's DNA and carry out the function of the errant gene in their cells. Ultimately, this would allow the patient's cells to make the proteins that are missing from their cells or are dysfunctional in some way.

Until recently, crippled viruses that could "infect" cells with an active gene were the main focus of vector research. However, controlling such biological vectors is not without problems, so several research groups around the world have turned to the possibility of using nanotechnology to build vectors for oligonucleotides.

One group of nano materials that could be used to transport gene therapy agents into cancer cells, for instance, are the poly(amido amine) (PAMAM) dendrimers. These are polymer type materials that instead of forming chains like conventional polymers are constructed with a central point from which the monomer building blocks branch out. The structure of a PAMAM dendrimer provides space between its branches and on its surface that can be loaded with other smaller molecules, including oligonucleotides.

PAMAM dendrimers are relatively easy to synthesise and are commercially available. This has made them the most studied dendrimer-based vectors for gene therapy.

Danani and his colleagues have now published two research papers that discuss computational results on the structures and optimisation of PAMAM dendrimer functionality and the molecules' interaction with different oligonucleotides.

The team's major findings concern simulation at the atomic level of 1st generation (G1) to sixth generation (G6) PAMAM dendrimers. Generations G1 to G6 have increasing degrees of polymer branching. These PAMAM dendrimers were dissolved in real solvents at different acidity and alkaline, or pH, conditions and were loaded with a test oligonucleotide, an siRNA.

This research has lead to the validation of the in silico models used for the simulations. It has also allowed the team to derive the free energy, or strength, of binding between G4-G6 PAMAM and siRNAs at the two physiological pH values relevant to delivery and intracellular trafficking. The team has also studied related PAMAM-like dendrimers with different cores to explore whether making the car-
Carrier molecules more flexible might improve how well they can bind to the gene therapy agent.

There are still many problems yet to be overcome concerning PAMAM dendrimers before this approach to gene therapy can be tested in clinical trials. Perhaps the most significant is that PAMAMs could have serious toxic side-effects. With this in mind, Danani and colleagues have also looked at alternative, but related, compounds known as functionalised dendrons. These compounds can have biologically compatible molecules such as spermine added, which may ultimately reduce their toxicity without affecting their carrier ability.

As such, the team has simulated the binding between such dendrons and a test gene therapy agent, ds-DNA, in presence of different salt concentrations. They found that for smaller dendron generations, DNA binding is adversely affected by increasing levels of salt at the concentrations found in the body. However, for higher generations a compensation process takes place.

The team also found that some of the spermine molecules can sacrifice themselves and so screen the target DNA from the potentially harmful effects of the carrier dendron. This concept of ligand sacrifice and binding site screening represents a new paradigm that could one day allow nanovectors to operate therapeutically without toxic side-effects.

Other work presently in progress concerns the study of different kind of dendrimers as well as dendrons, with various architecture and functionalisation, together with their interactions with nucleic acids and the organic system in general, proteins, membranes, etc.

Molecular model of first generation (G1) spermine dendron in complex with DNA (represented as orange and blue ribbons). The solute is immersed in a periodic water box (water molecules in cyan) in the presence of 150 millimolar sodium chloride solution. Sodium ions are represented as purple spheres and chloride ions as green.
**Supernova Models and the Prediction of Observables from Different Explosion**
Prof. Matthias Liebendoerfer, University of Basel, Switzerland

**The Multi-Dimensional Supernova**

Super computers at CSCS allowed Matthias Liebendoerfer and colleagues at the University of Basel to simulate in multiple dimensions the core-collapse of a supernova explosion at the end of the life of a massive star. This work provides new insights into distant cosmic phenomena and may also give scientists access to an understanding of exotic physics.

"The theoretical understanding of the mechanism of stellar explosions (supernovae) is crucial for the understanding of the stellar lifecycle," explains Liebendoerfer. Supernovae emit a broad spectrum of electromagnetic waves, neutrinos, cosmic rays and gravitational waves. As such, they can be observed using different astronomical instruments, including light and radio telescopes and increasingly sensitive neutrino detectors. A quantitative understanding of the supernova explosion mechanism, including its emissions and heavy element formation, may allow astronomers to observe matter under extreme conditions where novel physics might arise.

Historical supernovae have been observed by human eyes for centuries, if not millennia. Their sudden rare appearance in the sky was unexplained to our ancestors and was often considered to represent a mystical omen. With a good telescope and a systematic approach, however, astronomers can...
detect supernovae at (very) far distances every night. Modern astronomers know supernovae to be "simply" exploding stars, although that description belies a complexity that numerous research teams have uncovered in recent years. Liebendoerfer and his colleagues, Stuart Whitehouse, Simon Scheidegger and Roger Kaeppeli, are continuing the tradition of revealing the inner secrets of supernovae.

Until recently, calculations of the evolution and explosion of stars based on growing amounts of data had to rely on modelling with spherical symmetry. "It is not yet fully explained in detail by which mechanisms these explosions occur," explains Liebendoerfer, "Our models take part in the quest for the explanation of these stellar explosions by attempting to model these events on the computer in three dimensions." Increasing computing power and instrument sensitivity has facilitated the fully three-dimensional calculations that take into account fluid instabilities, magnetic fields and rotation of a stellar object are now producing much more realistic simulations of supernovae.

Liebendoerfer and colleagues, for instance, have carried out the largest 3D parameter study concerning the prediction of gravitational waves from supernovae with models that include microscopic input physics. They have also obtained the first results from 3D models that include the neutrino emission after core-bounce in the dynamical model of supernova evolution.

The work will provide new insights into stellar evolution. "One knows that many heavy elements are produced and ejected during a supernova explosion," adds Liebendoerfer. "During Galactic Evolution, new stars are formed from this polluted interstellar matter and the heavy elements accumulate to the presently seen abundance distributions. Hence, the research on supernovae attempts to explain the element abundances in the solar system and on Earth by understanding their astrophysical origin."

The same work, given adequately detailed observations for a supernova occurring in our Galaxy, can also allow the scientists to "constrain" the input physics and thus uncover fundamental phenomena. "The matter in supernovae is extremely dense and hot," says Liebendoerfer. Therefore, physics that normally cannot occur at the low-energy scales found on Earth can be observed and studied under the constraints of a supernova’s much more energetic environment. "The study and observation of very energetic astrophysical processes is a complementary approach to the expensive construction of large particle accelerators," he adds.

By focusing on neutrino emission, gravitational wave signals, and the formation of heavy elements, nucleosynthesis, the researchers hope to see through the outer layers of the explosion to the core of the supernovae and so learn something of the internal conditions close to the heart of the explosion.

Looking to the future, Liebendoerfer points out that supernova studies have always been at the cutting edge of available supercomputer performance. "They serve as a suitable platform and challenge to develop the numerical tools that will be required to later model even more challenging astrophysical scenarios, like the merger of neutron stars and black holes, or the accretion of matter on to rotating compact objects," he says.
**Computational Nanoscience at Surface and Interfaces**
Dr. Daniele Passerone, EMPA Dübendorf, Switzerland

**Surface Simulations**

Daniele Passerone, Carlo Pignedoli, and Empa Dübendorf are used to working on a very small length scale - billionths of a metre in fact. Their computational science group is embedded in a well-established nanoscience laboratory carrying out research as diverse as metallic alloys, surface chemistry, and self-assembly process in which designer molecules piece themselves together to make complex functional structures.

As such, understanding the details of the processes involved in the self-assembling could allow scientists to rationally design novel tailored functional devices. The team is using the most advanced computer code, based on density functional theory (DFT), to build correct models of chemical systems containing a large number of atoms.

The team has recently used CSCS resources in connection with three particular experimental projects: the bottom-up engineering of surface-supported graphene based nanostructures, hydrogen-bonded molecular networks for making surface-supported organic devices, and stepped gold surfaces that could act as templates for nanostructure applications.

In the first project, the team focused on graphene. This novel material resembles a flattened out sheet of chicken-wire fencing, with a carbon atom at the corner of each hexagon in the mesh; essentially, it is a layer of graphite just a single carbon atom thick. Graphene has attracted attention because of its unique electronic, magnetic and optical properties, which might be exploited in future opto-electronics devices and computing.

Unfortunately, there is currently no easy way to handle the large-scale processing of individual sheets of graphene and the objects, nanoribbons or nanographenes, that can be made from them. The researchers have suggested that a convenient on-surface synthesis route would be a powerful alternative for making nanographene structures. They have now discovered and explained some surface-assisted chemical reactions on single crystal metal, copper, silver, or gold, surfaces that might be used to make such graphene structures.

They conducted an extensive study of the steps making up the reaction pathway using classical and DFT simulations. The classical simulations were run locally on a Linux computer cluster. The Cray systems at CSCS were used to model, within DFT, systems with more than 500 atoms. The simulations allowed the team to describe a reaction pathway that fits the experimental results as well as calculating the barriers for its activation. Critically, catalytic pathways seem to be concurrent with non-catalytic routes, the team says, while dispersive, van der Waals interactions, are crucial to enhancing the reaction's efficiency.

In the second project, the team has investigated hydrogen-bonded molecular networks that can be constructed on a surface with a view to using organic semiconductor materials to make future nanoelectronic devices. Organic materials are easy to handle and their electronic properties can be fine-tuned for particular applications by simply adding or removing specific chemical groups from the molecular skeleton; something that is not possible with conventional semiconductors like silicon.

The team explains that thin organic films are already used in solar cells and photosensors and as organic light emitting diodes (OLEDs). In future devices, technology will exploit the functionality of clusters of molecules or even single molecules. The study on hydrogen bonding shows how arrays of organic
molecules can be controlled on a surface, which bodes well for the development of such organic devices.

Specific work with 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) coadsorbed with amine functionalised molecules 4,4’-diamino-p-terphenyl (DATP) and 2,4,6-tris(4-aminophenyl)-1,3,5-triazine (TAPT) was characterised with scanning tunnelling microscopy (STM) and demonstrated that it is possible to create ordered arrays of the organic semiconductor nanostructures. Such systems might be useful as 2D quantum dots. The team then used computational work, including DFT, to shed light on the subtle energetic balance driving the formation of the arrays.

In the third project, the team carried out DFT simulations of the surface of gold using the code cp2k with models as big as 1700 atoms. They ran the simulations on 2048 Cray cores and describe them as among the most extensive ab initio calculations they have performed for revealing details about how gold surfaces behave at the atomic level and how they might be used in the kinds of research defined by the other two projects.
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<td>Metadynamics Study of Large-Scale pH-Induced Conformational Changes in Dengue Virus Envelope Protein</td>
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<td>Meuwly, Markus</td>
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<td>Extreme Scalability in µFEA of Human Bone Structures</td>
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<td>Three-Dimensional Direct Numerical Simulations of Spherical Expanding Flames</td>
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Activity Report
The overarching goal of the Swiss High-Performance and High-Productivity (HP2C) platform is to create simulation codes that make effective use of future supercomputing systems. The specific ambition of HP2C is to create several application teams to develop and run codes at scale on the generation of supercomputers to be procured in Switzerland in the 2012-15 timeframe, including the large petascale systems funded by the national strategy for High Performance Computing and Networking (HPCN). Hence, the HP2C platform is seeding the user network of HPCN and is thus a central element of the national strategy approved by Swiss Parliament on December 16, 2009.

Organisationally, the HP2C platform builds on the experience of interdisciplinary teams that developed early applications for the leadership computing facility at Oak Ridge National Laboratory, in particular the two teams of the Nanomaterials Theory Institute that delivered the first applications capable of sustaining petaflop/s performance under production conditions on general-purpose supercomputers. With the HP2C platform, application teams at Swiss universities, which typically are already established in method and code development, will receive support for HPC developers in order to engage in significant algorithmic and software refactoring efforts over the coming three years. These development activities will be linked to and supported by a core group of scientific computing researchers at CSCS and the University of Lugano (USI). Furthermore, the core team in Lugano will develop and operate prototype platforms in collaboration with the supercomputing industry.

Seventeen application teams responded to an open call for proposals last summer and were submitted to a rigorous external peer review in the fall of 2009. Eight projects were selected to receive funding for three years in January 2010 – four proposals are still under considerations. The topical areas of these projects range from Astrophysics and Cosmology to Plasma Physics, Chemistry, Materials Science, and Life Sciences, as well as earth system and biomedical modelling. An updated list of supported projects as well as further information pertaining to the program can be found at www.hp2c.ch.

New Organisation of CSCS

2009 was the year in which the implementation of the Swiss national HPCN strategy began. The setting up of the Cray XT5 “Monte Rosa” was the initial step in a series of supercomputer installations leading to petascale systems in 2012. The call for proposals for HP2C projects marks the beginning of a new quality of collaboration between the supercomputer centre and the research groups at the Swiss universities and research institutions, developing scientific applications for the aforementioned systems. Finally, the decision of ETH Zurich to re-house its institutional compute clusters in the new CSCS building from 2012 expanded the mandate of the centre to transfer its know-how of selecting, operating, and optimising very large computer systems beyond individual cases like MeteoSwiss or CHIPP.

New projects and new activities require an organisation to adapt its structure in order to maximise effectiveness and efficiency. The classical structure of...
a supercomputer centre is based on groups of different expertise working tightly together on delivering a single service. Typical components of such a structure are groups of system administrators and engineers, user support specialists, application analysts, and data management and visualisation experts. This successful organisational model was transferred to the new expanded mandate of the centre by organising CSCS along business areas. Each business area would be covered by a single section that comprises the full knowledge stack, from installing and operating the machine to supporting the customer in the use of applications for scientific simulations. Cross-organisational mechanisms fostering the exchange of knowledge and experience between the business areas ensure that these vertically integrated sections do not develop into segregated silos.

The leadership team of CSCS identified the following business areas:

- **Scientific Computing Research**: engaging with the scientists at the universities to develop new simulation applications and new supercomputer system architectures
- **National Supercomputing Service**: delivering the service for the national supercomputer
- **HPC Co-Location Service**: offering the know-how and the expertise of the National Supercomputing Service for large institutional computer systems of individual customers

These three business areas are supported by a fourth division called Business Services, integrating vital components for the centre such as facility services, local IT services, and administrative support services.

At the strategic level the leadership team, consisting of the director of CSCS, the general manager, as well as the associate directors responsible for the different business areas, leads the centre. The Scientific Computing Research division is led by the Director himself, whereas the three service units report to the General Manager.

The collaboration between CSCS and MeteoSwiss show-cases the cross-fertilisation mechanisms between the business areas: The current operational MeteoSwiss service is delivered by the HPC Co-
Location Services section, focusing on service reliability and efficiency. However, MeteoSwiss regularly improves its forecasting service by introducing a new forecasting suite every 5 to 8 years. The new forecasting suite improves aspects such as resolution of the model and representation of processes in the atmosphere. Such improvements can only be obtained by working on the code of the simulation application, i.e. by starting a collaboration project with the Scientific Computing Research division. Once the new code has been developed, the new suite, i.e. the new model data and the corresponding system programming, has to be developed and tested at scale with the help of the National Supercomputing Service. After an extensive testing and consolidation period, a new production hardware platform is selected in collaboration with the HPC Co-Location Service, which then takes responsibility for the operation of the new suite.

**HPC Co-Location Services**

HPC Co-Location Services (HCS) operate dedicated systems for individual customer institutions and provide tailored HPC services for these systems. HCS has contractual links with a number of institutions for these services, the most important ones being the Swiss Federal Office for Meteorology and Climatology MeteoSwiss and the Swiss Institute for Particle Physics CHIPP. During 2009 HCS has been involved in the following main activities:

**Internal Set-Up and Organisation**

During the second part of 2009, a major effort has been devoted to organise the new HPC Co-Location Services unit with a focus on service orientation and the ability to expand the service. HCS is internally organised in three groups. The Service Management group is responsible for the key account management to the external clients and in charge for the development of new services and the life cycle management. The Service Desk group is the single point of contact for the external users and provides direct support. Finally, the IT Operations group manages the computing infrastructure and manages the system architecture and its deployment.
MeteoSwiss

HCS was able to operate the services for MeteoSwiss according to the specified SLA and to migrate from a shared infrastructure with the national HPC services to a dedicated one. In this frame the existing Cray XT4 called “Buin” has been upgraded from dual core to quad core processors, thus doubling the computing power, and then was split into two separate systems called Buin and Dôle. Buin will be used as the main production system and Dôle as the fail-over system, as well as a R&D system for the development and tuning of the new versions of the National weather forecast suite.

CHIPP

HCS is operating a Sun cluster for CHIPP, called “Phoenix”, as tier 2 for the LHC experiment at CERN. During 2009 the agreed SLA has been met. By 2010 Phoenix will be a three year old system making a replacement and upgrade necessary. During the second part of 2009 the replacement process was begun so that the new system can be installed at the beginning of 2010.

CSCS New Building

As part of the national HPCN Strategy, it was foreseen that CSCS should have a new building capable of hosting supercomputers of the Petaflop class and beyond by 2012. Planning for this building thus started in early 2008.

Requirements

The rapidly increasing electricity costs, the ever-changing demands of new computers on building infrastructure and environmental concerns were driving motivations behind the planning of the new building. The plan that will be submitted for construction in 2010 thus concentrates on providing a functional structure that allows for the flexible attribution, adaptation and extension of spaces. The technical infrastructure allows for maximum flexibility in terms of power, cooling technology and floor space. The compute centre must achieve a PUE of no more than 1.25.

Lake water cooling

The land made available by the city of Lugano lies just 2.8km from the shore of lake Lugano and is therefore optimally situated to make use of this re-
source for free cooling. A piping circuit will pump lake water at 6°C from 40m under the surface of the lake to the new CSCS. This system will provide for up to 14MW of cooling capacity. Waste heat from the compute centre will be made available free of charge at a number of locations for use in urban heating networks or the heating of public infrastructures such as the local university or swimming pools.

**Further extension options**

In the event that the centre should require more than 14MW of cooling capacity, the facility has been planned to accommodate a subsequent installation of cooling machines and cooling towers. In the same way, a later installation of dynamic UPS or even diesel generators has been foreseen should the quality of electrical power supply degrade. Research projects by some of the computer vendors into “high-temperature” cooling have lead us to plan the space for a high temperature cooling loop to be added later.

**Work space**

The new office building provides working space for up to 55 employees. This glass-fronted building will be realised along the guidelines of the Minergie ECO label for sustainable constructions. The land around the building will be transformed into attractive recreational space.

**Funding**

The new building is funded by 4 different entities:

- ETH Zurich 29.97 mCHF
- Swiss Confederation 28.93 mCHF
- Canton Ticino 5.00 mCHF
- City of Lugano  Land lease of 50 years

**Timeline**

- Competition and selection of the construction team: 1st quarter 2010
- Site preparation, including demolition of a previous building: 1st quarter 2010
- Completion: 3rd - 4th quarter 2011
- Start of operation: 4th quarter 2011

**National Supercomputing Service**

The reorganisation of CSCS led to an amalgamation of the groups responsible for application support, system management and user interaction with the academic research community under the new title of the National Supercomputing Service. The members of the unit engaged in a number of activities with research groups in order to improve their ability to make best use of CSCS facilities, and also provided improvements to the user documentation and training portfolio. However, the activities of the national supercomputing services group during 2009 were dominated by the arrival of the Cray XT5 system called Monte Rosa.

At the beginning of the year, the two academic production science systems had a combined set of resources for computation that consisted of approximately 4,000 compute cores with 5 Terabytes of main memory which together had a theoretical peak performance of 22 Teraflop/s. During the year the facilities were consolidated into one HPC system, a Cray XT5 which was initially a 14,000 processor system when first installed during the summer, but...
which was later upgraded to a 22'000 processor machine. Reaching 21st place in the November 2009 edition of the top500 list of most powerful supercomputers in the world, Monte Rosa was the 4th most powerful machine in Europe.

To support the more powerful machine, further enhancements were made to the storage infrastructure on offer, with enhanced scratch space and I/O bandwidth on the new XT5, and a growth of the site-wide parallel file system.

At the end of 2009, both the Cray XT3 Palu and the IBM p5-575 Blanc were retired from service, with the XT5 Monte Rosa being the single HPC machine on offer for production science projects.

The introduction of the new Cray XT5 not only involved a change to the underlying hardware, but also an operating system migration to the Cray Linux Environment, and associated with this was the provision of a richer programming environment featuring a wider set of tools and compilers. Whilst the installation of the XT5 machine was technically an upgrade from the previous XT3, the combination of changes to hardware, system software and programming environment meant that the porting effort was equivalent to installing a completely new machine.

In order to smooth the transition for the CSCS user community, a very small test and development system was created with the temporary name of (mini) Rosa. The success of the porting effort and migration assistance that could be offered on the small test machine, together with the willingness of the CSCS user community to test their applications on this facility, meant that it took only a few hours from the announcement that the full 20 cabinet Cray XT5 Monte Rosa was open to researchers for the machine to be filled to 75% of its capacity.

As a further demonstration of the success of the CSCS porting effort and the preparations for the new machine carried out by the CSCS user community, it should be noted that in the first three months after the Cray XT5 had completed its acceptance procedure, one third of the work on the system required more processors than had been available on the previous Cray XT3 machine, a figure that rose to over 40% during the last three months of 2009.

The large extra capacity provided by Monte Rosa offered CSCS the opportunity to make a special call for large-scale simulations that had not been possible on HPC facilities available in Switzerland before the introduction of the Cray XT5. This special call for proposals was targeted at problems requiring a large amount of compute power for a short period of time and resulted in projects in earthquake modelling, turbulent flows, combustion, materials science and astrophysics.

The upgrade of our main production system and the associated changes to the operating and programming environments gave us the ideal opportunity to simplify the user documentation, and further measures taken in order to smooth the transition for the user community were the hosting of a PRACE code porting workshop and an introduction to Rosa course, both delivered by Cray personnel.

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<thead>
<tr>
<th>System</th>
<th>Palu</th>
<th>Blanc</th>
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<th>Rosa</th>
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<td>22128</td>
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<td>1.8</td>
<td>5.1</td>
<td>29.5</td>
<td>5.8 X</td>
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<td>Peak Tflop/s</td>
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<td>4.5</td>
<td>21.8</td>
<td>212</td>
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Outreach

January 2009
A warm and grateful Farewell Party is held at CSCS on January 9 to honor the departing director Marco Baggiolini. He had led CSCS for two challenging years.

February 2009
CSCS initiates plans for a new home base. The current building has reached its maximum capacity in terms of power and machine cooling. Plans for a new building have thus gained top priority in CSCS’ future strategy and are an equally important matter for the city of Lugano, the Canton Ticino and the Swiss Confederation.

March 2009
Mario Valle, CSCS Visualisation and Data Analysis scientist, is co-author of a NATURE paper reporting about a special form of sodium.

The annual User Assembly is held on March 20 at the Kultur- und Kongresszentrum (KKL) in Lucerne. CSCS illustrated ongoing activities, its strategy and other important news to the user community.

The final decision about CSCS new home base is taken. The new building will be located in Cornaredo, Lugano.

April 2009
Pascal Couchepin, then member of the Swiss Federal Council and head of the Federal Department of Home Affairs, pays a brief visit to CSCS on April 2nd. This visit is a welcome opportunity for CSCS to illustrate to federal government its strategic plans within the HPCN initiative, and, in particular, pending supercomputer upgrades and details about the new building.

HP2C, the Swiss Platform for High-Performance and High-Productivity Computing, takes off following approval of funding from the Swiss Confederation.

May 2009
ROSA, the new Cray XT5 named after “Monte Rosa”, at 141.6 teraflops the most powerful supercomputer in Switzerland, goes into service. The installation is completed successfully on May 25, less than three months after the decision was taken to upgrade the then current facilities.

Swiss Government approves funding of the HPCN (High-Performance Computing and Networking) initiative on May 29. CSCS is designated to lead the initiative.

June 2009
The new Cray XT5 leverages CSCS’ position among the leading supercomputer centres in the world. On June 23, CSCS is reported to rank 23rd in the world and 4th in Europe, as communicated in the TOP500 list on the International Supercomputing Conference in Hamburg.

July 2009
Rosa fully passes acceptance on July 1 and becomes CSCS’ major production system.

CSCS organises an introductory course on July 2-3, to make the user community familiar with the characteristics of the new Cray XT5.

CSCS and Cray organise a code porting workshop on July 13-15. Luiz DeRose and John Levesque introduce into the peculiarities of the new Cray XT architecture.
CSCS helps to organise the CECAM symposium “Structural Transitions in Solids: Theory, Simulations, Experiments and Visualisation Techniques” which is held July 8-11 at Università della Svizzera Italiana (USI), Lugano. The symposium presents the state of the art in theory and experiment. It fosters dialog between scientists, thus seeding novel ideas for future investigation.

CSCS airs live on radio on July 30. The event is part of the program “VisionSchweiz. Vision Suisse. Visione Svizzera. Visun Svizra”, dedicated to the future of the country and broadcast by all four national radio stations. Michele De Lorenzi presents CSCS and its road to the future to an Italian speaking audience on RETE UNO, Dominik Ulmer to a German speaking audience on DRS1, and Ladina Gilly to a Rumantsch speaking audience on Radio Rumantsch.

**August 2009**

CSCS holds the annual “Parallel Programming” workshop on August 11-13.

On August 20, CSCS receives a delegation of the Swiss National Assembly, headed by then President Chiara Simoneschi-Cortesi. Following a brief oral presentation, CSCS offers a tour of the centre and shows its machine room. The president was very pleased to show to her colleagues the crowning achievement of her home canton.

On August 26, CSCS hosts the annual reunion of the Arma Swiss. Vice president of ETH Zurich Roman Boutellier led the commission.

CSCS adds a fourth cooling system on August 26 to accommodate the earlier upgrade of computer resources.

**September 2009**

CSCS organises the First European Workshop on HPC infrastructure, held at the Origlio Country Club from September 2-4. Prime focus is on the increasing demands of modern supercomputer architecture in terms of electrical and cooling power, and custom-fit building design.
On September 11, CSCS organises its annual User Day, which is again held at the Radisson Hotel in Lucerne. This event fosters contacts between CSCS staff and users, and provides a forum to inform about research projects and about computational needs. Keynote speaker Jeff Hammonds (Argonne) speaks about "New frontiers in quantum chemistry using supercomputers".

ROSA, the new Cray XT5 supercomputer, is inaugurated on September 18 by Fritz Schiesser, President of the ETH Board, and Ralph Eichler, President of ETH Zurich. ETH professor Marcella Carollo delivers a spectacular keynote speech on experimental and computational research in astronomy, and a festive aperitif rounds off this very special day.

Some 250 people visit CSCS the next day. The open day "A date with the cervellone" attracts visitors with guided tours of the computer and infrastructure rooms, "scientific experiments" in the kids corner and a quiz competition.

**October 2009**

CSCS participates in the CECAM workshop "Algorithmic Re-Engineering for Modern Non-Conventional Processing Units", organised by Alessandro Curioni and Teodoro Laino of IBM Rueschlikon, and held from September 30 to October 2 at USI Lugano. Central theme is the enormous gain in performance of current and future massively parallel supercomputer architectures, which require substantial algorithmic engineering to tap their full potential in production applications.

CSCS organises the LinkSCEEM workshop held in beautiful Cyprus from October 6 - 8. The linking "Scientific Computing in Europe and the Eastern Mediterranean" initiative wants to create an open forum where users and providers of HPC alike can meet and exchange their views and ideas.

**November 2009**

Following ROSA’s upgrade from quad- to hexacore processors, CSCS moves up two ranks (now 21) in...
the TOP500 list of supercomputers, published during
the annual ISC conference in Portland, Oregon (USA).
On November 24, also at the ISC conference,
CSCS director Thomas Schulthess is awarded the
Gordon-Bell Prize for the second time in a row. The
award recognises a simulation run at a speed of
1.84 petaflops, which is used to analyze magnetic
systems and, in particular, temperature effects on
magnets.

The Swiss HPC Service Provider "Community"
opens its web portal on November 25 (www.hpc-
ch.org). The goal of hpc-ch is to create a platform
for exchange of knowledge between HPC system
providers and Swiss universities.

CSCS becomes one of the founding members of
the new Hybrid Multicore Consortium, the others
being Oak Ridge National Lab, Berkeley National
Lab, Los Alamos National Lab and Georgia Tech
University. The consortium explores hybrid multicore
architectures as a significant, yet unrealised, prom-
ise for delivering high-end production computing
capabilities for the most demanding applications in
science.

Buin and La Dôle are the two new supercomputers
dedicated to MeteoSwiss. They are based on the
earlier Cray XT4 platform of Buin, which has been
upgraded from dual- to quad-cores and split into
two distinct and redundant supercomputers. The
name La Dôle refers - in the tradition of CSCS - to a
Swiss mountain, located in the Vaudoise Jura.
Coincidentally, one of the three Swiss meteorologi-
cal radars is actually located on that mountain (the
other two being on Albris near Zurich and Lema near
Lugano).

December 2009

Cray launches the European Exascale Research initi-
ative on December 2, naming CSCS one of two ini-
tial partners. This initiative aims at exploring new
ideas and technologies necessary to achieve sus-
tained exaflop performance, i.e. one quintillion
mathematical operations per second.

On December 10 the canton of Ticino decides to
subsidise the construction of the new CSCS build-
ing in Cornaredo, Lugano, with 5 million Swiss
Francs.

The Swiss Federal Parliament passes funding for
the new CSCS building definitively on December 16.
The great news has been communicated personally
by Fritz Schiesser, President of ETH Board. The
construction is now expected to begin in February
2010.

On December 20, the Swiss Platform for High-
Performance and High-Productivity Computing,
HP2C, chooses the first eight scientific projects to
develop highly scalable applications for the next
generation of supercomputers available from 2013.
Facts & Figures

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<td><strong>Investments</strong></td>
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<td><strong>Material/Goods/Services</strong></td>
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<td>Economic stabilisation measures 10'000'000.00</td>
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<td><strong>Personnel</strong></td>
<td><strong>Third-party contributions projects</strong></td>
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<td>6'284'972.98</td>
<td>1'400'976.66</td>
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<td>Payroll</td>
<td>European projects 581'838.81</td>
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<tr>
<td>4'753'785.70</td>
<td>Other projects (Ticino in Rete /</td>
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<td>HP2C 500'000.00</td>
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<td>Other (education, travel etc.)</td>
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<td>2'449'364.79</td>
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<td>Administrative expenses</td>
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</tr>
<tr>
<td>55'593.93</td>
<td></td>
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<tr>
<td>Hardware, software, services</td>
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<td>2'208'301.20</td>
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<td>Services &amp; remunerations</td>
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<td>93'431.86</td>
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<td>46'828.38</td>
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The balance is rolled over to the 2010 budget.

## Overview Expenses 2005-2009

![Chart showing expenses over the years](chart.png)
### Cost Analysis

**Breakdown of costs per customer**

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<tr>
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**Distribution Direct Costs**

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<th>IT Depreciation</th>
<th>Personnel Costs</th>
<th>Personnel Costs</th>
<th>IT Expenses and Maintenance</th>
<th>IT Expenses and Maintenance</th>
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<th>Total Direct Costs</th>
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<td>277</td>
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<td>518</td>
<td>51</td>
<td>60</td>
<td>58</td>
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<td>728</td>
<td>113</td>
<td>164</td>
<td>127</td>
<td>14</td>
<td>57</td>
<td>365</td>
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<tr>
<td>3'218</td>
<td>518</td>
<td>548</td>
<td>462</td>
<td>85</td>
<td>300</td>
<td>1'270</td>
<td>177</td>
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</table>

**Distribution Overhead**

<table>
<thead>
<tr>
<th>Overhead Infrastructure</th>
<th>Overhead Infrastructure</th>
<th>Overhead Management</th>
<th>Overhead Management</th>
<th>Technical Overhead</th>
<th>Technical Overhead</th>
<th>Total Cost Overhead</th>
<th>Total Cost Overhead</th>
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</tr>
<tr>
<td>3'218</td>
<td>518</td>
<td>548</td>
<td>462</td>
<td>85</td>
<td>300</td>
<td>1'270</td>
<td>177</td>
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</table>

**Total costs**

<table>
<thead>
<tr>
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</thead>
<tbody>
<tr>
<td>3'723.65</td>
<td>3'824.43</td>
<td>5'082.06</td>
<td>4'945.62</td>
<td>17'575.75</td>
<td>25.58</td>
<td>11'248.87</td>
<td>11'248.87</td>
<td>4'753.79</td>
<td>755.26</td>
<td>775.92</td>
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### Cost Distribution

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<th>Q3</th>
<th>Q4</th>
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<td>7.67</td>
<td>0.00</td>
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<td>Salaries</td>
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<td>1'123.80</td>
<td>1'248.50</td>
<td>1'281.73</td>
<td>4'753.79</td>
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<td>Contribution social insurances</td>
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<td>174.69</td>
<td>187.86</td>
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<td>Other personnel costs</td>
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<td>161.62</td>
<td>183.54</td>
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<td>1'620.90</td>
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<td>6'284.97</td>
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<td>108.76</td>
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<td>105.16</td>
<td>284.00</td>
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<td>348.49</td>
<td>475.98</td>
<td>631.84</td>
<td>1'956.76</td>
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<td>16.72</td>
<td>29.93</td>
<td>20.28</td>
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<td>Hardware, Software, Services</td>
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<td>606.79</td>
<td>604.76</td>
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<td>5'082.06</td>
<td>4'945.62</td>
<td>17'575.75</td>
</tr>
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All figures are given in kCHF, deviations may occur, they are due to round ups/downs
## Usage Statistics

### Usage by research fields

<table>
<thead>
<tr>
<th>Research Field</th>
<th>Cray XT3 PALU</th>
<th>Cray XT4 BUIN</th>
<th>Cray XT5 ROSA</th>
<th>IBM P5 BLANC</th>
<th>SUN Cluster RIGI</th>
<th>HP Cluster HORUS</th>
<th>Total</th>
</tr>
</thead>
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<td>19.62%</td>
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<td>28.89%</td>
<td>12.29%</td>
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<td>0.00%</td>
<td>20.56%</td>
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<td>9.45%</td>
<td>14.72%</td>
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<td>0.00%</td>
<td>0.00%</td>
<td>13.65%</td>
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<td>18.44%</td>
<td>82.53%</td>
<td>6.97%</td>
<td>5.48%</td>
<td>46.10%</td>
<td>7.79%</td>
<td>11.40%</td>
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<td>8.88%</td>
<td>6.10%</td>
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<td>4.41%</td>
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<td>0.79%</td>
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<td>81.57%</td>
<td>3.30%</td>
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<td><strong>Total Usage CPU Hours per machine</strong></td>
<td>13'576'800</td>
<td>3'410'090</td>
<td>72'019'670</td>
<td>5'161'987</td>
<td>326'505</td>
<td>33'133</td>
<td>94'528'185</td>
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### Usage by customer

<table>
<thead>
<tr>
<th>Customer</th>
<th>Cray XT3 PALU</th>
<th>Cray XT4 BUIN</th>
<th>Cray XT5 ROSA</th>
<th>IMB P5 BLANC</th>
<th>SUN Cluster RIGI</th>
<th>HP Cluster HORUS</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>ETH Zurich</td>
<td>51.82%</td>
<td>17.33%</td>
<td>41.30%</td>
<td>48.55%</td>
<td>6.11%</td>
<td>17.99%</td>
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<td>University of Zurich</td>
<td>12.22%</td>
<td>0.03%</td>
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<td>15.03%</td>
<td>0.00%</td>
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<td>0.05%</td>
<td>9.39%</td>
<td>1.22%</td>
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<td>0.00%</td>
<td>9.50%</td>
</tr>
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<td>0.30%</td>
<td>7.40%</td>
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<td>EPF Lausanne</td>
<td>7.16%</td>
<td>0.00%</td>
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<td>15.55%</td>
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<td>3.21%</td>
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<td>0.00%</td>
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<td>1.86%</td>
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<td>2.44%</td>
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<td>1.86%</td>
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<td>0.06%</td>
<td>1.78%</td>
<td>0.07%</td>
<td>9.22%</td>
<td>81.57%</td>
<td>1.45%</td>
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<tr>
<td>University of Bern</td>
<td>1.66%</td>
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<td>0.00%</td>
<td>0.00%</td>
<td>0.81%</td>
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<td>Others</td>
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<td>45.17%</td>
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<td>0.61%</td>
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<tr>
<td><strong>Total Usage CPU Hours per machine</strong></td>
<td>13'576'800</td>
<td>3'410'090</td>
<td>72'019'670</td>
<td>5'161'987</td>
<td>326'504</td>
<td>33'133</td>
<td>94'528'185</td>
</tr>
</tbody>
</table>
CPU Usage per Research Field in 2009

- Physics: 25%
- Chemistry: 14%
- Material Sciences: 11%
- Earth and Environmental Sciences: 10%
- Biosciences: 7%
- Fluid Dynamics: 7%
- Nanosciences: 7%
- Internal: 3%
- Astronomy: 3%
- Mechanical Engineering: 2%

CPU Usage per Institution in 2009

- ETH Zurich: 42%
- University of Zurich: 21%
- PSI: 14%
- University of Basel: 10%
- EPF Lausanne: 7%
- University of Geneva: 7%
- MeteoSwiss: 7%
- EMPA: 3%
- Cray: 3%
- CSCS: 2%
- University of Bern: 2%
- Others: 1%
## Compute Infrastructure

<table>
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<tr>
<th>Vendor &amp; Model</th>
<th>CPU Type</th>
<th>No. of Processors</th>
<th>No. of Nodes</th>
<th>Interconnect type</th>
<th>Interconnect peak bandwidth (GB/sec)</th>
<th>Total memory size (GB)</th>
<th>Year of installation</th>
<th>Core Peak Performance (Gflops)</th>
<th>Peak Performance (Tflops)</th>
<th>LINPACK Performance (Tflops) Nov. 09</th>
<th>Top500 position Nov. 09</th>
<th>Produced (consumed) CPU hours</th>
<th>Average Utilisation (%)</th>
<th>Annual direct costs in 2009 (kCHF)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CRAY XT5 Rosa</td>
<td>AMD Opteron 2.4 GHz</td>
<td>22128</td>
<td>1844</td>
<td>CRAY SeaStar 2+</td>
<td>57.6</td>
<td>29504</td>
<td>2009</td>
<td>9.6</td>
<td>212.43</td>
<td>169</td>
<td>21</td>
<td>72,019,670.00*</td>
<td>88.4</td>
<td>3'094</td>
</tr>
<tr>
<td>CRAY XT4 Buin</td>
<td>AMD Opteron 2.3 GHz</td>
<td>1040</td>
<td>260</td>
<td>CRAY SeaStar 2</td>
<td>45.6</td>
<td>2080</td>
<td>2009</td>
<td>9.2</td>
<td>9.57</td>
<td>-</td>
<td>-</td>
<td>3'410'090.00</td>
<td>43.8</td>
<td>1'404</td>
</tr>
<tr>
<td>IBM p575 Blanc</td>
<td>IBM Power5 1.5 GHz</td>
<td>768</td>
<td>48</td>
<td>Infiniband 4X SDR</td>
<td>-</td>
<td>1650</td>
<td>2006</td>
<td>6</td>
<td>4.61</td>
<td>-</td>
<td>-</td>
<td>5'161'986.00</td>
<td>76.7</td>
<td>1383</td>
</tr>
<tr>
<td>HP-XC Cluster</td>
<td>AMD Opteron 2.4 GHz</td>
<td>34</td>
<td>16</td>
<td>Infiniband 4X SDR</td>
<td>1</td>
<td>128</td>
<td>2007</td>
<td>9.6</td>
<td>0.16</td>
<td>-</td>
<td>-</td>
<td>33'133.16</td>
<td>11.1</td>
<td>205</td>
</tr>
<tr>
<td>SUN Cluster</td>
<td>AMD Opteron 2.6 GHz</td>
<td>104</td>
<td>26</td>
<td>Infiniband 4X SDR</td>
<td>2</td>
<td>208</td>
<td>2007</td>
<td>14</td>
<td>0.54</td>
<td>-</td>
<td>-</td>
<td>326'504.64</td>
<td>35.8</td>
<td>200</td>
</tr>
</tbody>
</table>

* The indications for Cray XT5 are valid from July 1, 2009 until December 31, 2009

### Evolution of CPU usage in 2009

![Graph showing CPU usage evolution in 2009](image)
Job size for research fields on Cray-XT5 for the time period of 01.07.2009 – 31.12.2009

Job size in cores on Cray XT5 for the time period 01.07.2009 - 31.12.2009
Report of the Auditors

to CSCS Directorate

CSCS – SWISS NATIONAL SUPERCOMPUTING CENTRE
6928 Manno

Based on the assigned mandate we have audited the accounting records and the financial reporting of the CSCS – Swiss National Supercomputing Centre, Manno, for the year ended December 31, 2009.

CSCS Directorate and the Vice President Human Resources and Infrastructure are responsible for the financial reporting. Our responsibility is to express an opinion on this financial reporting based on our audit. We confirm that we meet the legal requirements concerning professional qualification and independence.

Our audit was conducted in accordance with Swiss auditing standards which require that an audit has to be planned and performed to obtain reasonable assurance about whether the financial reporting are free of material misstatement. We have examined, on a test basis, evidence supporting the amounts and disclosures in the financial reporting. We have also assessed the accounting principles used and significant estimates made as well as the overall financial reporting presentation. We believe that our audit provides a reasonable basis for our opinion.

We recommend that the financial reporting submitted to you be approved.

Bellinzona, February 25, 2010

Claudio G. Fantana
Auditor in charge

FIDECONTO REVISIONI SA

Financial reporting
<table>
<thead>
<tr>
<th>Publication</th>
<th>Impact factor</th>
<th>Principal investigator</th>
<th>Application field</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bernet, ML; Miniati, F; Lilly, SJ, et al. Strong magnetic fields in normal galaxies at high redshift; NATURE, 45 (7202) 302-304 (2008)</td>
<td>31.434</td>
<td>Francesco Miniati</td>
<td>Astrophysics</td>
</tr>
<tr>
<td>Raiteri, P; Bussi, G; Cucinotta, CS, et al. Unraveling the shuffling mechanism in a photoswitchable multicomponent bistable rotaxane; ANGEWANDE CHEMIE INTERNATIONAL EDITION, 47 (19) 3536-3539 (2008)</td>
<td>10.879</td>
<td>Michele Parrinello</td>
<td>Material Science / Nanochemistry</td>
</tr>
<tr>
<td>Joos, F; Spahn, R. Rates of change in natural and anthropogenic radiative forcing over the past 20,000 years; PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 105 (5) 1425-1430 (2008)</td>
<td>9.380</td>
<td>Fortunat Joos</td>
<td>Climate</td>
</tr>
<tr>
<td>Domene, C; Klein, ML; Branduardi, D, et al. Conformational changes and gating at the selectivity filter of Potassium channels; JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 130 (29) 9474-9480 (2008)</td>
<td>8.091</td>
<td>Michele Parrinello</td>
<td>Biosciences</td>
</tr>
<tr>
<td>Gossens, C; Tavernelli, L; Rothlisberger, U. DNA structural distortions induced by ruthenium-arene anticancer compounds; JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 130 (33) 10921-10928 (2008)</td>
<td>8.091</td>
<td>Ursula Rothlisberger</td>
<td>Biosciences</td>
</tr>
</tbody>
</table>

Source: ISI Web of Knowledge SM
**Personnel**

FTE per Unit on December 31, 2009

![Pie chart showing FTE distribution across various units and services]

**Customer Satisfaction (2009)**

CSCS services portfolio

![Bar chart showing satisfaction levels for various services]

- Network performance available
- Performance of the parallel file system
- Storage capacity of parallel file system
- Archiving performance available
- Availability of archiving capacity
- Availability of memory per core IBM
- Availability of memory per core Cray
- Availability of computing resources

Legend:
- Insufficient
- Barely sufficient
- Sufficient
- Ample
- More than needed
Quality of user support in the following fields

```
<table>
<thead>
<tr>
<th>Field</th>
<th>Quality of application portfolio</th>
<th>Quality of software environment</th>
<th>Response/turnaround time for technical support</th>
<th>Quality of technical support</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physics &amp; CFD</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Material Sciences</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Engineering</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Climate</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Biology/Chemistry</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
</tbody>
</table>
```

Application and user support

```
<table>
<thead>
<tr>
<th>Field</th>
<th>Quality of application portfolio</th>
<th>Quality of software environment</th>
<th>Response/turnaround time for technical support</th>
<th>Quality of technical support</th>
</tr>
</thead>
<tbody>
<tr>
<td>Information services</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Interaction with CSCS via user events</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Info about efficiency and amount of used resources</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Supplied information on systems and on web</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
</tbody>
</table>
```

Information services

```
<table>
<thead>
<tr>
<th>Field</th>
<th>Quality of application portfolio</th>
<th>Quality of software environment</th>
<th>Response/turnaround time for technical support</th>
<th>Quality of technical support</th>
</tr>
</thead>
<tbody>
<tr>
<td>Training course and events</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Organisation of the courses and events</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Quality of the offered training</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
<tr>
<td>Information about courses and events</td>
<td>Poor</td>
<td>Average</td>
<td>Good</td>
<td>Very good</td>
</tr>
</tbody>
</table>
```

The participation at the User Day was

```
<table>
<thead>
<tr>
<th>Field</th>
<th>Quality of application portfolio</th>
<th>Quality of software environment</th>
<th>Response/turnaround time for technical support</th>
<th>Quality of technical support</th>
</tr>
</thead>
<tbody>
<tr>
<td>The participation at the User Assembly was</td>
<td>Not useful</td>
<td>Somewhat useful</td>
<td>Moderately useful</td>
<td>Useful</td>
</tr>
<tr>
<td>The participation at the User Assembly was</td>
<td>Not useful</td>
<td>Somewhat useful</td>
<td>Moderately useful</td>
<td>Useful</td>
</tr>
</tbody>
</table>
```
Software support and development

Future expectations and wishes (next 3 years)

For achieving the scientific results the contribution of CSCS was:
Publications

Papers published by CSCS users in 2009

Dr. Andreas Adelmann:


Prof. Wanda Andreoni:


Prof. Peter Arbenz:


Prof. Alfons Baiker:


Prof. Andrea Danani:


Dr. Christos Frouzakis:


Prof. Stefan Goedecker:


Prof. Andreas Hauser:


Prof. Jürg Hutter:


Prof. Andrew Jackson:


Prof. Fortunat Joos:


Dr. Daniel Jung:


Prof. Michele Parrinello:


Prof. Markus Meuwly:


Prof. Alfredo Pasquarello:

forearm fracture risk in postmenopausal women. Osteoporosis International (accepted).


Dr. Helena van Swygenhoven:


Prof. Laurent Villard:


Prof. Viola Vogel:


[3] William Little, Ruth Schwartzander, Michael Smith, Delphine Gourdon and Viola Vogel, Stretched fibronectin fibers turn fouling and are functionally rescued by the chaperones albumin and casein, Nanoletters, in press.


Dr. Tomasz Wesolowski:


Papers published by CSCS employees in 2009

John Biddiscombe:


Jean Favre:


Fotis Georgatis:


Maria Grazia Giuffreda:


Thomas Schuttel:


*DCA++: a case for science driven application development for leadership computing platforms*, Summers MS, Gonzalez A, Meredith J, Maier TA, and Schuttel TC, JOURNAL OF PHYSICS: CONFERENCE SERIES, Volume: 190, Article Number: 012077, Published: 2009


Tim Stitt:


Mario Valle:


Ugo Varetto:


Invited talks and seminars

Jean Favre:


Fotis Georgatis:


Maria Grazia Giuffreda and Ugo Varetto:


Tim Stitt:

An introduction to Chapel: a next-generation high productivity parallel programming language; Computer Science Seminar, Queen’s University Belfast, Northern Ireland, May 2009.
Towards a European HPC Training and Education Infrastructure for Petascale Computing; PRACE/DEISA Scientific Symposium, Amsterdam, Netherlands, May 2009

Parallel Performance Optimization and Behavior Analysis Tools: A Comparative Evaluation on the Cray XT Architecture; Cray User Group, Atlanta, May 2009

Scaling the Peak of High-Performance Computing; 1st Annual Workshop on Computational Economics and Finance, University of Zurich, September 2009

Introduction to High-Performance Computing; LinkSCEEM HPC Conference, Cyprus, October 2009

Mario Valle:

Introduzione alla visualizzazione scientifica; CINECA — Scuola estiva di visualizzazione e computer graphics; June 16, 2009

Visualizzare per comunicare; CINECA — Scuola estiva di visualizzazione e computer graphics; June 17, 2009

General Visualization using AVS/Express; ETH Zürich — AVS User Meeting May 7, 2009

La matematica? Non è come pensate! Convegno AMITE – Associazione Montessori Italia Europa: “Infanzia e Adolescenza – pensiero e ambiente” (Milano); November 14, 2009

Foster Insight by Integrating Advanced Visualization with Data Analysis Stony Brook University (Stony Brook, USA) – Solid State Seminar series October 9, 2009

Crystal fingerprint space: a novel paradigm to study crystal structures sets; CECAM (Lugano) — for the workshop: Structural Transitions in Solids: Theory, Simulations, Experiments and Visualization Techniques July 8-11, 2009

From Tradition to Insight – Do Chemistry Visualization Tools Measure Up? Keynote for the 24th Philippine Chemistry Congress (Tagbilaran, Philippines) April 15, 2009
Members of Advisory Board

Anwar Osseyran, SARA Computing and Networking Services, Netherlands, Chairman of the Board
Guy Brasseur, Climate Service Centre (CSC), Germany
Mehdi Jazayeri, Università della Svizzera Italiana (USI), Switzerland
Klaus Schulten, University of Illinois, Urbana-Champaign, USA
Horst Simon, Lawrence Berkeley National Laboratory, USA

Impressum

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Fax +41 (0) 91 610 82 09
http://www.cscs.ch

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