CSCS
Swiss National Supercomputing Centre

Annual Report

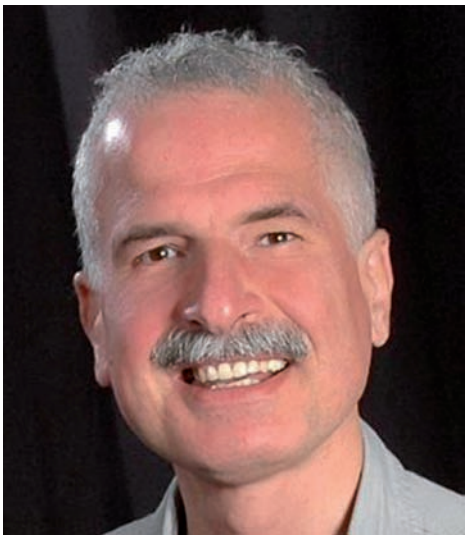
Annual Report 2009

CSCS
Swiss National Supercomputing Centre

Annual Report 2009

Content

Research Digest



Dr. Anwar Osseyran, Chairman of the Advisory Board, Managing Director of SARA, Computing and Networking Services

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 CO_2 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-compute 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 supernodes.

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 tradeoffs 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 “Outcompute 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

Prof. Petros Koumoutsakos

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.

Presentation of Three Production 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 2009 projects on page 18.

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

Nanovectors for Drug Delivery in Oncology

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-

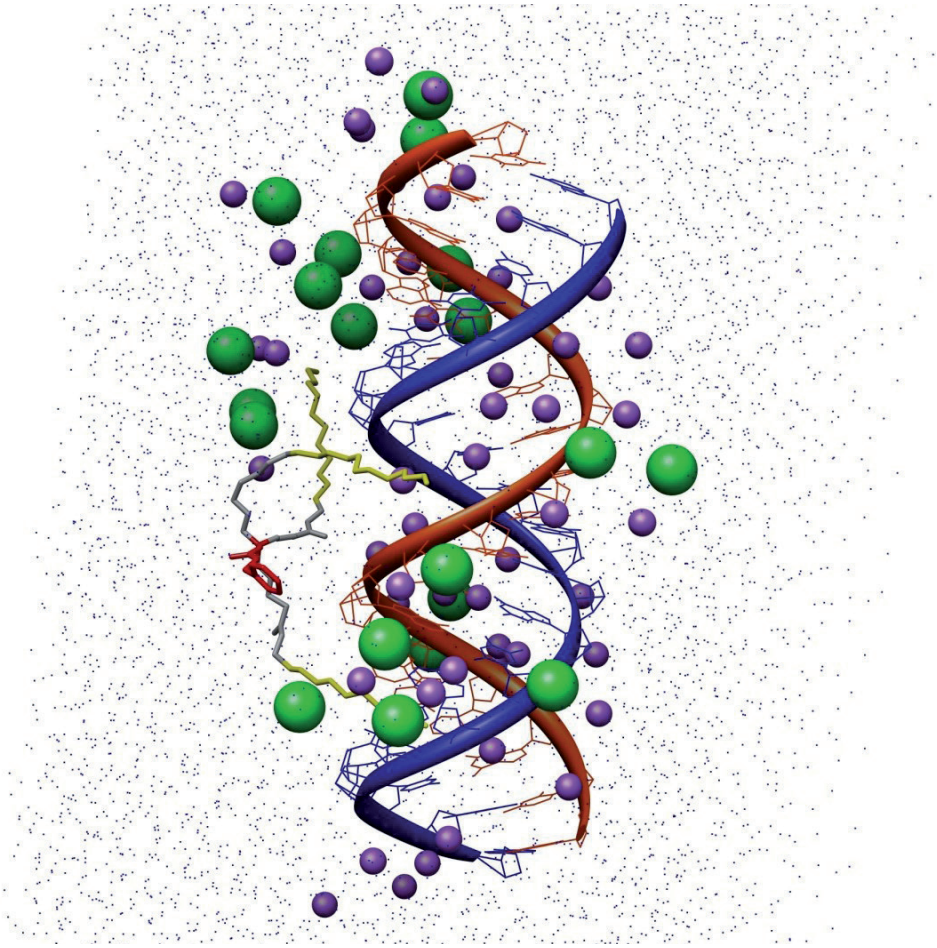
rier molecules more flexible might improve how well they can bind to the gene therapy agent.

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

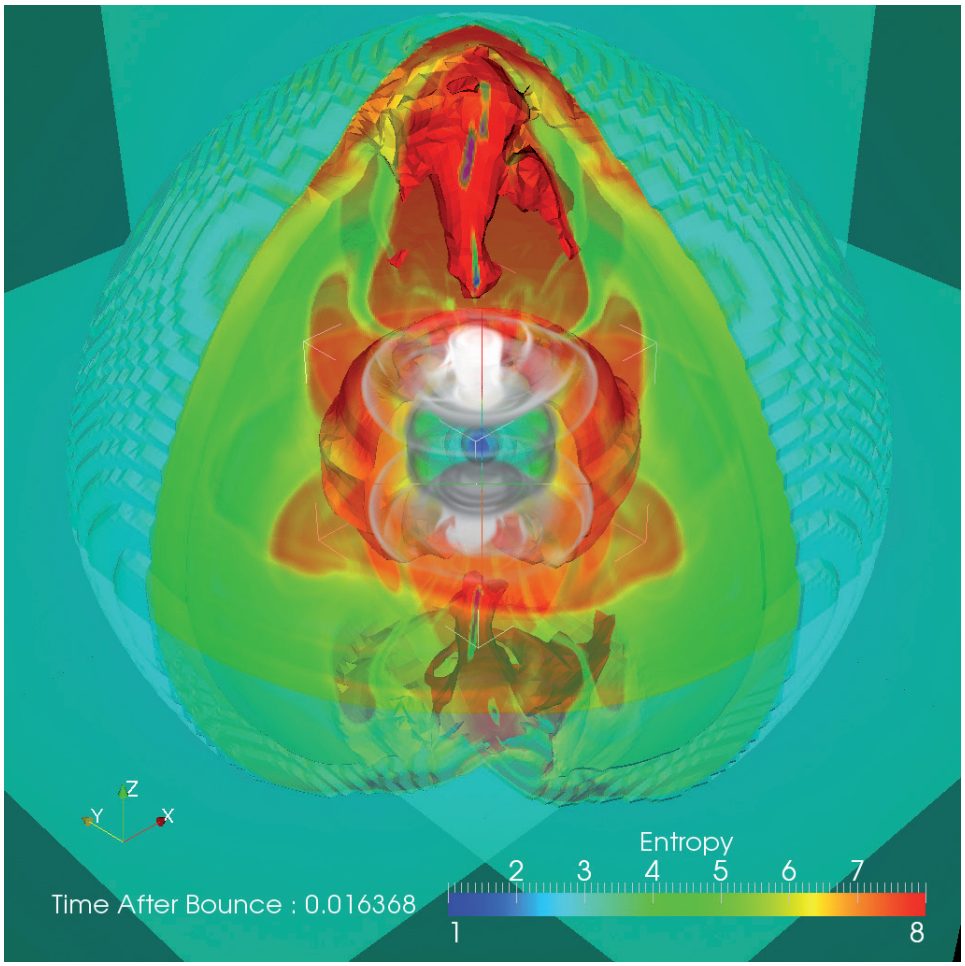
Prof. Matthias Liebendoerfer, University of Basel, Switzerland

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



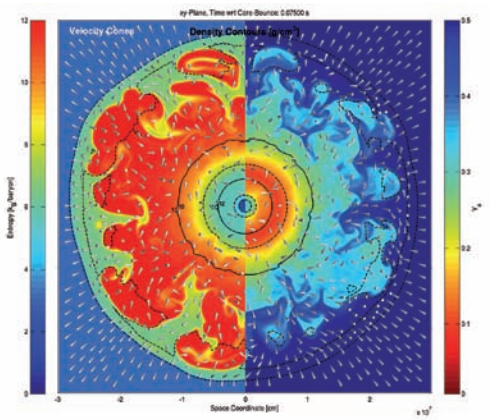
Three-dimensional computer simulation of a magneto-rotational supernova explosion mechanism that is obtained by setting an extremely large initial magnetic field. Mildly relativistic bipolar jets (red balloon) form above the neutron star (bluish central region) and push through the outrunning shock wave (turquoise shell). [Viz. J. A. Biddiscombe, CSCS]

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.”



Three-dimensional computer simulation of the neutrino-driven supernova explosion mechanism showing vigorous convection between the neutron star (enclosed by the black density contour at 10^{12} g/cm^3) and the outrunning shock wave at about 250 km radius.

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.

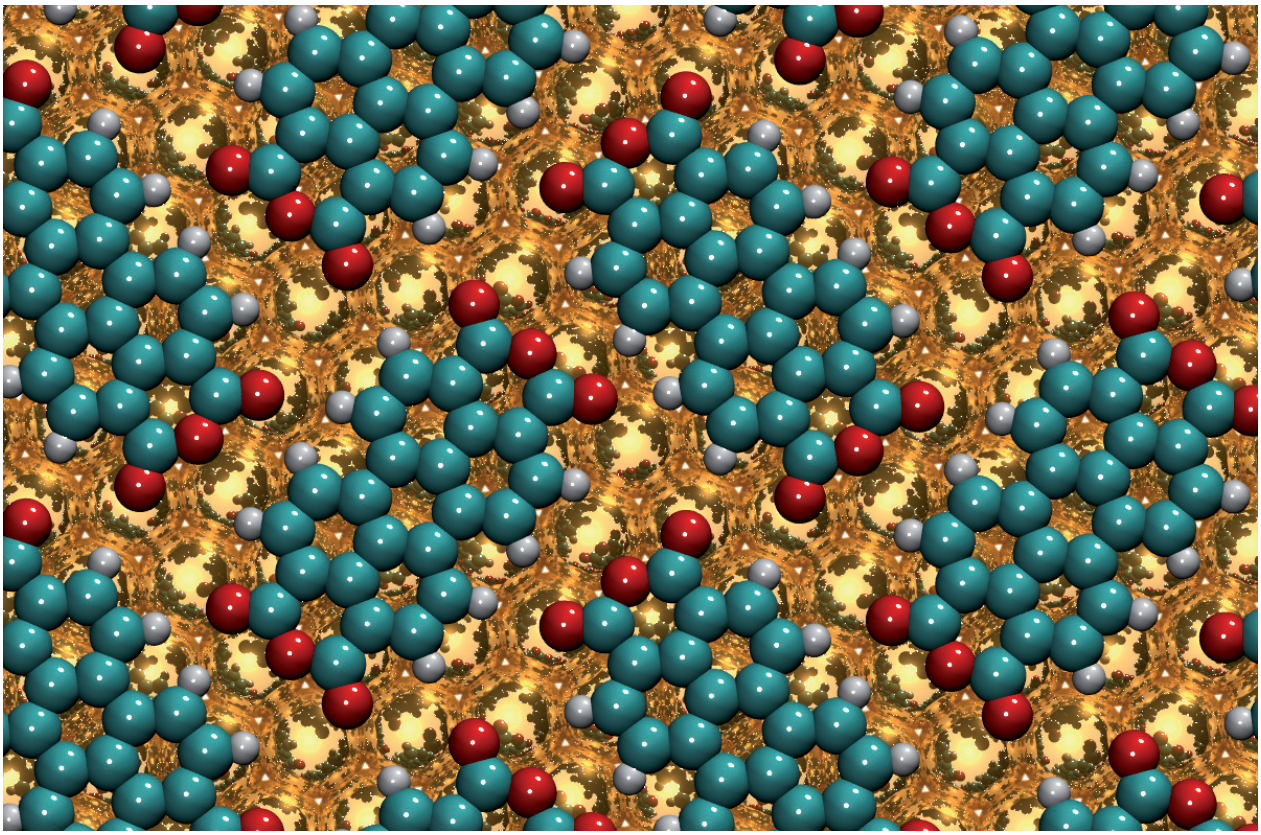
In the second project, the team has investigated hydrogen-bonded molecular networks that can be constructed on a surface with a view to using organic semiconductor materials to make future nanoelectronic devices. Organic materials are easy to handle and their electronic properties can be fine-tuned for 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.



Model of PTCDA/Au(111) herringbone structure

List of Production Projects 2009

Name	Organisation	Project Title
Adelmann, Andreas	PSI	Beam Dynamics for the PSI-XFEL and the High Power Cyclotron Upgrade
Arbenz, Peter	ETH Zurich	Multi-level Micro-Finite Element Analysis for Human Bone Structures
Arbenz, Peter	ETH Zurich	Multi-level Micro-Finite Element Analysis for Embedded Human Bones
Baiker, Alfons	ETH Zurich	Nature of Chemical Reactivity of Nano-Sized Materials and Environmental Catalysts
Bakowies, Dirk	ETH Zurich	Energies from Ab initio Calculations without Empirical Corrections
Bernèche, Simone	University of Basel	Influence of FAB Fragments on the Structure and Dynamics of the KcsA Channel
Brunner, Dominik	EMPA	Regional Scale Impacts of Changing Anthropogenic Emissions on Aerosols and Climate
Carollo, Marcella	ETH Zurich	The Build-up of Massive Galaxies in the Early Universe
Carollo, Marcella	ETH Zurich	Galaxy Formation in the Cosmic Web-Analysis and Visualization Follow-up
Cooper, W. Anthony	EPF Lausanne	Computation of Stellarator Coils, Equilibrium, Stability and Transport
Cucinotta, Clotilde	ETH Zurich	Material Science for the H Storage and Use
Fichtner, Wolfgang	ETH Zurich	Computational Science and Engineering in Nanoelectronics
Goedecker, Stefan	University of Basel	Atomistic Simulations and Electronic Structure
Hauser, Andreas	University of Geneva	Photophysics and Photochemistry of Transition Metal Compounds: Theoretical Approaches
Hutter, Juerg	University Zurich	Applications of Ab initio Molecular Dynamics
Hutter, Juerg	University Zurich	New Algorithms for Large-Scale DFT
Jackson, Andrew	ETH Zurich	Convection and Magnetic Field Generation in the Earth
Jackson, Andrew	ETH Zurich	Convection in Earth with Inhomogeneous Boundary Conditions
Joos, Fortunat	University of Bern	CARBOCLIM II. Modelling CARBOn Cycle CLIMate Feedbacks
Khaliullin, Rustam	ETH Zurich	A Molecular Dynamics Study of the Phase Diagrams of Carbon, Sodium, and Iron Employing Neural Network Potentials
Kleiser, Leonhard	ETH Zurich	Numerical Simulation of Transitional, Turbulent and Multiphase Flows
Koumoutsakos, Petros	ETH Zurich	Aircraft Wake Evolutionary Optimisation
Koumoutsakos, Petros	ETH Zurich	Multiphysics/Scale Simulations using Particle Methods: I. Algorithms and Parallel Computing. II. Biology, Nanotechnology, Fluids and their Interfaces
Lehning, Michael	SLF Davos	High Resolution Simulation of Flow and Meteorology in Steep Terrain

Name	Organisation	Project Title
Limongelli, Vittorio	ETH Zurich	Simulating the Undocking Process of the Inhibitor SC-558 in COX Structures
Liebendoerfer, Matthias	University of Basel	Multi-Dimensional Supernova Models and the Prediction of Observables from Different Explosion Mechanisms
Lodziana, Zbigniew	EMPA	Materials for Hydrogen Storage
Lohmann, Ulrike	ETH Zurich	Role of Anthropogenic versus Natural Forcing on Decadal Scales in Global Climate Models
Luethi, Hans Peter	ETH Zurich	Ab initio Molecular Dynamics of the Reaction Mechanisms for New Donors for 1-2cis Glycosylations
Maddocks, John	EPF Lausanne	Analysis and Simulation of Mulitiscale Mechanics of DNA
Mareda, Jiri	University of Geneva	Molecular Modelling of Multifunctional Supramolecular Assemblies
Mayer, Lucio	University of Zurich	Co-Evolution of Galaxies and Supermassive Black Holes
Meher, Ayalasomayajula	ETH Zurich	Metadynamics Study of Large-Scale pH-Induced Conformational Changes in Dengue Virus Envelope Protein
Meuwly, Markus	University of Basel	Influence of Dimerization on Allostery of Multidomain Proteins
Meuwly, Markus	University of Basel	Electronic Structure Calculations for Chemical Reactions Involving Transition Metals
Mila, Frederic	EPF Lausanne	Simulating Frustrated Quantum-Magnetic Materials
Parrinello, Michele	ETH Zurich	Linear-Scaling Molecular Dynamics: Development and Applications
Parrinello, Michele	ETH Zurich	Ab-initio Study of Crystallization Processes in Phase Change Alloys
Pasquarello, Alfredo	EPF Lausanne	Band and Defect-Level Alignments at Semiconductor-Oxide Interfaces through the Use of Hybrid Density Functionals
Passerone, Daniele	EMPA	Computational Nanoscience at Surface and Interfaces
Pfaendtner, Jim	ETH Zurich	Metadynamics Investigation of Opening and Closing of the Nucleotide Binding Cleft in Actin and Actin-Like Proteins
Raible, Christoph	University of Bern	Modelling and Reconstruction of North Atlantic Climate System Variability (MONALISA III)
Roethlisberger, Ursula	EPF Lausanne	Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Studies of Biological System
Schaer, Christoph	ETH Zurich	Regional Climate Modelling on European to Alpine Scales
Seneviratne, Sonia	ETH Zurich	Land-climate Interactions: Modelling and Analysis
Van Lenthe, Harry	ETH Zurich	Hierarchical Multi-Level Analyses of Age-Related Bone Loss and Bone-implant Interaction over Time
Van Swygenhoven Helena	PSI	The Atomistic Modelling of Size Effects in Plasticity
Vogel, Viola	ETH Zurich	Simulating Integrin Junctions under Tension: from the Extracellular Matrix to the Cytoskeleton

Name	Organisation	Project Title
Wesolowski,Tomasz	University of Geneva	Electronic Structure of Chemical Molecules in Condensed-Phase
Zoppi, Laura	University of Zurich	Organic Molecules on Metal Surfaces: from Supramolecular Arrangement to Electron Transport across the Interface by First-Principle Theoretical Approaches

List of High Impact Projects 2009

Name	Organisation	Project Title
Arbenz, Peter	ETH Zurich	Extreme Scalability in μFEA of Human Bone Structures
Frouzakis, Christos	ETH Zurich	Three-Dimensional Direct Numerical Simulations of Spherical Expanding Flames
Giardini, Domenico	ETH Zurich	Site-Specific Numerical Simulations of Earthquake Rupture Dynamics and Strong Ground Motion: Application to Swiss NPP's
Goedecker, Stefan	University of Basel	Atomistic Simulations and Electronic Structure
Kleiser, Leonhard	ETH Zurich	Massively-Parallel Simulation of the Particle Settling in an Estuary
Koumoutsakos, Petros	ETH Zurich	Direct Numerical Simulations of a Turbulent Vortex Ring
Liebendoerfer, Matthias	University of Basel	3D Supernova Model with Spectral Neutrino Transport
Moore, Ben	University of Zurich	On the Origin of the Hubble Sequence of Galaxies
Vande Vondele, Joost	University of Zurich	From Level Structure to Charge Injection in Dye Sensitized Solar Cells: Insight from Realistic Models and Hybrid Density Functional Simulations

List of Early User Projects 2009

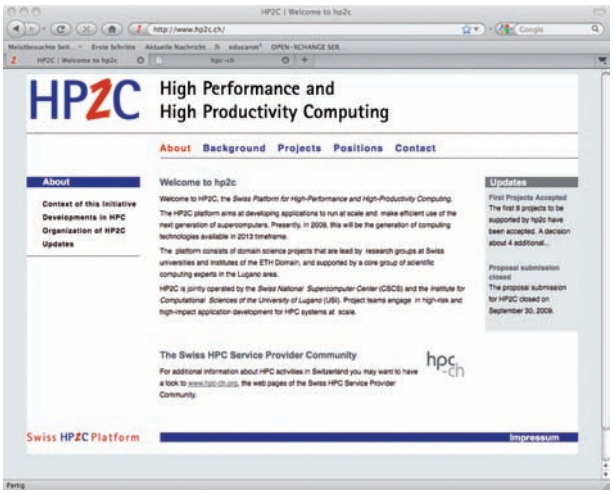
Name	Organisation	Project Title
Bernèche, Simon	University of Basel	Simulation of Membrane Protein Complexes: KcsA-Antibodies and AmtB Trimer
Danani, Andrea	SUPSI	Nanovectors for Drug Delivery in Oncology: a Combined Modelling/Experimental Study
Frouzakis, Christos	ETH Zurich	Direct Numerical Simulation of Instabilities and Long-Term Evolution of Propagating Premixed Flame Fronts
Jung, Daniel	ETH Zurich	Investigations on the Building Blocks of Complex Metal Alloys and their Interactions
Hu, Ming	ETH Zurich	MD Modelling of Heat Transfer at Solid-Solid and Solid-Liquid Interfaces
Villard, Laurent	EPF Lausanne	ORB5-TURB

Activity Report

HP2C

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



HP2C homepage under www.hp2c.ch

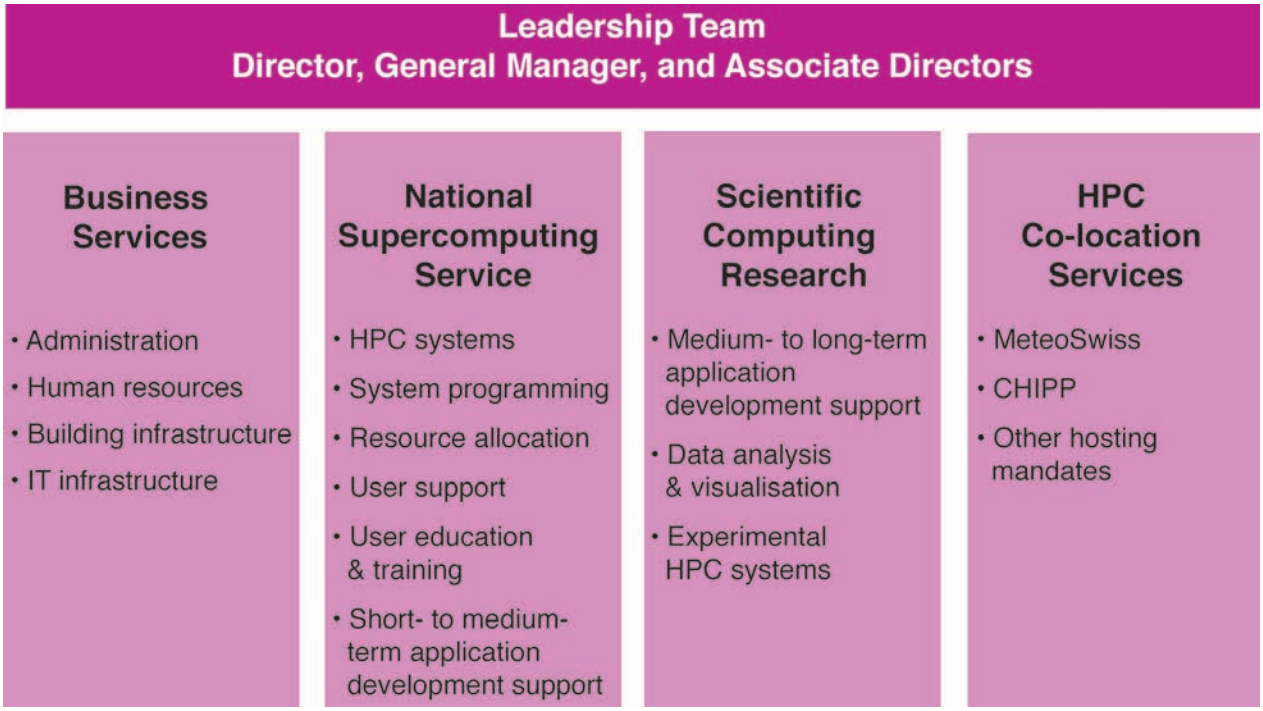
over the coming three years. These development activities will be linked to and supported by a core group of scientific computing researchers at CSCS and the University of Lugano (USI). Furthermore, the core team in Lugano will develop and operate prototype platforms in collaboration with the supercomputing 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



Organisational chart

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-

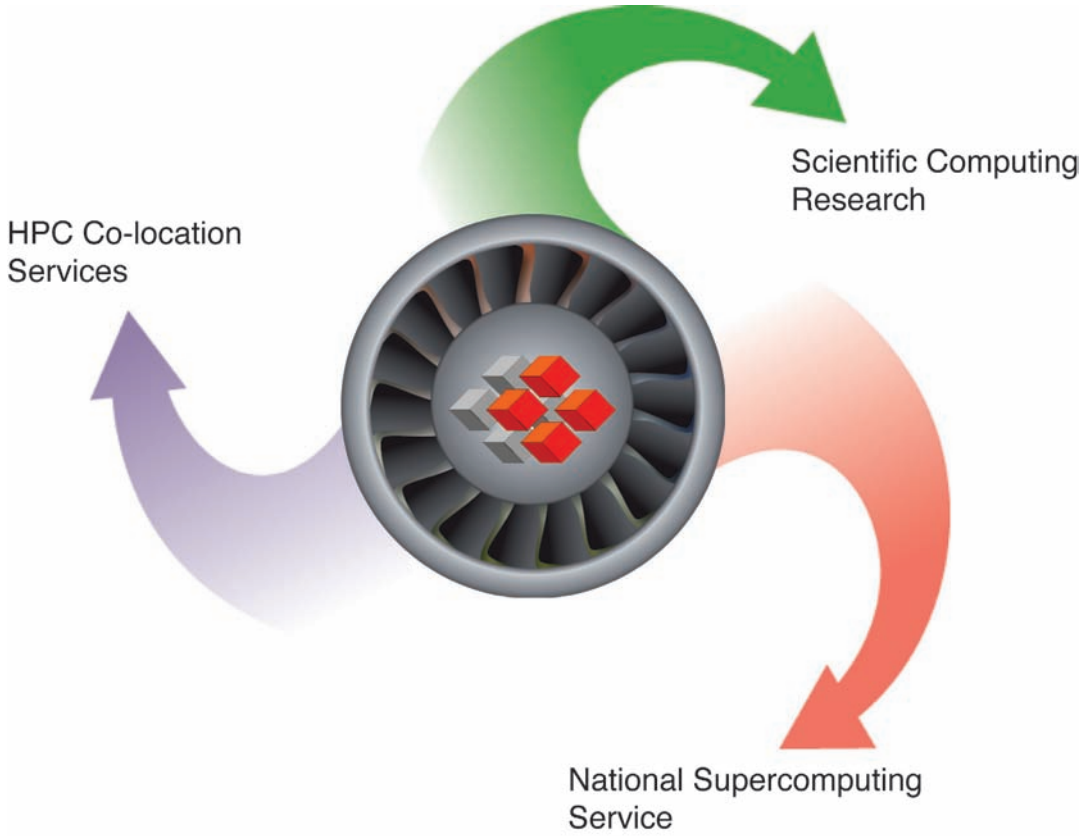
Location Services section, focussing on service reliability and efficiency. However, MeteoSwiss regularly improves its forecasting service by introducing a new forecasting suite every 5 to 8 years. The new forecasting suite improves aspects such as resolution of the model and representation of processes 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.



Business Model

Front view plan of the new building

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

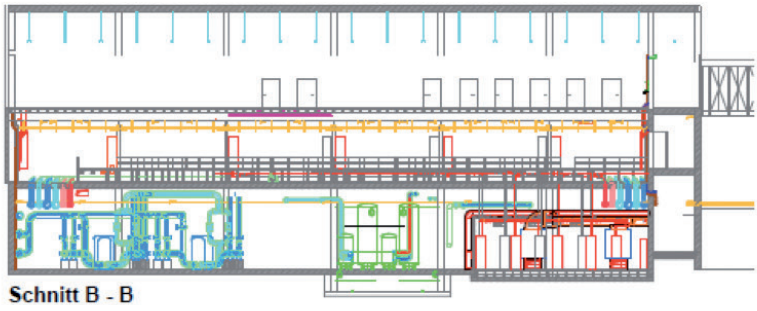
Timeline

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



Sheer plan of the new building

System	Palu	Blanc	Old Systems Combined	Rosa	Improvement
Processors	3328	768	4096	22128	5.4 X
Memory (TB)	3.3	1.8	5.1	29.5	5.8 X
Peak Tflop/s	17.3	4.5	21.8	212	9.7 X

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.

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.

Pascal Couchepin, Member of Swiss Federal Council, at CSCS

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.

Impressions of the First European HPC Infrastructure Workshop

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

User Assembly at KKL in Lucerne, Switzerland

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, promise 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 meteorological radars is actually located on that mountain (the other two being on Albis near Zurich and Lema near Lugano).

December 2009

Cray launches the Eurpean Exascale Research initiative on December 2, naming CSCS one of two initial partners. This initiative aims at exploring new ideas and technologies necessary to achieve sustained 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 building 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

Income & Expenditure Flow (1.1.2009-31.12.2009)

Expenditures		Income	
Investments	**11'540'846.95**	**Basic Budget**	**24'000'000.00**
		Contribution ETH Zurich	14'000'000.00
Material/Goods/Services	**16'328.72**	Economic stabilisation measures	10'000'000.00
Personnel	**6'284'972.98**	**Third-party contributions projects**	**1'400'976.66**
Payroll	4'753'785.70	European projects	581'838.81
Employer's contributions	755'262.40	Other projects (Ticino in Rete / AAA Switch 08)	319'137.85
Other (education, travel etc.)	775'924.88	HP2C	500'000.00
Other material expenses	**5'399'155.85**	**Third-party contributions services**	**2'449'364.79**
Floor space	209'016.63	CHIPP hosting	1'348'691.77
Maintenance	888'709.22	MeteoSwiss	815'174.60
Energy & media	1'956'757.12	PSI, part upgrade Cray XT3	254'742.10
Administrative expenses	55'593.93	Other income	30'756.32
Hardware, software, services	2'208'301.20		
Services & remunerations	93'431.86		
Other	-12'654.11		
Extraordinary incom/expenditures	**60'063.13**		
Membership fees	13'234.75		
Overhead	46'828.38		
Expenses total	**23'301'367.18**	**Income total**	**27'850'341.45**
Balance			**4'548'974.27**

– The balance is rolled over to the 2010 budget.

Overview Expenses 2005-2009

Cost Analysis

Breakdown of costs per customer

Customer	ETHZ	EPFL	PSI	Univ. Basel	Univ. Bern	Univ. Geneva	Univ. Zurich	EMPA	Meteo CH	CHIPP	EU Proj.	Other	CSCS	TOTAL
Income Federal Base Funding	24'000	0	0	0	0	0	0	0	0	0	0	0	0	24'000
Income Third Party Funds	500	0	255	0	0	0	0	0	815	1'349	582	350	0	3'851
Distribution Direct Costs														
IT Depreciation	1'972	354	324	277	44	177	812	114	806	696	0	111	109	5'795
Personnel Costs	518	51	60	58	27	66	93	31	358	116	705	138	584	2'807
IT Expenses and Maintenance	728	113	164	127	14	57	365	32	55	0	0	43	53	1'752
Total Direct Costs	3'218	518	548	462	85	300	1'270	177	1'219	812	705	292	746	10'352
Distribution Overhead														
Overhead Infrastructure	0	0	0	0	0	0	0	0	0	0	0	0	3'537	3'537
Overhead Management	0	0	0	0	0	0	0	0	0	0	137	0	1'805	1'942
Technical Overhead	0	0	0	0	0	0	0	0	0	0	6	0	1'737	1'743
Total Cost Overhead	0	0	0	0	0	0	0	0	0	0	143	0	7'079	7'222
Total costs	3'218	518	548	462	85	300	1'270	177	1'219	812	848	292	7'825	17'576

Cost Distribution

Cost element	Q1	Q2	Q3	Q4	Total
Materials	**8.66**	**0.00**	**7.67**	**0.00**	**16.33**
Salaries	1'098.76	1'123.80	1'249.50	1'281.73	4'753.79
Contribution social insurances	177.90	174.69	187.86	214.81	755.26
Other personnel costs	191.86	161.62	183.54	238.91	775.92
Total costs of personnel	**1'468.53**	**1'460.10**	**1'620.90**	**1'735.45**	**6'284.97**
Floor space	11.80	108.76	41.33	47.12	209.02
Maintenance	93.04	305.16	284.00	206.52	888.71
Energy & Media	500.44	348.49	475.98	631.84	1'956.76
Adminstrative expenses	-11.34	16.72	29.93	20.28	55.59
Hardware, Software, Services	535.46	461.26	606.79	604.76	2'208.30
Services & remunerations	18.69	37.40	12.64	24.70	93.43
Other costs	1.50	-3.32	-11.86	1.02	-12.65
Depreciation of investments	1'084.99	1'089.89	2'001.71	1'673.12	5'849.71
Total costs of materials	**2'234.62**	**2'364.37**	**3'440.53**	**3'209.35**	**11'248.87**
Extraordinary costs	**11.85**	**0.00**	**12.95**	**0.77**	**25.58**
Total costs	**3'723.65**	**3'824.43**	**5'082.06**	**4'945.62**	**17'575.75**

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

Usage Statistics

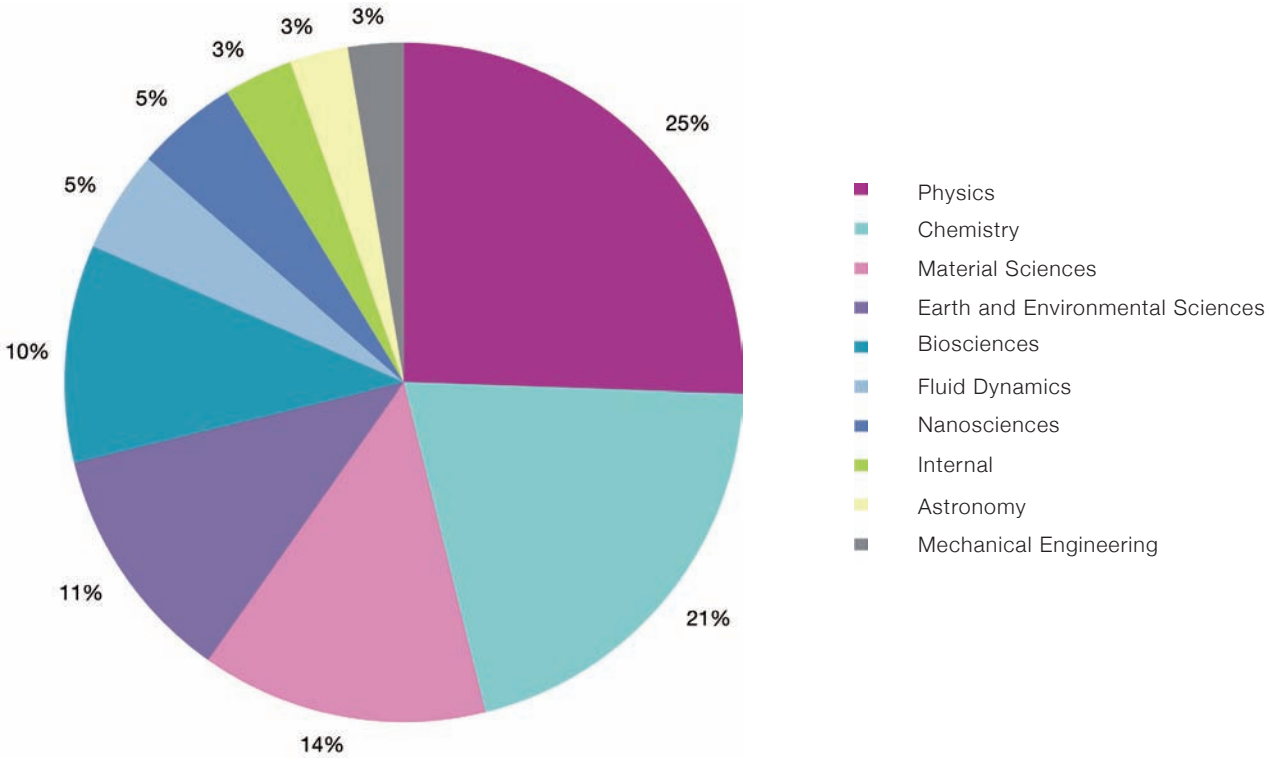
Usage by research fields

	Cray XT3 PALU	Cray XT4 BUIN	Cray XT5 ROSA	IBM P5 BLANC	SUN Cluster RIGI	HP Cluster HORUS	Total
Physics	19.62%	0.05%	28.89%	12.29%	0.36%	0.14%	25.50%
Chemistry	12.80%	4.59%	21.29%	42.78%	0.00%	0.00%	20.56%
Material Sciences	6.38%	9.45%	14.72%	21.59%	0.00%	0.00%	13.65%
Earth & Environmental S.	18.44%	82.53%	6.97%	5.48%	46.10%	7.79%	11.40%
Biosciences	21.56%	1.06%	8.88%	6.10%	30.73%	4.41%	10.34%
Fluid Dynamics	11.04%	2.26%	3.71%	6.79%	0.79%	6.08%	4.87%
Nanoscience	3.90%	0.00%	5.28%	4.85%	0.00%	0.00%	4.85%
Internal	0.18%	0.06%	4.22%	0.04%	9.22%	81.57%	3.30%
Astronomy	6.08%	0.00%	2.46%	0.04%	0.00%	0.00%	2.75%
Mechanical Engineering	0.00%	0.00%	3.49%	0.00%	0.00%	0.01%	2.66%
Economics	0.00%	0.00%	0.09%	0.00%	0.00%	0.00%	0.07%
Computer Sciences	0.00%	0.00%	0.01%	0.03%	12.63%	0.00%	0.06%
Engineering	0.00%	0.00%	0.00%	0.00%	0.16%	0.00%	0.00%
Total Usage CPU Hours per machine	13'576'800	3'410'090	72'019'670	5'161'987	326'505	33'133	94'528'185

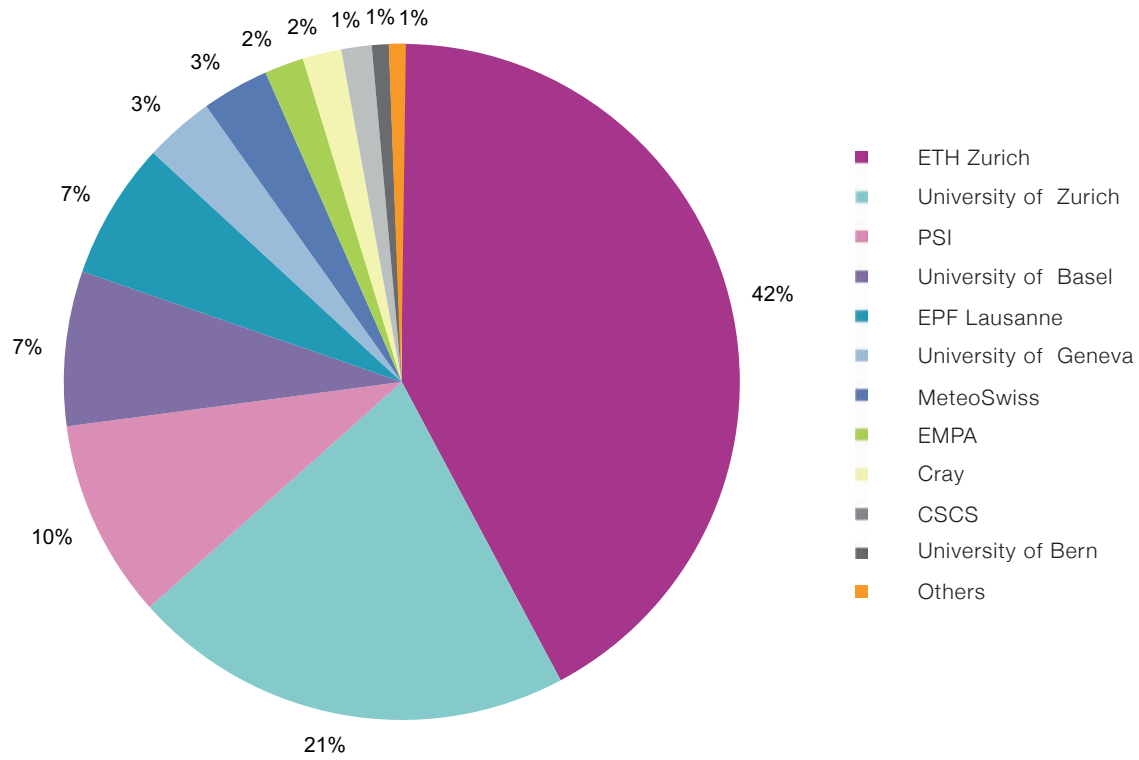
Usage by customer

	Cray XT3 PALU	Cray XT4 BUIN	Cray XT5 ROSA	IMB P5 BLANC	SUN Cluster RIGI	HP Cluster HORUS	Total
ETH Zurich	51.82%	17.33%	41.30%	48.55%	6.11%	17.99%	42.21%
University of Zurich	12.22%	0.03%	24.42%	15.03%	0.00%	0.14%	21.18%
PSI	15.85%	0.05%	9.39%	1.22%	0.00%	0.00%	9.50%
University of Basel	6.88%	0.00%	8.11%	4.19%	0.36%	0.30%	7.40%
EPF Lausanne	7.16%	0.00%	6.14%	15.55%	0.00%	0.00%	6.55%
University of Geneva	2.34%	0.00%	3.38%	7.68%	0.00%	0.00%	3.33%
MeteoSwiss	0.66%	82.53%	0.01%	0.00%	39.13%	0.00%	3.21%
EMPA	1.23%	0.00%	1.81%	5.88%	0.00%	0.00%	1.88%
Cray	0.00%	0.00%	2.44%	0.00%	0.00%	0.00%	1.86%
CSCS	0.18%	0.06%	1.78%	0.07%	9.22%	81.57%	1.45%
University of Bern	1.66%	0.00%	0.63%	1.81%	0.00%	0.00%	0.81%
Others	0.00%	0.00%	0.60%	0.00%	45.17%	0.00%	0.61%
Total Usage CPU Hours per machine	13'576'800	3'410'090	72'019'670	5'161'987	326'504	33'133	94'528'185

CPU Usage per Research Field in 2009



CPU Usage per Institution in 2009

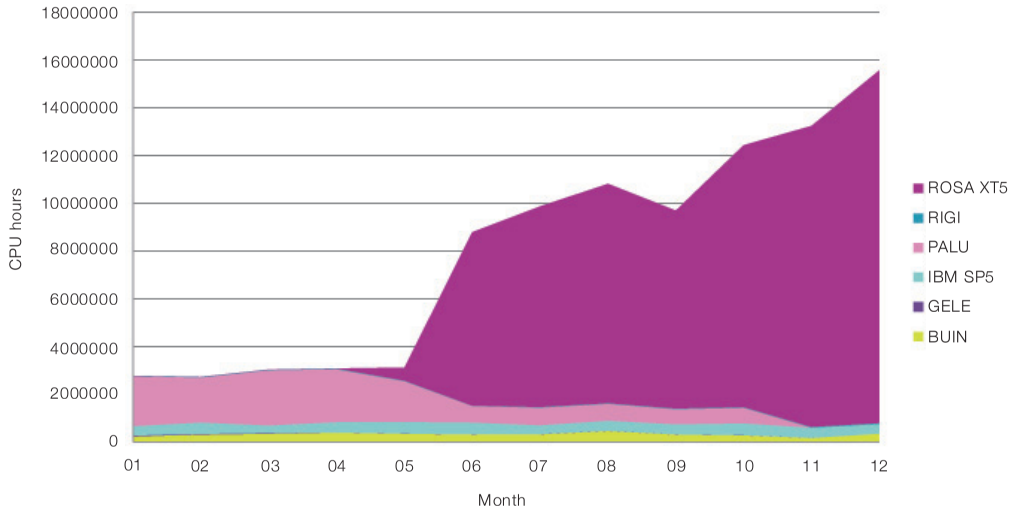


Compute Infrastructure

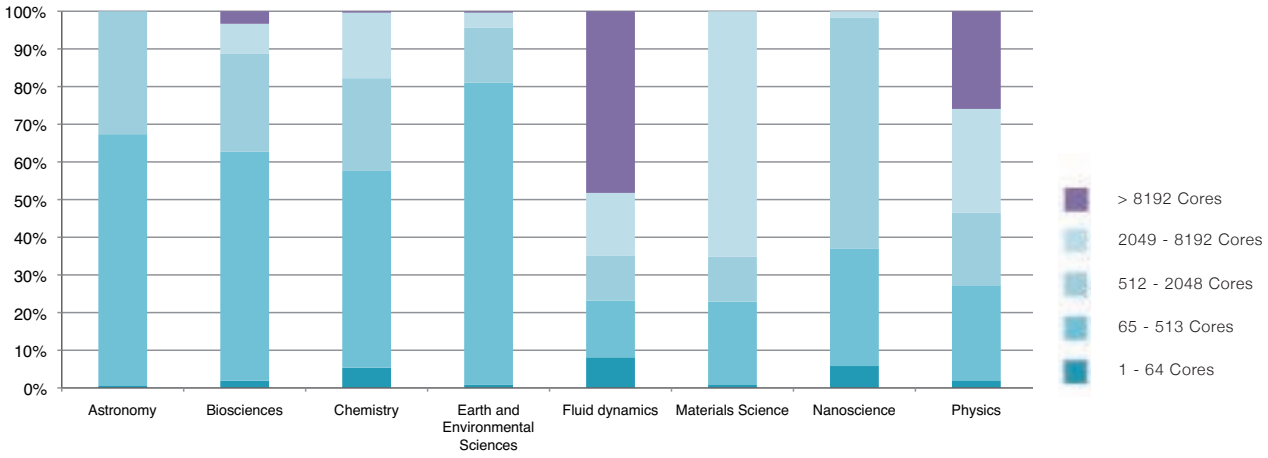
Vendor & Model	CPU Type	No. of Processors	No. of Nodes	Inter-connect type	Interconnect peak bandwidth (GB/sec)	Total memory size (GB)	Year of installation	Core Peak Performance (Gflops)	Peak Performance (Tflops)	LINPACK Performance (Tflops) Nov. 09	Top500 position Nov. 09	Produced (consumed) CPU hours	Average Utilisation (%)	Annual direct costs in 2009 (kCHF)
CRAY XT5 Rosa	AMD Opteron 2.4 GHz	22128	1844	CRAY Seastar2+	57.6	29504	2009	9.6	212.43	169	21	72,019,670.00*	88.4	3'094
CRAY XT4 Buin	AMD Opteron 2.3 GHz	1040	260	CRAY Seastar2	45.6	2080	2009	9.2	9.57	-	-	3'410'090.00	43.8	1'404
IBM p575 Blanc	IBM Power5 1.5 GHz	768	48	Infiniband 4X SDR	-	1650	2006	6	4.61	-	-	5'161'986.00	76.7	1'383
HP-XC Cluster	AMD Opteron 2.4 GHz	34	16	Infiniband 4X SDR	1	128	2007	9.6	0.16			33'133.16	11.1	205
SUN Cluster	AMD Opteron 2.6 GHz	104	26	Infiniband 4X SDR	2	208	2007	14	0.54			326'504.64	35.8	200

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

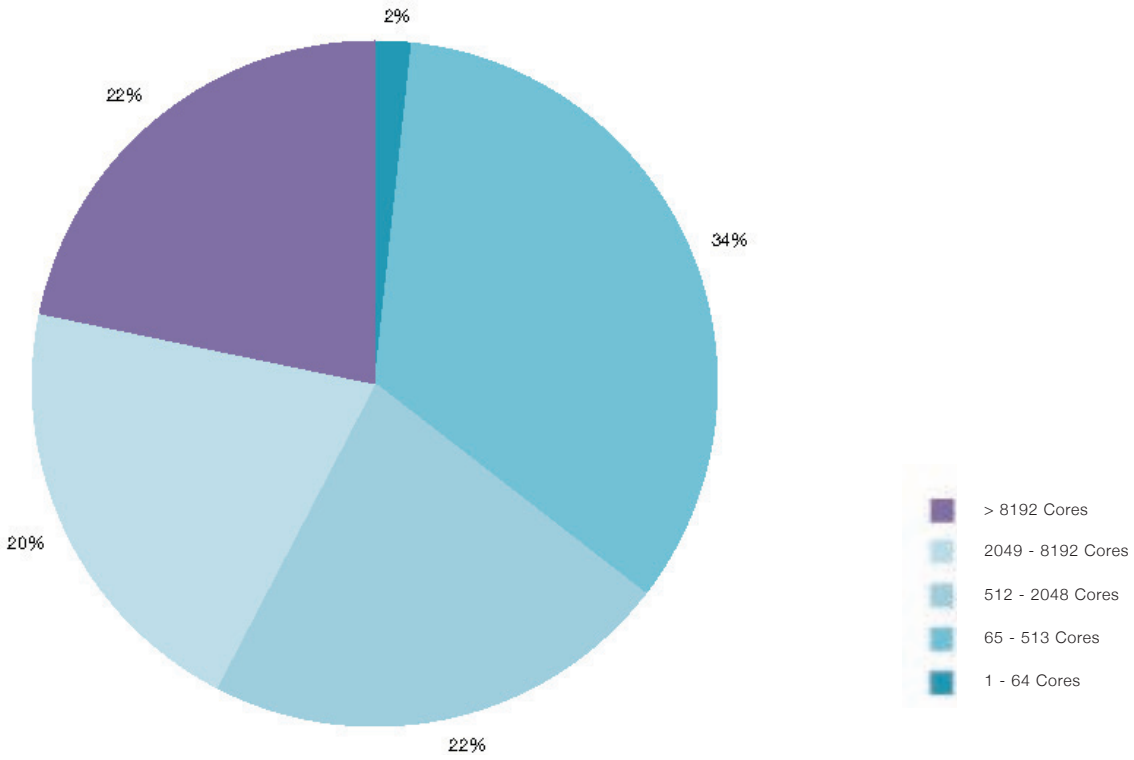
Evolution of CPU usage in 2009



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



fideconto revisioni

Fideconto Revisioni SA
Società di revisione

Report of the auditors
to CSCS Directorate

CSCS – SWISS NATIONAL SUPERCOMPUTUNG 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 indipendence.

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

FIDECONTO REVISIONI SA

Claudio G. Fontana
Auditor in charge

Andrea Pedrotti

Financial reporting

SEDE | CH-6500 Bellinzona
via Canc. Molo 11
Tel. +41 91 820 67 00

SUCCURSALE | CH-6600 Locarno
via Ciseri 23
Tel. +41 91 756 02 00

www.fideconforevisioni.com • info@fidecontorevisioni.com • N. IVA 361 013

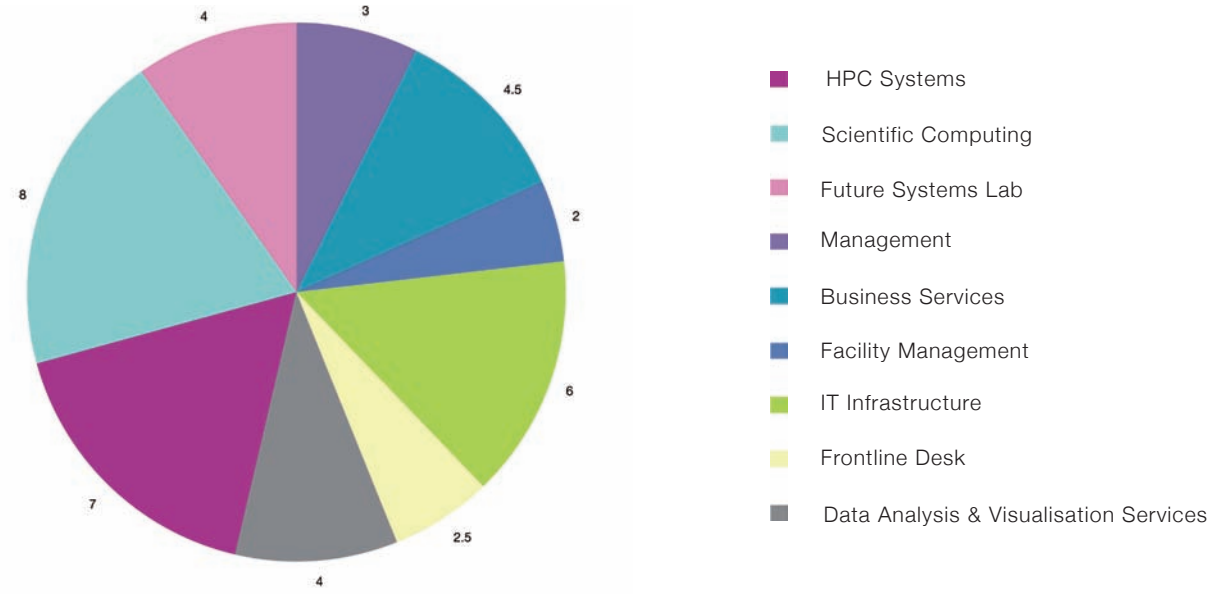
Journal Impact Factor for Papers Listed in the 2008 Annual Report

Publication	Impact factor	Principal investigator	Application field
Bernet, ML; Miniati, F; Lilly, SJ, et al. Strong magnetic fields in normal galaxies at high redshift; NATURE, 45 (7202) 302-304 (2008)	31.434	Francesco Miniati	Astrophysics
Raiteri, P; Bussi, G; Cucinotta, CS, et al. Unravelling the shuttling mechanism in a photoswitchable multicomponent bistable rotaxane; ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, 47 (19) 3536-3539 (2008)	10.879	Michele Parrinello	Material Science / Nanochemistry
Urakawa, A; Maeda, N; Baiker, A. Space-and time-resolved combined DRIFT and Ramen; Spectrocopy: monitoring dynamic surface and bulk processes during NO_x storage reduction; ANGEWANDTE CHEMIE-INTERNATIONAL EDITION, 47 (48) 9256-9259 (2008)	10.879	Alfons Baiker	Material Science
Milos, M; Kairouani, S; Rabaste, S, et al. Energy migration within the E-2 state of Cr^{3+}; COORDINATION CHEMISTRY REVIEWS, 252 (23-24) 2540-2551 (2008)	10.588	Andreas Hauser	Chemistry
Joos, F; Spahni, 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)	9.380	Fortunat Joos	Climate
Van Vuuren, DP; Meinshausen, M; Plattner, GK, et al. Temperature increase of 21st century mitigation scenarios; PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA, 105 (40) 15258-15262 (2008)	9.380	Fortunat Joos	Climate
Zhuang, W; Kasemi, E; Ding, Y, et al. Self-folding of charged single dendronized polymers; ADVANCED MATERIALS, 20 (17) 3204-3210 (2008)	8.191	Martin Kroeger	Material Science
Bonomi, M; Branduardi, D; Gervasio, FL, et al. The unfolded ensemble and folding mechanism of the C-terminal GB1 beta-hairpin; JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 130 (42) 13938-13944(2008)	8.091	Francesco Gervasio	Biosciences
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)	8.091	Michele Parrinello	Biosciences
Gossens, C; Tavernelli, I; Rothlisberger, U. DNA structural distortions induced by ruthenium-arene anticancer compounds; JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 130 (33) 10921-10928 (2008)	8.091	Ursula Roethlisberger	Biosciences
Masson, F; Laino, T; Tavernelli, I, et al. Computational study of thymine dimer radical anion splitting in the self-repair process of duplex DNA; JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 130 (11) 3443-3450 (2008)	8.091	Juerg Hutter / Ursula Roethlisberger	Biosciences
Mobian, P; Nicolas, C; Francotte, E, et al. Synthesis, resolution, and VCD analysis of an enantiopure diazaoxatricornan derivative; JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 130 (20) 6507-6514 (2008)	8.091	Thomas Buergi	Nanoscience
Xiao, W; Passerone, D; Ruffieux, P, et al. C-60/corannulene on CU (110): A surface-supported bistable buckybowl-buckyball host-guest system; JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, 130 (14) 4767-4771 (2008)	8.091	Daniele Passerone	Material Science

Source: ISI Web of Knowledge SM

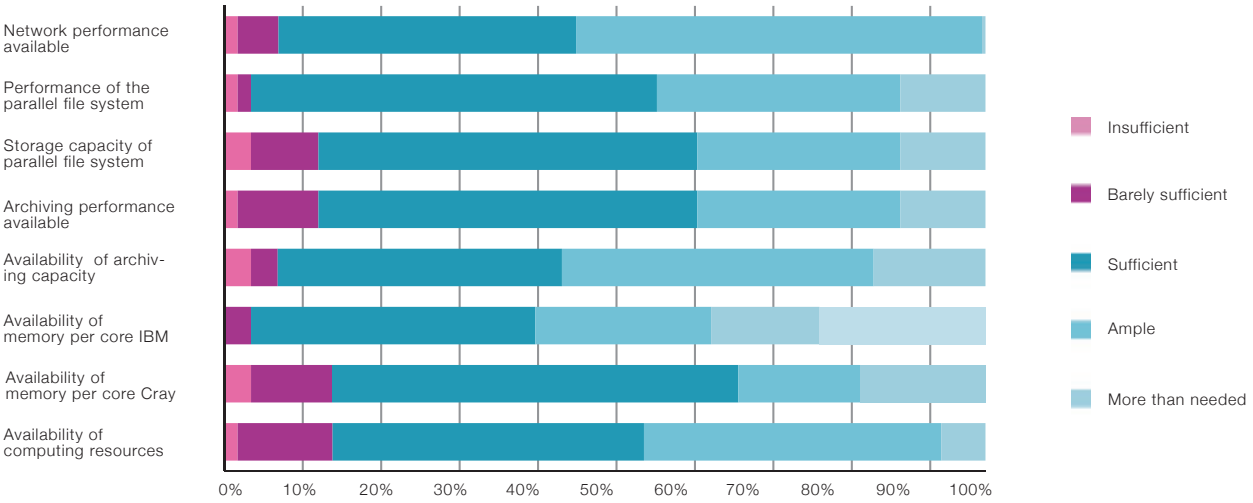
Personnel

FTE per Unit on December 31, 2009

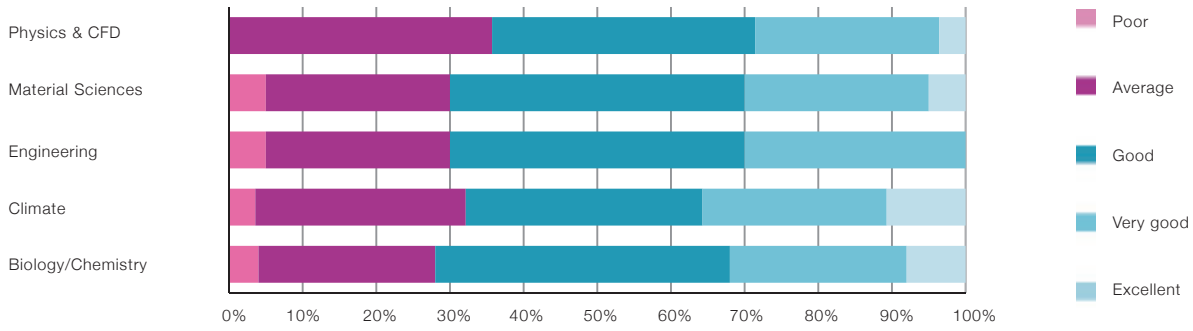


Customer Satisfaction (2009)

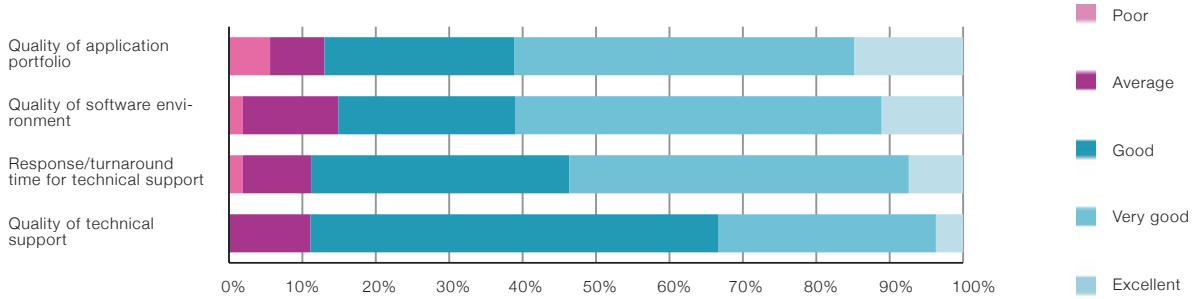
CSCS services portfolio



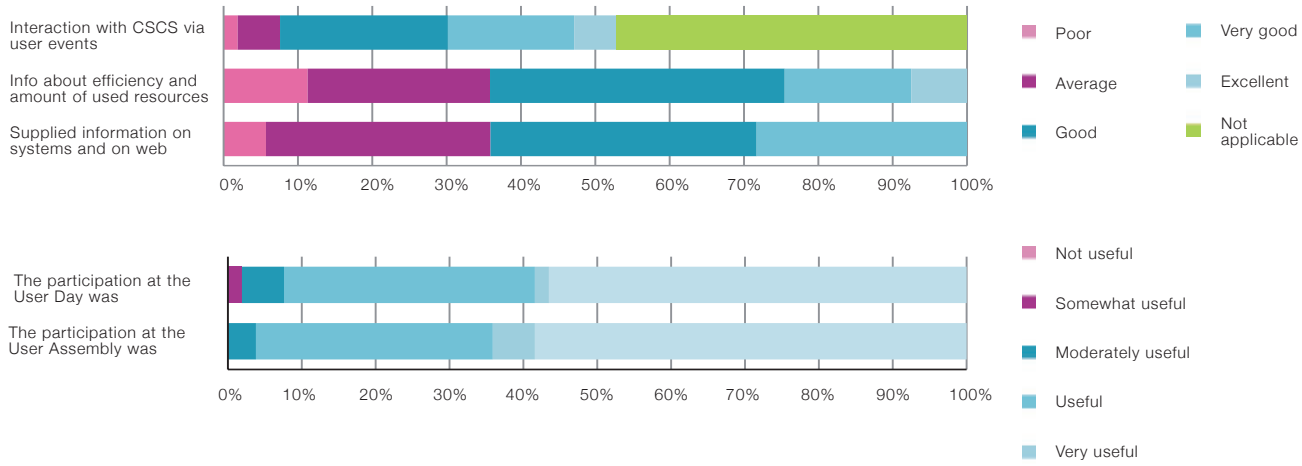
Quality of user support in the following fields



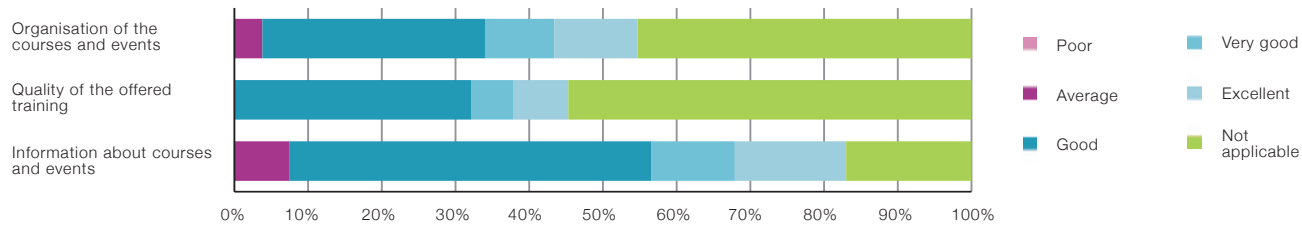
Application and user support



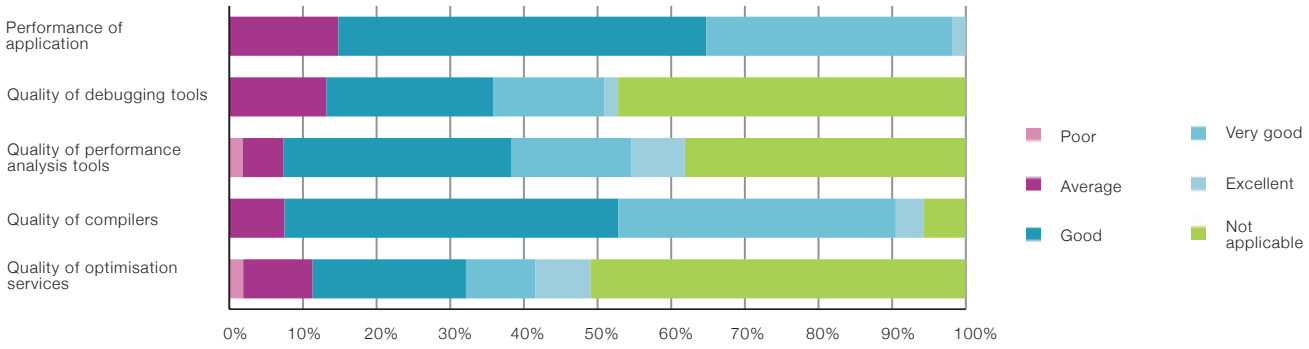
Information services



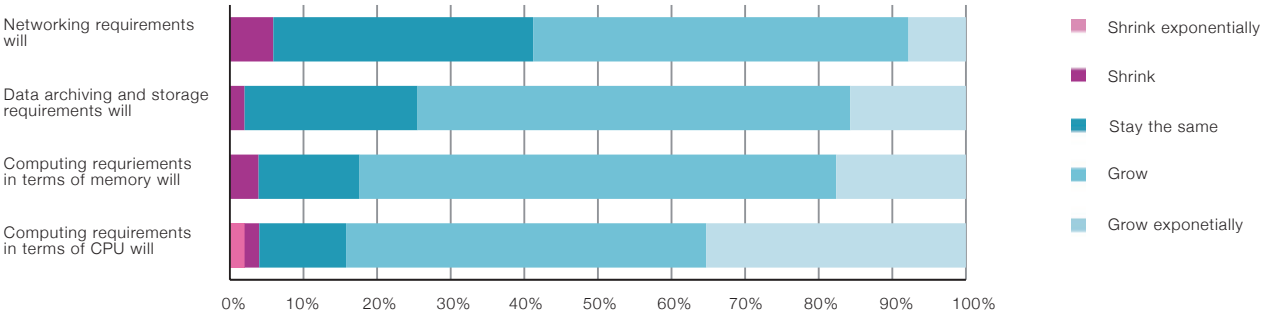
Training course and events



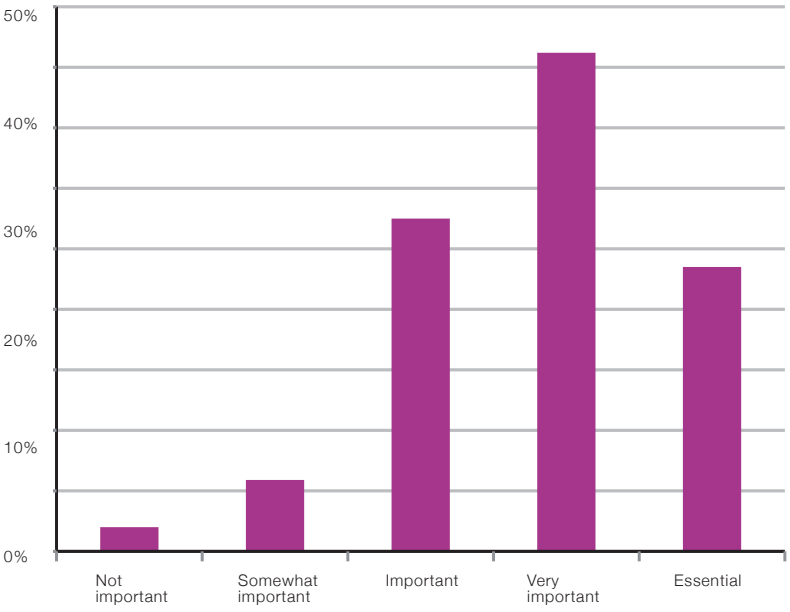
Software support and development



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:

[1] A. Adelmann, P. Arbenz, and Y. Ineichen: “A Fast Parallel Poisson Solver on Irregular Domains Applied to Beam Dynamic Simulations”, July 2009, 21pp. e-Print: arXiv:0907.4863 [physics.comp-ph].

Prof. Wanda Andreoni:

[1] P. Clausen, W. Andreoni, A. Curioni, E. Hughes, ”Water Adsorption at a Sodium Smectite Clay Surface: an ab initio Study of the First Stage ”, J. Chem. Phys. 2009.

Prof. Peter Arbenz:

[1] S. Paranjape, M. Kaufmann, P. Arbenz: “WebParFE: A a Web interface for the High-Performance Parallel Finite Element Solvent ParFE”. Technical Report 654, Chair of Computational Science, ETH Zürich, December 2009.

[2] A.J. Wirth, Th.L. Mueller, W. Vereecken, C. Flaig, P. Arbenz, R. Müller, G.H. van Lenthe: Mechanical competence of bone-implant systems can accurately be determined by image-based micro-finite element analyses. Appl. Mech., online 29.10.2009, doi:10.1007/s00419-009-0387-x.

[3] P. Arbenz, J. Bryner, Ch. Tobler: Parallelized transient elastic wave propagation in orthotropic structures. Accepted for publication in the proceedings of the 8th Conference on Parallel Processing and Applied Mathematics. Wroclaw, Poland, Sept 13-16, 2009.

[4] A. Adelmann, P. Arbenz, and Y. Ineichen: “A Fast Parallel Poisson Solver on Irregular Domains Applied to Beam Dynamic Simulations”, July 2009, 21pp. e-Print: arXiv:0907.4863 [physics.comp-ph].

Prof. Alfons Baiker:

[1] P. Haider, J.D. Grunwaldt, and A. Baiker: “Gold Supported on Mg, Al and Cu containing Mixed Oxides: Relation between Surface Properties and Catalytic Behavior in Aerobic Oxidation of 1-Phenylethanol”. Catal. Today, 141, 349 (2009).

[2] F. Jutz, J.D. Grunwaldt, and A. Baiker: ”In situ XAS Study of the Mn(III)(salen)Br Catalyzed Synthesis of Cyclic Organic Carbonates from Epoxides and CO_2,” J. Mol. Catal. A, 297, 63 (2009).

[3] T. Seki, J.D. Grunwaldt, and A. Baiker: ”In Situ Attenuated Total Reflection Infrared Spectroscopy of Imidazolium-Based Ionic Liquids under Supercritical CO_2,” J. Phys. Chem. B, 113, 114 (2009).

[4] B. Kimmerle, P. Haider, J.D. Grunwaldt, A. Baiker, P. Boye, and C. G. Schroer: ”High Throughput Cell for X-ray Absorption Spectroscopy Applied to Study the Effect of Au on Rh-Catalyzed Partial Oxidation of Methane,” Appl. Catal. A, 353, 36 (2009).

[5] S. Roy, and A. Baiker: ”NO_x Storage-Reduction Catalysis: From Mechanism and Materials Properties to Storage-Reduction Performance,” Chem. Rev., 109, 4054 (2009).

[6] L. Aschwanden, T. Mallat, J.D. Grunwaldt, F. Krumeich, and A. Baiker: ”Gold Catalyzed Aerobic Oxidation of Dibenzylamine: Homogeneous or Heterogeneous Catalysis?,” J. Mol. Catal. A., 300, 111 (2009).

[7] R. Büchel, R. Strobel, F. Krumeich, A. Baiker, and S.E. Pratsinis: ”Influence of Pt Location on $BaCO_3$ or Al_2O_3 during NO_x Storage-Reduction,” J. Catal., 261, 201 (2009).

[8] M. O. Symalla, A. Drochner, H. Vogel, R. Büchel, S. E. Pratsinis, and A. Baiker: ”Structure and NO_x-Storage Behaviour of Flamemade $BaCO_3$ and $Pt/BaCO_3$ Nanoparticles,” Appl. Catal. B, 89, 41 (2009).

[9] B. Kimmerle, J.D. Grunwaldt, A. Baiker, P. Glatzel, P. Boye, S. Stephan, C. G. Schroer: ”Visualisation of the Ignition of Catalytic Partial Oxidation of Methane,” J. Phys.Chem. C, 113, 3037 (2009).

[10] S. Marx and A. Baiker: ”Beneficial Interaction of Gold and Palladium in Bimetallic Catalysts for the Selective Aerobic Oxidation of Benzyl Alcohol”, J. Phys. Chem. C, 113, 6191 (2009).

[11] B. Panella, A. Vargas, and A. Baiker: ”Magnetically Separable Pt Catalyst for Asymmetric Hydrogenation”, J. Catal., 261, 88 (2009).

[12] Y. Jiang, J. Huang, B. Kasumaj, G. Jeschke, M. Hunger, T. Mallat, and A. Baiker: ”Adsorption-Desorption Induced Structural Changes of Cu-MOF Evidenced by Solid State NMR and EPR Spectroscopy”, J. Amer. Chem. Soc., 131, 2058 (2009).

[13] F. Hoxha, N. van Vegten, A. Urakawa, F. Krumeich, T. Mallat, and A. Baiker: ”Remarkable Particle Size Effect in Rh–Catalyzed Enantioselective Hydrogenations”, J. Catal., 261, 224 (2009).

[14] P. Haider, A. Urakawa, E. Schmidt, and A. Baiker: ”Selective Blocking of Active Sites on Supported Gold Catalysts by Adsorbed Thiols and its Effect on the Catalytic Behaviour. A Combined Catalytic, in situ ATR and DFT Study”, J. Mol. Catal. A: Chemical, 305, 161 (2009).

[15] L. Aschwanden, T. Mallat, F. Krumeich, and A. Baiker: ”Simple Preparation of an Efficient Heterogeneous Gold Catalyst for Amine Oxidation”, J. Mol. Catal. A: Chemical, 309, 57 (2009).

[16] I. Hermans, E. Spiers, U. Neuenschwander, N. Turra, and A. Baiker: ”Selective Oxidation Catalysis: Opportunities and Challenges”, Top. Catal., 52, 1162 (2009).

[17] T. Seki and A. Baiker: ”Catalytic Oxidations in Dense Carbon Dioxide”, Chem. Rev., 109, 2409 (2009).

[18] L. Aschwanden, B. Panella, P. Rossbach, B. Keller, and A. Baiker: ”Magnetically Separable Gold Catalyst for Aerobic Oxidation of Amines”, Chem. Cat. Chem., 1, 111 (2009).

[19] D. Ferri and A. Baiker: ”Advances in Infrared Spectroscopy of Catalytic Solid-Liquid Interfaces: The Case of the Selective Alcohol Oxidation”, Top. Catal., 52, 1323 (2009).

[20] D.M. Meier, A. Urakawa, R. Mäder and A. Baiker: ”Design and Performance of a Flow-Through Polarization-Modulation Infrared Reflection-Absorption Spectroscopy Cell for Time-Resolved Simultaneous Surface and Liquid Phase Detection under Concentration and Temperature Perturbations”, Rev. Sci. Instrum., 80, 094101 (2009).

[21] J.D. Grunwaldt, B. Kimmerle, A. Baiker, P. Boye, C. Schroer, P. Glatzel, C. Borca, and F. Beckmann: ”Catalysts at Work: From Integral to Spatially Resolved X-ray Absorption Spectroscopy”, Catal. Today, 145, 267 (2009).

[22] A. Urakawa and A. Baiker: ”Space–Resolved Profiling Relevant in Heterogeneous Catalysis”, Top. Catal., 52, 1312 (2009).

[23] H. Hesske, A. Urakawa, and A. Baiker: "Ab Initio Assignments of FIR, MIR, and Raman Bands of Bulk Ba Species Relevant in NO_x Storage-Reduction", J. Phys. Chem. C, 113, 12286 (2009).

[24] W. Kleist, F. Jutz, M. Maciejewski and A. Baiker: "Mixed-Linker Metal-Organic Frameworks as Catalysts for the Synthesis of Propylene Carbonate from Propylene Oxide and CO_2", Eur. J. Inorg. Chem., 3552 (2009).

[25] C. Mondelli, A. Vargas, G. Santarossa, and A. Baiker: "Fundamental Aspects of the Chiral Modification of Platinum with Peptides: Asymmetric Induction in Hydrogenation of Activated Ketones", J. Phys. Chem. C. 113, 15246 (2009).

[26] T. Seki, J.M. Andanson, F. Jutz, and A. Baiker:"Tracing the Acetalization in CO_2-Expanded Alcohols by In Situ Attenuated Total Reflection Infrared Spectroscopy", Appl. Spectrosc., 63, 1008 (2009).

[27] Supercritical CO2 / Ionic Liquid Systems: What Can We Extract from Infrared and Raman Spectra? , by J.M. Andanson, F. Jutz, and A. Baiker, J. Phys. Chem. B, 113, 10249 (2009).

[28] S. Hannemann, J.D. Grunwaldt, B. Kimmerle, A. Baiker, P. Boye, and C. Schroer: "Axial Changes of Catalyst Structure and Temperature in a Fixed-Bed Microreactor during Noble Metal Catalyzed Partial Oxidation of Methane", Top. Catal., 52, 1360 (2009).

[29] M. Kamperman, A. Burns, R. Weissgraeber, N. van Vegten, S. C. Warren, S. M. Gruner, A. Baiker, and U. Wiesner: "Integrating Eight Length Scales in Porous High Temperature Ceramics with Catalytic Function", Nano Lett., 9, 2756 (2009).

[30] E. Schmidt, A. Vargas, T. Mallat and A. Baiker: "Shape-Selective Enantioselective Hydrogenation on Pt Nanoparticles", J. Amer. Chem. Soc., 131, 12358 (2009).

[31] D.M. Meier, A. Urakawa, and A. Baiker: "Polarization-Modulation Infrared Reflection-Absorption Spectroscopy Affording Time-Resolved Simultaneous Detection of Surface and Liquid Phase Species at Catalytic Solid-Liquid Interfaces", Analyst, 134, 1779 (2009).

[32] N. van Vegten, P. Haider, M. Maciejewski, F. Krumeich, and A. Baiker: "Chemisorption of Methyl Mercaptane on Titania Supported Au Nanoparticles: Viability of Au Surface Area Determination", J. Colloid Interface Sci., 339, 310 (2009).

[33] N. Maeda, A. Urakawa, and A. Baiker: "Support Effects and Chemical Gradients along the Catalyst Bed in NO_x Storage-Reduction Studied by Space- and Time-Resolved in situ DRIFTS", J. Phys. Chem. C, 113, 16724 (2009).

[34] B. Panella, A. Vargas, D. Ferri, and A. Baiker: "Chemical Availability and Reactivity of Functional Groups Grafted to Magnetic Nanoparticles Monitored insitu by ATR-IR Spectroscopy", Chem. Mater., 21, 4316 (2009).

[35] R. Büchel, R. Strobel, A. Baiker, and S.E. Pratsinis: "Flamemade Pt/K/Al_2O_3 for NO_x Storage-Reduction (NSR) Catalysts", Top. Catal., 52, 1799 (2009).

[36] J.D. Grunwaldt, M. Beier, B. Kimmerle, A. Baiker, B. Griesebock, D. Lützenkirchen-Hecht, and R. Frahm: "Dynamic Structural Changes during the Ignition and Extinction of the Partial Oxidation of Methane Studied with Advanced QEXAFS Techniques", Phys. Chem. Chem. Phys., 11, 8779 (2009).

PD Dr. Dirk Bakowies:

[1] Bakowies D., "Ab initio thermochemistry with high-level isodesmic corrections: Validation of the ATOMIC protocol for a large set of compounds with first-row atoms (H, C, N, O, F)", J. Phys. Chem. A 2009.

[2] Bakowies, D., "Ab initio thermochemistry using optimal-balance models with isodesmic corrections: The ATOMIC protocol ", J. Phys. Chem. C 2009, 113, 15218-15225.

Dr. Alessandro Barducci:

[1] M. Bonomi, A. Barducci, M. Parrinello, "Reconstructing the equilibrium Boltzmann distribution from well-tempered metadynamics", J. Comput. Chem. 2009, 30, 1615-1621

Prof. Simon Bernèche

[1] C. Wirth, G. Condemine, C. Boiteux, S. Bernèche, T. Schirmer, and C. M. Peneff, "NanC crystal structure, a model for outer membrane channels of the acidic sugar-specific KdgM proin family", J.Mol. Biol. Doi:10.1016/j.jmb.2009.09.054 (2009).

Dr. Dominik Brunner:

[1] C. Knote, G. Bonafe, F. Di Giuseppe, "Leaf Area Index Specification for Use in Mesoscale Weather Prediction Systems", Monthly Wearger Review, 137 (10), 3535-3550.

[2] D. Brunner, P. Siegmund, P. T. May, L. Chappel, C. Schiller, R. Müller, T. Peter, S. Fueglistaler, A. R. MacKenzie, A. Fix, H. Schlager, G. Allen, A. M. Fjaeraa, M. Streibel, and N. R. P. Harris, "The SCOUT-O3 Darwin Aircraft Campaign: rationale and meteorology", Atmos. Chem. Phys., 9, 93-117, 2009.

[3] O. R. Cooper, S. Eckhardt, J. H. Crawford, C. C. Brown, R. C. Cohen, T. H. Bertram, P. Wooldridge, A. Perring, W. H. Brunner, X. Ren, D. Brunner, and S. L. Baughcum (2009), "Summertime buildup and decay of lightning NO_x and aged thunderstorm outflow above North America", J. Geophys. Res., 114, D01101, doi:10.1029/2008JD010293, 2009.

[4] G. Allen, G. Vaughan, D. Brunner, P. T. May, W. Heyes, P. Minnis, and J. K. Ayers, "Modulation of tropical convection by breaking Rossby waves", Q. J. R. Met. Soc., 135, 125-137, doi:10.1002/qj.349, 2009.

Dr. Wilfred Anthony Cooper:

[1] W. Anthony Cooper, Steven P. Hirshman, Peter Merkel, Jonathan P. Graves, Johann Kisslinger, Horst F. G. Wobig, Yoshiro Narushima, Shoichi Okamura, and Kiyomasa Y. Watanabe, "Three-dimensional anisotropic pressure free boundary equilibria", In Computer Physics Communications, volume 180, number 9, pages 1524-1533, 2009.CRPP-ARTICLE-2009-.

[2] J. P. Graves, M. Jucker, et al., "A new theory of sawtooth control by off-axis toroidally propagating ICRF waves and experimental tests of its predictions in the JET tokamak", Invited paper presented at European Fusion Theory Conference. Riga, Latvia, (2009).

Dr. Clotilde Cucinotta:

[1] C. S. Cucinotta, G. Miceli, P. Raiteri, M. Krack, T. Kühne, M. Bernasconi, and M. Parrinello, Superionic Conduction in Substoichiometric LiAl Alloy: an Ab–Initio Study, Phys. Rev. Lett., 103 (12), 125901 (2009).

[2] C. S. Cucinotta, M. Kosa, A. Cavalli, P. Melchiorre and F. L. Gervasio, Bifunctional Catalysis by Cinchona Alkaloids: a Mechanism Explained, Chem. Eur. Jour. 15 (32), 7913-7921 (2009).

Prof. Andrea Danani:

[1] G. Ambrosetti, N. Johner, C. Grimaldi, T. Maeder, P. Ryser and A. Danani, "Electron Tunneling in conductor-insulator composites with spherical fillers", Journal of Applied Physics, 106, 016103 (2009)

[2] Pavan G.M., Danani A., Pricl S., Smith D.K., "Modeling the Multivalent Recognition between Dendritic Molecules and DNA: Understanding How Ligand Sacrifice and Screening Can Enhance Binding", JACS-Journal of the American Chemical Society 2009, 131(28):9686-94

Prof. Wolfgang Fichtner:

[1] B. Sahli, K. Vollenweider, W. Fichtner "Ab initio Calculations for Point Defect Clusters with P, As, and Sb in Si" Physical Review B, vol. 80, pp. 075208, Aug 2009

[2] K. Vollenweider, B. Sahli, W. Fichtner, Ab Initio Study of Fluorine in Silicon: Large Clusters and the Dominant Mobile Defect Physical Review Letters, vol. 103, pp. 075503, Aug 2009

[3] K. Vollenweider, B. Sahli, N. Zographos, C. Zechner Fluorine Clustering and Diffusion in Silicon: Ab Initio Calculations and Kinetic Monte Carlo Model Proc. of Insight - 2009, Napa, CA, USA, pp. 317-323, Apr 2009

[4] A. Esposito, M. Luisier, M. Frey, A. Schenk A Nonparabolicity Model Compared to Tight-Binding: The Case of Square Silicon Quantum Wires Solid-State Electronics, vol. 53, no. 3, pp. 376-382, Jan 2009

[5] V. Peikert, A. Schenk A First Analysis of a New Fixed Point Iteration of the Boltzmann Equation: Application to TCAD, International Conference on Ph.D. Research in Microelectronics & Electronics 2009 (PRIME), Cork, Ireland, 14 Jul 2009

[6] M. Frey, A. Esposito, A. Schenk Boundary Conditions for Incoherent Quantum Transport Proc. of 13th International Workshop on Computational Electronics (IWCE-13), Beijing, China, pp. 17-20, May 2009

Dr. Christos Frouzakis:

[1] Dynamics of premixed flames in a narrow channel with a step-wise wall temperature, Combust. Flame, 156(11):2190-2200, 2009 (with VN Kurdyumov, G Pizza, J Mantzaras).

[2] Method of invariant grid for model reduction of hydrogen combustion, Proc. Comb. Inst 32(1):519-526, 2009 (with E Chiavazzo, IV Karlin, K Boulouchos)

[3] Suppression of combustion instabilities of premixed hydrogen/air flames in microchannels using heterogeneous reactions, Proc. Comb. Inst. 32(2):3051-3058, 2009 (with G. Pizza G, J. Mantzaras J, A. Tomboulides, K. Boulouchos).

Prof. Stefan Goedecker:

[1] X. Gonze et al.:ABINIT: First-principles approach to material and nanosystem properties, Computer Physics Communications 180 2582 (2009).

[2] Luigi Genovese, Matthieu Ospici, Thierry Deutsch, Jean-Francois Mohaut, Alexey Neelov and Stefan Goedecker: Density functional theory calculation on many-cores hybrid central processing unit-graphic processing unit architectures, J. Chem. Phys. 131, 034103 (2009).

[3] Shantanu Roy, Stefan Goedecker, Martin J. Field and Evgeni Penev: A Minima Hopping Study of All-Atom Protein Folding and Structure Prediction, J. Phys. Chem. B, 113, 7315 (2009).

[4] Maximilian Amsler, S. Alireza Ghasemi, Stefan Goedecker, Alexey Neelov and Luigi Genovese: Adsorption of small NaCl clusters on surfaces of silicon nanostructures, Nanotechnology 20, 445301 (2009).

[5] Sandro E. Schoenborn, Stefan Goedecker, Shantanu Roy: The performance of Minima Hopping and Evolutionary Algorithms for cluster structure prediction, J. Chem. Phys. 130, 144108 (2009).

[6] Kuo Bao, Stefan Goedecker, Kenji Koga, Frederic Lancon, and Alexey Neelov: Structure of large gold clusters obtained by global optimization using the minima hopping method, Phys. Rev. B 79 041405 (2009).

Prof. Andreas Hauser:

[1] A. Vargas, A. Hauser, L. M. Lawson Daku "Influence of guest-host interactions on the structural, energetic and Mössbauer spectroscopy properties of iron(II)tris(2,2'-bipyridine) in the the low-spin and high-spin states : a density-functional theory study of the zeolite-Y embedded complex." J. Chem. Theory Comput. 2009, 5, 97-115.

[2] L. M. Lawson Daku A. Castaings, J.-C. Marchon "Density-functional theory study of the stereochemistry of chloroiron(III) and chloromanganese(III) complexes of a bridled chiroporphyrin." Inorg. Chem. 2009, 48, 5164-5176.

[3] V. Mishra, R. Mukherjee, J. Linares, F. Varret, M. Lawson Daku. "Spin-transition in nearly cubic site in [FeII(L)3][PF6]2", Hyperfine Interactions, 2009, 188, 71-78

Prof. Jürg Hutter:

[1] "Magnetic linear response properties calculations with the Gaussian and augmented-plane-wave method" V. Weber, M. Iannuzzi, S. Giani, J. Hutter, R. Declerck, M. Waroquier; J. Chem. Phys. 131 014106 (2009).

[2] "Low-Barrier Pathway for endo-Cleavage Induced Anomerization of Pyranosides with N-Benzyl-2,3-trans-oxazolidinone Groups" H. Satoh, J. Hutter, H. P. Luethi, S. Manabe, K. Ishii, Y. Ito; Europ. J. Org. Chem. 8 1127-1131 (2009).

[3] "A Scheme for the Evaluation of Electron Delocalization and Conjugation Efficiency in Linearly pi- Conjugated Systems" M. Bruschi, P. A. Limacher, J. Hutter, H. P. Luethi; J. Chem. Theo. Comp. 5 506-514 (2009).

[4] "A QM/MM Investigation of Thymine Dimer Radical Anion Splitting Catalyzed by DNA Photolyase" F. Masson, T. Laino, U. Rothlisberger, J. Hutter; Chem. Phys. Chem. 10 400-410 (2009).

Prof. Andrew Jackson:

[1] Livermore, P. W., Ierley, G. and Jackson, A. (2009) "The construction of exact Taylor states. I: The full sphere", Geophys. J. Int. , 179, 923-928.

[2] Stockmann, R., Finlay, C.C. and Jackson, A. (2009) "Imaging Earth's crustal magnetic field with satellite data: a regularized spherical triangle tessellation approach", Geophys. J. Int. , 179, 929-944.

[3] While, J., Biegert, E. and Jackson, A. (2009) "Generalized sampling interpolation of noisy gravity/gravity gradient data", Geophys. J. Int, 178, 638-650.

[4] Buffett, B.A., Mound, J. and Jackson, A. (2009) “Inversion of torsional oscillations for the structure and dynamics of Earth’s core”, Geophys. J. Int, 177, 878-890.

Prof. Fortunat Joos:

[1] Cao, L., M. Eby, A. Ridgwell, K. Caldeira, D. Archer, A. Ishida, F. Joos, K. Matsumoto, U. Mikolajewicz, A. Mouchet, J. C. Orr, G.-K. Plattner, R. Schlitzer, K. Tokos, I. Totterdell, T. Tschumi, Y. Yamanaka, and A. Yooll, ”The role of ocean transport in the uptake of anthropogenic CO_2”, Biogeosciences, 6/3, 375-390,2009

[2] Elsig, J., J. Schmitt, D. Leuenberger, R. Schneider, M. Eyer, M. Leuenberger, F. Joos, H. Fischer, T. F. Stocker, ”Stable isotope constraints on Holocene carbon cycle changes from an Antarctic ice core”, Nature, 461, 507-510,2009

[3] Fischer, H., J. Schmitt, D. Lüthi, T. Tschumi, P. Parekh, F. Joos, T.F. Stocker, P. Köhler, C. Völker, R. Gersonde, C. Barbante, M. Le Floch, D. Raynaud, J. Chappellaz, E. W. Wolff, ”The role of Southern Ocean processes on orbital and millenial CO_2 variations - a synthesis”, Quaternary Science Reviews, in press, 2009

[4] Frank, D.C., J. Esper, C.C. Raible, U. Büntgen, V. Trouet, B. Stocker, F. Joos, Ensemble reconstruction constraints of the global carbon cycle sensitivity to climate, Nature, resubmitted, 2009

[5] Frölicher, T. L., F. Joos, G.-K. Plattner, M. Steinacher, S. C. Doney, ”Natural variability and anthropogenic trends in oceanic oxygen in a coupled carbon cycle-climate model ensemble”, Global Biogeochemical Cycles, 23/GB1003, 2009

[6] Frölicher, T. L., F. Joos, ”Reversible and irreversible impacts of greenhouse gas emissions in multi-century projections with a comprehensive climate-carbon model”, Climate Dynamics, submitted, 2009

[7] Gerber, M., F. Joos, M. Vázquez-Rodriguez, F. Touratier, C. Goyet, ”Regional air-sea fluxes of anthropogenic carbon inferred with an Ensemble Kalman Filter”, Global Biogeochemical Cycles, 23/GB1013, 2009

[8] Gerber, M., F. Joos, ”Carbon sources and sinks from an Ensemble Kalman Filter ocean data assimilation”, Global Biogeochemical Cycles, submitted, 2009

[9] Gruber, N., M. Gloor, S. Mikaloff Fletcher, S. Doney, S. Dutkiewicz, M. Follows, M. Gerber, A. Jacobson, F. Joos, K. Lindsay, D. Menemenlis, A. Mouchet, S. Müller, J. Sarmiento, T. Takahashi, ”Oceanic sources, sinks, and transport of atmospheric CO2”, Global Biogeochemical Cycles, 23/GB1005, 2009

[10] Gattuso, J.-P., L. Hansson, J. Bijma, H. Elderfield, P. Burkill, T. Tyrrell, M. Edwards, S. Widdicombe, U. Riebesell, M. Steinacher, F. Joos, T. L. Frölicher, C. Turley, K. Boot, K.-M. Davidson, D. Laffoley, P. Saugier, ”European Project on Ocean Acidification (EPOCA): objectives, products and scientific highlights”, Oceanogaphy, accepted, 2009

[11] Köhler, P., R. Bintanja, H. Fischer, F. Joos, G. Lohmann, V. Masson-Delmotte, ”What caused Earth’s temperature variations during the last 800,000 years?”, Quaternary Science Reviews, in press, 2009

[12] Ritz, S. P., T. F. Stocker, F. Joos, ”A three-dimensional coupled ocean-atmosphere model of reduced complexity for paleoclimate studies”, Journal of Climate, submitted, 2009

[13] Steinacher, M., F. Joos, T. L. Frölicher, G.-K. Plattner, S. C. Doney, ”Imminent ocean acidification in the Arctic projected with the NCAR global coupled carbon cycle-climate model”, Biogeosciences, 6/4, 515-533,2009

[14] Steinacher, M., F. Joos, T. L. Frölicher, L. Bopp, P. Cadule, S. C. Doney, M. Gehlen, B. Schneider, J. Segschneider, ”Projected 21st century decrease in marine productivity: a multi-model analysis”, Biogeosciences Discuss, 6, 7933-7981,2009

[15] Strassmann, K. M., G.-K. Plattner, F. Joos, ”CO_2 and non-COðð radiative forcings in climate projections for twenty-first century mitigation scenarios”, Climate Dynamics, 33/6, 737-749,2009

Dr. Daniel Jung:

[1] Conrad, M., Harbrecht, B., Weber, T., Jung, D.Y, and Steurer, W. (2009). “Large, larger, largest – a family of cluster-based tantalum-copper-aluminides with giant unit cells. Part B: The cluster structure”, Acta Crystallographica Section B-Structural Science, 65:318–325.

Dr. Rustam Khaliullin:

[1] R.Z. Khaliullin, A.T. Bell, M. Head-Gordon Chem. Eur. J., 2009, 15(4), 851-855 “Electron donation in the water-water hydrogen bond”

Prof. Leonhard Kleiser:

[1] F. Keiderling, L. Kleiser, and C. Bogey, “Numerical study of eigenmode forcing effects on jet flow development and noise generation mechanisms”, Phys. Fluids, 21:045106, 2009.

[2] J. Ziefle and L. Kleiser, “Large-eddy simulation of a round jet in crossflow”, AIAA J., 47(5):1158–1172, 2009. AIAA 0001-1452.

Prof. Petros Koumoutsakos:

[1] Falcón B.L., Hashizume H., Koumoutsakos P., Chou J., Bready J.V., Coxon A., Oliner J.D., McDonald D.M., Contrasting Actions of Selective Inhibitors of Angiopoietin-1 and Angiopoietin-2 on the Normalization of Tumor Blood Vessels, The American J. of Pathology, 175, 5, 2009.

[2] Gebäck T., Koumoutsakos P., Edge detection in microscopy images using curvelets, BMC Bioinformatics, 10,75, 2009.

[3] Gebäck T., Schulz M.M.P., Koumoutsakos P., Detmar M.,TScratch: a novel and simple software tool for automated analysis of monolayer wound healing assays, BioTechniques, 46, 265, 2009.

[4] N. Hansen, A. S.P. Niederberger, L.Guzzella, P. Koumoutsakos, A Method for Handling Uncertainty in Evolutionary Optimization with an Application to Feedback Control of Combustion, IEEE Trans. Evolutionary Computation, 180-197, 13, 2009.

[5] Zambrano H.A., Walther J.H., Koumoutsakos P., Sbalzarini I.F., Thermophoretic Motion of Water Nanodroplets Confined inside Carbon Nanotubes, Nano Letters, 9,1,66-71, 2009.

[6] Kotsalis E.M., Walther J.H., Kaxiras E., Koumoutsakos P., Control algorithm for multiscale flow simulations of water, Physical Review E, 79,4, 2009.

[7] Bayati B., Chatelain P., Koumoutsakos P., D-leaping: Accelerating stochastic simulation algorithms for reactions with delays, J. of Computational Physics, 228, 5908-5916, 2009.

[8] Mjolsness E., Orendorff D., Chatelain P., Koumoutsakos P., An exact accelerated stochastic simulation algorithm, Journal of Chemical Physics, 130, 14, 2009.

[9] Morra G., Chatelain P., Tackley P., Koumoutsakos P., Earth curvature effects on subduction morphology: Modeling subduction in a spherical setting, Acta Geotechnica, 4, 95-105, 2009.

[10] Rossinelli D., Bergdorf M, Hejazialhosseini B. and Koumoutsakos P., Wavelet-based Adaptive Simulation of Complex Systems on Multicore Architectures, Euro-Par 2009 (Distinguished paper award), Delft , The Netherlands.

[11] Gonnet P., Walther J.H., Koumoutsakos P., ∂-SHAKE: An extension to SHAKE for the explicit treatment of angular constraints, Computer Physics Communications, 180, 360–364, 2009.

Prof. Simon Krichak:

[1] Krichak, S.O., Alpert, P Kunin, P. (2009) Numerical Simulation of Seasonal Distribution of Precipitation over the Eastern Mediterranean with a RCM. Climate Dynamics, DOI 10.1007/s00382-009-0649-x .

[2] Krichak, SO, P. Alpert, P. Kunin (2009) Projections of Climate Change over Non-boreal East Europe During First Half of Twenty-First Century According to Results of a Transient RCM Experiment, 2009, in pp. 55-62 in Regional Aspects of Climate-Terrestrial-Hydrologic Interactions in Non-boreal Eastern Europe, Springer, NATO Science for Peace and Security Series, Series C: Environmental Security, Edited by P. Ya. Groisman and S.V. Ivanov.

Dr. Martin Kröger:

[1] O. Peleg, M. Kröger, Y. Rabin Effect of network topology on phase separation in two-dimensional Lennard-Jones networks, Phys. Rev. E 79 (2009) 040401(R)

[2] M. Laso, N.C. Karayiannis, K. Foteinopoulou, M.L. Mansfield, M. Kröger, Random packing of model polymers: local structure, topological hindrance and universal scaling, Soft Matter 5 (2009) 1762-1770

[3] N.C. Karayiannis, M. Kröger Combined molecular algorithms for the generation, equilibration and topological analysis of entangled polymers: Methodology and performance Int. J. Mol. Sci. 10 (2009), 5054-5089

[4] N.C. Karayiannis, M. Laso, M. Kröger Detailed atomistic molecular-dynamics simulations of alpha-conotoxin AulB in water J. Phys. Chem. B 113 (2009) 5016-5024

[5] P. Ilg, H.C. Öttinger, M. Kröger Systematic time-scale-bridging molecular dynamics applied to flowing polymer melts Phys. Rev. E 79 (2009) 011802

[6] R.S. Hoy, K. Foteinopoulou, M. Kröger, Topological analysis of polymeric melts: Chain-length effects and fast-converging estimators for entanglement lengthPhys. Rev. E 80 (2009) 031803

[7] A. Halperin, M. Kröger, Ternary protein adsorption onto brushes: Strong versus weak Langmuir 25 (2009) 11621-11634

[8] Y. Guo, J. van Beek, B. Zhang, M. Colussi, P. Walde, A. Zhang, M. Kröger, A. Halperin, A.D. Schlüter Tuning polymer thickness: Synthesis and scaling theory of homologous series of dendronized polymers, J. Am. Chem. Soc. 131 (2009) 11841-11854

[9] K. Foteinopoulou, N.C. Karayiannis, M. Laso, M. Kröger Structure, dimensions, and entanglement statistics of long linear polyethylene chains J. Phys. Chem. B 113 (2009) 442-455

[10] Y. Ding, M. Kröger, Phase behavior and formation dynamics of helically wound networks: generalized Janus chain model, Macromolecules 42 (2009) 576-579

[11] M. Colangeli, M. Kröger, H.C. Öttinger Boltzmann equation and hydrodynamic fluctuations; Phys. Rev. E 80 (2009) 051202

Dr. Michael Lehning:

[1] Bavay, M., Lehning M., Jonas, T., Löwe, H., 2009. Simulations of future snow cover and discharge in Alpine headwater catchments, Hydrol. Processes, 22, DOI: 10.1002/hyp.7195.

[2] Phillips, M., Zenklusen-Mutter, E., Kern-Luetschg, M., Lehning, M., 2009. Rapid Degradation of Ground Ice in a Ventilated Talus Slope: Fluela Pass, Swiss Alps. Permafrost and Periglac. Processes, 20, DOI: 10.1002/ppp.638, 1-14.

[3] Harris, C., ….Lehning, M., et al., 2009. Permafrost and climate in Europe: Monitoring and modelling thermal, geomorphological and geotechnical responses, Earth Science Reviews, 92, DOI: 10.1016/j.earscirev.2008.12.002, 117-171.

[4] Helbig, N., Löwe, H., Lehning M., 2009. Radiosity approach for the shortwave surface radiation balance in complex terrain, J. Atmos. Sc., in press, DOI: 10.1175/2009JAS2940.1

[5] Blanchet, J., Marty, C., Lehning, M., 2009. Extreme value statistics of snowfall in the Swiss Alpine region, Wat. Res. Res., 45, W05424, doi:10.1029/2009WR007916.

[6] Wever, N., Lehning, M., Clifton, A., Rüedi, J.-D., Nishimura, K., Yamaguchi, S., Nemoto, M., Sato, A., 2009. Verification of moisture budgets during drifting snow conditions in a cold wind tunnel, Water Resources Res., 45, doi:10.1029/2008WR007522.

[7] Schirmer, M., Lehning, M., Schweizer, J. 2009. Statistical forecasting of avalanche danger using simulated snow cover data, J. Glaciol., 55/193, 761-768.

Prof. Matthias Liebendörfer:

[1] M. Liebendörfer, T. Fischer, M. Hempel, A. Mezzacappa, G. Pagliara, I. Sagert, J. Schaffner-Bielich, S. Scheidegger, F.-K. Thielemann, S. C.Whitehouse, Supernovae as Nuclear and Particle Physics Laboratories, Nucl. Phys. A 827, 573 [6 p.] (2009)

[2] I. Sagert, M. Hempel, G. Pagliara, J. Schaffner-Bielich, T. Fischer, A. Mezzacappa, F.-K. Thielemann, M. Liebendörfer, The strange prospects for astrophysics, J. Phys. G 36, 064009 (2009)

[3] M. Liebendörfer, S. Whitehouse, T. Fischer, The isotropic diffusion source approximation for supernova neutrino transport, ApJ 698, 1174 [17 p.] (2009)

[4] I. Sagert, T. Fischer, M. Hempel, G. Pagliara, J. Schaffner- Bielich, A. Mezzacappa, F.-K. Thielemann, M. Liebendörfer, Signals of the QCD phase transition in core-collapse supernovae, Phys. Rev. Lett. 102, 081101 [4 p.] (2009)

[5] T. Fischer, S. C. Whitehouse, A. Mezzacappa, F.-K. Thielemann, M. LiebendoÅNrfer, The neutrino signal from protoneutron star accretion and black hole formation, A&A 499, 1 [15 p.] (2009)

Dr. Vittorio Limongelli:

[1] Heckmann D, Laufer B, Marinelli L, Limongelli V, Novellino E, Zahn G, Stragies R, Kessler H. Breaking the dogma of the metal-coordinating carboxylate group in integrin ligands: introducing hydroxamic acids to the MIDAS to tune potency and selectivity. Angew. Chem. Int. Ed. Engl. 2009, 24, 4436-40

Prof. Ulrike Lohmann:

[1] Croft, B.,U. Lohmann, R. V. Martin, P. Stier, S. Wurzler, J. Feichter, R. Posselt, and S. Ferrachat, Aerosol size-dependent below-cloud scavenging by rain and snow in the ECHAM5-HAM, Atmos. Chem. Phys. 9, 46534675, 2009.

[2] Croft, B.,U. Lohmann, R. V. Martin, P. Stier, S. Wurzler, J. Feichter, U. Heikkil'a, A. van Donkelaar and S. Ferrachat, Influences of in-cloud aerosol scavenging parameterizations on aerosol concentrations and wet deposition in ECHAM5-HAM, Atmos. Chem. Phys. Discuss. 9, 22041-22101, 2009.

[3] Joos, H., P. Spichtinger, and U. Lohmann, Orographic cirrus in a future climate, Atmos. Chem. Phys. 9, 7825-7845, 2009.

[4] Kloster, S., F. Dentener, J. Feichter, F. Raes, U. Lohmann, E. Roeckner, and I. Fischer-Bruns, A GCM study of future climate response to air pollution reductions, Clim. Dyn. 33, doi:10.1007/s00382-009-0573-0, 2009.

[5] Lohmann, U. and C. Hoose, Sensitivity studies of different aerosol indirect effects in mixed-phase clouds, Atmos. Chem. Phys. Discuss. 9, 1504515081, 2009.

[6] Posselt, R. and U. Lohmann, Sensitivity of the total anthropogenic aerosol effect to the treatment of rain in a global climate model, Geophys. Res. Lett. 36, L02805, doi:10.1029/2008GL035796, 2009.

PD Dr. Hans-Peter Lüthi/Prof. Hiroko Satoh:

[1] H. Satoh, J. Hutter, H.P. Lüthi, S. Manabe, K. Ishii, Y. Ito "Low barrier pathway for endo-cleavage induced anomerization of pyranosides with N-benzyl-2,3-trans Oxazolidinone groups" Eur.J.Org.Chem. (2009) 1127-1131.

[2] M. Bruschi, P.A, Limacher, J. Hutter, H.P. Lüthi, "A scheme for the evaluation of electron delocalization and conjugation efficiency in linearly π–conjugated systems J.Chem.Theory.Comput. 5 (2009) 506-514.

[3] P.A. Limacher, K.V. Mikkelsen, H.P. Lüthi, "On the accurate calculation of polarizabilities and second hpyerpolarizabilities of poyacetylene oligomer chains using the CAM-B3LYP density functional", J. of Chem. Phys. 130 (2009) on-line, DOI: 10.1063/1.3139023

[4] S. Borini, P.A. Limacher, H.P. Lüthi, "A systematic analysis of the structure and (hyper)polarizability of donor-acceptor substituted polyacetylenes using a Coulomb-attenuating density functional", J. of Chem. Phys. 131 (2009) on-line, DOI: 10.1063/1.3216825

Prof. John Maddocks:

[1] R. Lavery, K. Zakrzewska, D. Beveridge, T.C. Bishop, D.A. Case, T. Cheatham III, S. Dixit, B. Jayaram, F. Lankas, Ch. Laughton, J.H. Maddocks, A. Michon, R. Osman, M. Orozco, A. Perez, T. Singh, N. Spackova, J. Sponer, "A systematic molecular dynamics study of nearest-neighbor effects on base pair and base pair step conformations and fluctuations in B-DNA", Nucleic Acids Research (2009) 1–15

[2] F. Lankas, O. Gonzalez, L. M. Heffler, G. Stoll, M. Moakher, J. H. Maddocks, "On the parameterization of rigid base and basepair models of DNA from molecular dynamics simulations", Phys. Chem. Chem. Phys. 11 (2009) 10565 - 10588

[3] D. Demurtas, A. Amzallag, E. Rawdon, J.H. Maddocks, J. Dubochet, A. Stasiak, "Bending modes of DNA directly addressed by Cryo-Electron Microscopy of DNA minicircles", Nucleic Acids Research, 37, 9 (2009) 2882-2893

[4] R. Lavery, M. Moakher, J.H. Maddocks, D. Petkeviciute, K. Zakrzewska, "Conformational analysis of nucleic acids revisited: Curves+", Nucleic Acids Res. 37 (2009); 5917-5929

Prof. Jiri Mareda:

[1] J. Mareda, S. Matile, Concept article in Chem. Eur. J., 2009, 15(1), 28-37.

[2] A. Fürstenberg, O. Kel, J. Gradinaru, T.R. Ward, D. Emery, G. Bollot, J. Mareda, E. Vauthey, ChemPhysChem 2009, 10(9-10), 1517-1532.

[3] R.S.K. Kishore, O. Kel, N. Benerji, D. Emery, G. Bollot, J. Mareda, A. Gomez-Casado, P. Jonkheijm, J. Huskens, P. Maroni, M. Borkovec, E. Vauthey, N. Sakai, S. Matile, J. Am. Chem. Soc. 2009, 131(31), 11106-11116.

[4] S. Sulzer-Mossé, A. Alexakis, J. Mareda, G. Bollot, G. Bernardinelli, Y. Filinchuk, Chem. Eur. J. 2009, 15(13), 3204-3220.

Prof. Lucio Mayer:

[1] Governato, F., Brook, C., Mayer, L., Brook, A., Rhee, G., Wadsley, J., Jonsson, P., Willman, B., Quinn, T., & Madau, P., "At the heart of the matter: the origin of bulgeless dwarf galaxies and dark matter cores", 2009, accepted to Nature

[2] Mayer, L., "The environment of dwarf spheroidal satellites; ram pressure, tides and external radiation fields", 2009, Invited Review, Advances in Astronomy (Special Issue on "Dwarf Galaxies and Cosmology"), in press

[3] Lokas, E., Klimentowski, J., Kazantzidis , S., Mayer, L., Mamon, G., & Prada, F., "The orientation and kinematics of inner tidal tails around dwarf galaxies orbiting the Milky Way", 2009, MNRAS,in press.

[4] Feldmann, R., Carollo, C. M., Mayer, L., Renzini, A., Lake, G., Quinn, T., Stinson, G. S., & Yepes, G., "The Evolution of Central Group Galaxies in Hydrodynamical Simulations", 2009, accepted to ApJ.

[5] Edouard J, Monelli, M., Gallart, C., Drozdovsky, I., Stetson, P. B., Aparicio, A., Cassisi, S., Mayer, L, et al., "The ACS LCID Project. I. Short-Period Variables in the Isolated Dwarf Spheroidal Galaxies Cetus and Tucana Bernard", 2009, ApJ, 699, 1742.

[6] Belokurov, V., Walker, M. G., Evans, N. W., Gilmore, G., Irwin, M. J., Mateo, M., Mayer, L., Olszewski, E., Bechtold, J., Pickering, T., "Segue 2: A Prototype of the Population of Satellites of Satellites", 2009, MNRAS, 397. 1748.

[7] Colpi, M., Callegari, S., Dotti, M., & Mayer, L., "Massive black hole binary evolution in gas-rich mergers", 2009, Classical and Quantum Gravity, 26, Issue 9, pp. 094029.

[8] Callegari, S., L. Mayer, et al., "Pairing of supermassive black holes in minor mergers", 2009, ApJ Letters, 696, L89.

[9] Mayer, L., "Formation via disk instability" 2009, invited refereed chapter, in press for book "Exoplanet formation and interactions", edited by R. Barnes, Wiley-VCH.

[10] Read, J.I., Mayer, L.. Governato, F., Brooks, A., & Lake, G., "A dark matter disc in three cosmological simulations of Milky Way mass galaxies", 2009, MNRAS, 397, 44.

[11] Governato, F., Brook, C.B., Brooks, A., Mayer, L., Willman, B., Jonsson, P., & Stilp, A., "Forming a large disk galaxy from a z< 1 major merger", 2008, MNRAS, 398, 312.

[12] Agertz, O. et al., "Large scale galactic turbulence: can self-gravity drive the observed HI velocity dispersions?", 2009, MNRAS, 392, 294.

[13] Lokas, E., Klimentowski, J., Kazantzidis, S., & Mayer, L., "The anatomy of Leo I: how tidal tails affect the kinematics", 2008, MNRAS, 390, 625.

[14] Klimentowski, J., Lokas, E., Kazantzidis,S., & Mayer, L., "Tidal evolution of a disky dwarf galaxy in the Milky Way potential: the formation of a dwarf spheroidal", 2009, MNRAS, in press.

Prof. Markus Meuwly:

[1] I. Tubert-Brohman, M. Schmid and M. Meuwly Molecular Mechanics Force Field for Octahedral Organometallic Compounds with Inclusion of the Trans Influence JCTC 5, 530 (2009)

[2] M. Meuwly Studying Chemical Reactions with Molecular Mechanics Conference Information: International Conference on Computational Methods in Science and Engineering, SEP 25-30, 2008 Hersonissos, Greece Comp. Meth. Sci. Eng., Vol 1 - Adv. Comp. Sci., AIP Conference Proceedings 1108, 138 (2009)

[3] N. Plattner and M. Meuwly Higher order multipole moments for molecular dynamics simulations J. Mol. Model., 15, 687 (2009)

[4] M. Devereux and M. Meuwly Structural Assignment of Spectra by Characterization of Conformational Substates in Bound MbCO Biophys. J., 39, 4363 (2009)

[5] S. Mishra and M. Meuwly Nitric Oxide Dynamics in Truncated Hemoglobin: Docking Sites, Migration Pathways, and Vibrational Spectroscopy from Molecular Dynamics Simulations Biophys. J., 96, 2105 (2009)

[6] G. Buffa, L. Dore and M. Meuwly State-to-state rotational transition rates of the HCO^+ ion by collisions with Helium MNARS, 397, 1909-1914 (2009)

[7] M. Devereux, N. Plattner and M. Meuwly Application of Multipolar Charmge Models and Molecular Dynamics Simulations to Study Stark Shifts in Inhomogeneous Electric Fields J. Phys. Chem. B, in print (2009)

[8] M. Devereux and M. Meuwly Anharmonic Coupling in Molecular Dynamics Simulations of Ligand Vibrational Relaxation in Bound Carbonmonoxy Myoglobin J. Phys. Chem. B, 39, 13061-13070 (2009)

[9] J. D. Doll and J. E. Gubernatis and N. Plattner and M. Meuwly and P. Dupuis and H. Wang A Spatial Averaging Approach to Rare-Event Sampling J. Chem. Phys, in print, (2009)

[10] S. Lutz, K. Nienhaus, G. U. Nienhaus and M. Meuwly Ligand Migration between Internal Docking Sites in Photodissociated Carbonmonoxy Neuroglobin J. Phys. Chem. B, in print (2009)

[11] K. Nienhaus, S. Lutz, M. Meuwly and G. U. Nienhaus Structural Identification of Spectroscopic Substates in Neuroglobin ChemPhysChem, in print (2009)

Prof. Michele Parrinello:

[1] Phase selection and energetics in chiral alkaline earth tartrates and their racemic and meso analogues: synthetic, structural, computational and calorimetric studies L.N. Appelhand, M. Kosa, A.V. Radha, P. Simoncic, A. Navrotsky, M. Parrinello and A.K. CheethamJ. Am. Chem. Soc. 2009, 131, 15375-15386

[2] Ensemble of transition state structures for the Cis-Trans Isomerization of N-Methylacetamide Y.A. Mantz, D. Branduardi, G. Bussi and M. Parrinello J. Phys. Chem. B 2009, 113, 12521-12529

[3] Superionic conduction in substoichiometric LiAl alloy: an Ab initio study C.S. Cucinotta, G. Miceli, P. Raiteri, M. Krack, T.D. Kühne, M. Bernasconi and M. Parrinello Phys. Rev. Lett. 2009, 102, 125901

[4] PLUMED: a portable plugin for free-energy calculations with molecular dynamics M. Bonomi, D. Branduardi, G. Bussi, C. Camilloni, D. Provasi, P. Raiteri, D. Donadio, F. Marinelli, F. Pietrucci, R. A. Broglia and M. Parrinello Comp. Phys. Comm. 2009, 180, 1961-1972

[5] A molecular dynamics study of the early stages of calcium carbonate growth G. A. Tribello, F. Bruneval, C. C. Liew, M. Parrinello J. Phys. Chem. B. 2009, 113, 11680-11687

[6] Nuclear quantum effects in solids using a colored-noise thermostat M. Ceriotti, G. Bussi, M. Parrinello Phys. Rev. Lett. 2009, 103 (3), 030603

[7] Nucleotide-dependent conformational states of actin J. Pfaendtner, D. Branduardi, M. Parrinello, T. D. Pollard, G. A. Voth PNAS 2009, 106 (31), 12723-12728

[8] Reconstructing the equilibrium Boltzmann distribution from well-tempered metadynamics M. Bonomi, A. Barducci, M. Parrinello J. Comput. Chem. 2009, 30, 1615-1621

[9] First-principles study of crystalline and amorphous Ge2Sb2Te5 and the effects of stoichiometric defects" S. Caravati, M. Bernasconi, T.D. Kühne, M. Krack, M. Parrinello J. Phys.: Condens. Matter 2009, 21, 255501

[10] Unravelling the mechanism of pressure induced amorphization of phase change materials S. Caravati, M. Bernasconi, T.D. Kühne, M. Krack, M. Parrinello Phys. Rev. Lett. 2009, 102, 205502

[11] Binding of calcium and carbonate to polyacrylates G.A. Tribello, C.C. Liew, M. Parrinello J. Phys. Chem. B 2009, 113, 7081-7085

[12] Protein conformational transitions: the closure mechanism of a kinase explored by atomistic simulations A. Berteotti, A. Cavalli, D. Branduardi, F.L. Gervasio, M. Recanatini, M. Parrinello J. Am. Chem. Soc. 2009, 131, 244-250

[13] Langevin equation with colored noise for constant-temperature molecular dynamics simulations M. Ceriotti, G. Bussi, M. Parrinello Phys. Rev. Lett. 2009, 102, 020601

[14] Static and dynamical properties of liquid water from first principles by a novel Car-Parrinello-like approach T.D. Kuehne, M. Krack , M. Parrinello J. Chem. Theory and Comput. 2009, 5 (2), 235-241

[15] Isothermal-isobaric molecular dynamics using stochastic velocity rescaling G. Bussi, T Zykova-Timan, M. Parrinello J. Chem. Phys. 2009, 130, 074101

Prof. Alfredo Pasquarello:

[1] Medium-range structure of vitreous SiO2 obtained through first-principles investigation of vibrational spectra, L. Giacomazzi, P. Umari, and A. Pasquarello, Physical Review B 79, 064202 (2009).

[2] First principles investigation of defect energy levels at semiconductor-

oxideinterfaces: Oxygen vacancies and hydrogen interstitials in the Si-SiO_2-HfO_2 stack, P. Broqvist, A. Alkauskas, J. Godet, and A. Pasquarello, Journal of Applied Physics 105, 061603 (2009).

[3] Band offsets at the Ge/GeO_2 interface through hybrid density functionals, P. Broqvist, J. F. Binder, and A. Pasquarello, Applied Physics Letters 94, 141911 (2009).

[4] Atomic structure of the two intermediate phase glasses $GeSe_4$ and $SiSe_4$, C. Massobrio, M. Celino, P. S. Salmon, R. A. Martin, M. Micoulaut, and A. Pasquarello, Physical Review B 79, 174201 (2009).

[5] Atomistic model structure of the Ge(100)-GeO_2 interface, P. Broqvist, J. F. Binder, and A. Pasquarello, Microelectronic Engineering 86, 1589 (09).

[6] First principles study of substoichiometric germanium oxides J. F. Binder, P. Broqvist, and A. Pasquarello, Microelectronic Engineering 86, 1760 (2009).

[7] O. V. Yazyev and A. Pasquarello, Magnetoresistive junctions based on epitaxial graphene and hexagonal boron nitride, Physical Review B 80, 035408 (2009).

[8] Z. Sljivancanin, H. Brune, and A. Pasquarello, Nitrogen fixation at passivated Fe nanoclusters supported by an oxide surface: Identification of viable reaction routes using density functional calculations, Physical Review B 80, 075407 (2009). Hybrid-functional calculations with plane-wave basis sets: Effect of singularity correction on total energies, energy eigenvalues, and defect energy levels, P. Broqvist, A. Alkauskas, and A. Pasquarello, Physical Review B 80, 085114 (2009).

[9] Quantum ESPRESSO: a modular and open-source software project for quantum simulations of materials, P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni,D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch Journal of Physics: Condensed Matter 21, 395502 (2009)

Dr. Daniele Passerone:

[1] M. Farnesi Camellone, T. Kühne and D. Passerone Density functional theory study of self-trapped holes in disordered SiO_2 Phys. Rev. B 80, 330203 (2009).

[2] Parschau, M., Passerone, D., Rieder, K.-H., Hug, H. J. & Ernst, K.-H. Switching the chirality of single adsorbate complexes Angew. Chem. Int. Ed. doi:10.1002/anie.200805740 (2009).

[3] M. Treier, M.-T. Nguyen, N. V. Richardson, C. Pignedoli, D. Passerone, R. Fasel, D. Passerone and R. Fasel Tailoring low-dimensional organic semiconductor nanostructures Nano Lett. 9(1):126-31 (2009)

Dr. Jim Pfaendtner:

[1] Nucleotide-dependent conformational states of actin J. Pfaendtner, D. Branduardi, M. Parrinello, T. D. Pollard, G. A. Voth PNAS 2009, 106 (31), 12723-12728.

Prof. Dimos Poulikakos/ Dr. Ming Hu:

[1] Ming Hu, Javier V. Goicochea, Bruno Michel, and Dimos Poulikakos, “Thermal rectification at water functionalized silica interfaces”, Appl. Phys. Lett., 95, 151903 (2009).

[2] Ming Hu, Pawel Keblinski, and Patrick Schelling, “Kapitza conductance of silicon–amorphous polyethylene interfaces by molecular dynamics simulations”, Phys. Rev. B, 79, 104305 (2009).

Dr. Cristoph Raible:

[1] Fleitmann, D., H. Cheng, S. Badertscher, R. L. Edwards, M. Mudelsee, O. M. Goektuerk, A. Fankhauser, R. Pickering, C. C. Raible, A. Matter, J. Kramers, O. Tueysuez, 2009: Timing and climatic imprint of Dansgaard-Oeschger events in stalagmites from Northern Turkey, GRL, GRL, 36, L19707.

[2] Yoshimori, M., C. C. Raible, M. Renold,and T. F. Stocker, 2010: Simulated decadal oscillations of the Atlantic meridional overturning circulation in a cold climate state, Clim. Dyn., 34, 101-121

[3] Spangehl,T., U. Cubasch, C. C. Raible, U. Langematz, S. Schimanke, J. Koerper, and D. Hofer, 2009: Transient climate simulations from the Maunder Minimum to present day: the role of the stratosphere, J. Geophy. Res. - CAWSES special issue, Quat. Sci. Rev., 29, 101-112.

[4] Renold, M., C. C. Raible, T. F. Stocker and M. Yoshimori, 2009: Simulated resumption of the North Atlantic meridional overturning circulation, Quat. Sci. Rev., in press.

Prof. Ursula Röthlisberger:

[1] I.Tavernelli, I.C. Lin, and U. Rothlisberger Multicenter-type corrections to standard DFT exchange and correlation functionals Phys. Rev. B 79, 045106 (2009)

[2] P. Aeberhard, J. S. Arey, I. C. Lin, and U. Rothlisberger Accurate DFT descriptions for weak interactions of molecules containing sulfur J. Chem. Theor. Comp.5, 23-28 (2009)

[3] I. C. Lin, A. P. Seitsonen, M. Coutinho-Neto, I.Tavernelli, and U. Rothlisberger Importance of weak interactions in liquid water J. Phys. Chem. B 113, 1127-1131 (2009)

[4] F. Masson, T. Laino, U. Rothlisberger, and J. Hutter A QM/MM Investigation of Thymine Dimer Repair by DNA Photolyase ChemPhysChem 10, 400-410 (2009)

[5] I. Tavernelli, E. Tapavicza, and U. Rothlisberger Non-adiabatic coupling vectors within linear response time-dependent density functional theory J. Chem. Phys. 130, 124107 (2009)

[6] J. S. Arey, P. Aeberhard, I. C. Lin, and U. Rothlisberger Hydrogen bonding described using dispersion-corrected density functional theory J. Phys. Chem. B 113, 4726-4732 (2009)

[7] T. Bessho, E. Yoneda, J.H. Yum, M. Guglielmi, I. Tavernelli, U. Rothlisberger, H. Imai, M. K. Nazeeruddin, and M. Grätzel New Paradigm in Molecular Engineering of Sensitizers for Solar Cell Applications J. Am. Chem. Soc. 131, 5930-5934 (2009)

[8] M. Guglielmi, Tavernelli, and U. Rothlisberger On the Proton Transfer Mechanism in Ammonia-Bridged 7-Hydroxyquinoline: a First-Principles TDDFT Molecular Dynamics Study PCCP 11, 4549-4555 (2009)

[9] S. Vanni, I. Tavernelli, M. Neri, and U. Rothlisberger Observation of ”Ionic Lock” Formation in Molecular Dynamics Simulations of Wild Type ß1 and ß2 Adrenergic Receptors Biochemistry 48, 4789-4797 (2009)

[10] M. –E. Moret, I. Tavernelli, and U. Rothlisberger A combined QM/MM and Classical Molecular Dynamics Study of [Ru(bpy)3]2] in Water J. Phys. Chem. B, 113 (22), 7737–7744 (2009)

[11] A.K. Renfrew, A.D. Phillips, E. Tapavicza, R. Scopelliti, U. Rothlisberger, and P.J. Dyson Tuning the efficacy of ruthenium(II)-arene (RAPTA) antitumour compounds with fluorinated arene ligands Organometallics 28, 5061-5071 (2009)

[12] D. Bucher, L. Guidoni, P. Maurer, and U. Rothlisberger Developing Improved Charge Sets for the Modeling of the KcsA K^+ Channel Using QM/MM Electrostatic Potentials J. Chem. Theor. Comp.5, 2173-2179 (2009)

[13] I. Tavernelli, E. Tapavicza, and U. Rothlisberger Ab Initio Excited State Properties and Dynamics of a Prototype sigma- Bridged-Donor-Acceptor Molecule J. Phys. Chem. A 113, 9595-9602 (2009)

[14] M. Cascella, I.C. Lin, I. Tavernelli, and U. RothlisbergerDispersion-Corrected Atom-Centered Potentials for Phosphorous J. Chem. Theor. Comp. 5, 2930-2934 (2009)

[15] I.Tavernelli, E. Tapavicza, U. Rothlisberger Non-adiabatic Dynamics Using Time-Dependent Density Functional Theory: assessing the Coupling Strengths J. Mol. Struc. 914, 22-29 (2009)

[16] C. Gossens, I. Tavernelli, and U. Rothlisberger Binding of Organometallic Ruthenium(II) Anticancer Compounds to Nucleobases: A Computational Study J. Phys. Chem. A, 113, 11888-11897 (2009)

Prof. Christoph Schär:

[1] Fischer E.M. and C. Schär, 2009a: Futuer changes in daily summer temperature variability: driving processes and role for temperature extremes. Clim. Dyn., 33 (7), 917-935,, DOI 10.1007/s00382-008-0473-8

[2] Hohenegger, C., P. Brockhaus, C. Bretherton and C. Schär, 2009: The soil moisture-precipitation feedback in simulations with explicit and parameterized convection. J. Climate, J. Clim., 22 (19), 5003–5020

[3] Schwierz, C., P. Heck, E. Zenklusen, D.N. Bresch, C. Schär, P.L. Vidale and M. Wild, 2009: Modelling European winter storm losses in current and future climates. Climatic Change, in press

Prof. Sonia Seneviratne:

[1] Mahecha, M.D., et al., 2009: Comparing observations and process-based simulations of biosphere atmosphere exchanges on multiple time scales. J. Geophys. Res. – Biogeosciences, in press. Piao, S., et al., 2009: Summer soil moisture regulated by precipitation frequency in China. Environ. Res. Lett., in press.

[2] Corti, T., V. Muccione, P. Köllner-Heck, D. Bresch, and S.I. Seneviratne, 2009: Simulating past droughts and associated building damages in France. HESS, 13, 1739-1747.

[3] Jaeger, E.B., R. Stöckli, and S.I. Seneviratne, 2009: Analysis of planetary boundary layer fluxes and land-atmosphere coupling in the Regional Climate Model CLM. J. Geophys. Res. - Atmospheres, 114, D17106.

[4] Pitman, A.J., et al., 2009: Uncertainties in climate responses to past land cover change: first results from the LUCID intercomparison study. Geophys. Res. Lett., 36, L14814, doi:10.1029/2009GL039076.

[5] Teuling, A.J., R. Uijlenhoet, B. van den Hurk, and S.I. Seneviratne, 2009: Parameter sensitivity in LSMs: An analysis using stochastic soil moisture models and ELDAS soil parameters. J. Hydrometeorology, 10 (3), 751-763, doi:10.1175/2008JHM1033.1.

[6] Teuling, A.J., et al., 2009: A regional perspective on trends in continental evaporation. Geophys. Res. Lett., 36, L02404, doi:10.1029/2008GL036584

Dr. Joost VandeVondele:

[1] Paier J; Diaconu CV; Scuseria GE; Guidon M; VandeVondele J; Hutter J. 2009 Accurate Hartree-Fock energy of extended systems using large Gaussian basis sets. PHYSICAL REVIEW B 80(17): 174114

[2] Guidon M; Hutter J; VandeVondele J. 2009 Robust Periodic Hartree-Fock Exchange for Large-Scale Simulations Using Gaussian Basis Sets. JOURNAL OF CHEMICAL THEORY AND COMPUTATION 5(11): 3010-3021

[3] Schmidt J; VandeVondele J; Kuo IFW; Sebastiani D; Siepmann JI; Hutter J; Mundy CJ. 2009. Isobaric-Isothermal Molecular Dynamics Utilizing Density Functional Theory: An Assessment of the Structure and Density of Water at Near-Ambient Conditions. JOURNAL OF PHYSICAL CHEMISTRY B 113(35): 11959-11964

[4] Trinh. TT; Jansen APJ; van Santen RA; VandeVondele J; Meijer EJ. 2009. Effect of Counter Ions on the Silica Oligomerization Reaction. CHEMPHYSCHEM 10(11): 1775-1782

[5] Adriaanse C; Sulpizi M; VandeVondele J; Sprik M. 2009. The electron attachment energy of the aqueous hydroxyl radical predicted from the detachment energy of the aqueous hydroxide anion. JOURNAL OF THE AMERICAN CHEMICAL SOCIETY 131(17): 6046–6047

Prof. Harry van Lenthe:

[1] Mueller T.L., Stauber M., Kohler T., Eckstein F., Müller R. and van Lenthe G.H. (2009). Non-invasive bone competence analysis by high-resolution pQCT: An in vitro reproducibility study on structural and mechanical properties at the human radius. Bone 44: 364-371.

[2] Gerhard F.A., Webster D.J., van Lenthe G.H. and Müller R. (2009). In silico biology of bone modeling and remodelling - Adaptation. Philosophical Transactions of the Royal Society A 367: 2011-2030.

[3] Kirmani S., Christen D., van Lenthe G.H., Fischer P.R., Bouxsein M.L., McCready L.K., Melton L.J., Riggs B.L., Amin S., Müller R. and Khosla S. (2009). Bone structure at the distal radius during adolescent growth. J. Bone Miner. Res. 24:1033-1042.

[4] Voide R., Schneider P., Stauber M., Wyss P., Stampanoni M., Sennhauser U., van Lenthe G.H. and Müller R. (2009). Time-lapsed assessment of microcrack initiation and propagation in murine cortical bone at submicrometer resolution. Bone 45: 164-173.

[5] Mueller T.L., van Lenthe G.H., Stauber M., Gratzke C., Eckstein F. and Müller R. (2009). Regional, age and gender differences in architectural measures of bone quality and their correlation to bone mechanical competence in the human radius of an elderly population. Bone 45: 882-891.

[6] Cohen A., Dempster D.W., Müller R., Guo X.E., Nickolas T.L., Liu X.S., Zhang X.H., Wirth A.J., van Lenthe G.H., Kohler T., McMahon D.J., Zhou H., Rubin M.R., Bilezikian J.P., Lappe J.M., Recker R.R. and Shane E. (2009). Assessment of trabecular and cortical architecture and mechanical competence of bone by high-resolution peripheral Computed Tomography: comparison with transiliac bone biopsy. Osteoporosis International: (accepted).

[7] Melton L.J., Christen D., Riggs B.L., Achenbach S.J., Müller R., van Lenthe G.H., Amin S., Atkinson E.J. and Khosla S. (2009). Assessing

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

[8] Wirth A.J., Mueller T.L., Vereecken W., Müller R. and van Lenthe G.H. (2009). Mechanical competence of bone-implant structures - experimental validation of image-based micro-finite element analyses. Archive of Applied Mechanics (accepted).

Dr. Helena van Swygenhoven:

[1] Atomistic Simulations of Dislocations in Confined Volumes Derlet PM, Gumbsch P, Hoagland R, Li J, McDowell DL, Van Swygenhoven H MRS BULLETIN 34 (3):184-189 2009

Prof. Laurent Villard:

[1] J. Chowdhury, R. Ganesh, J. Vaclavik, S. Brunner, L. Villard, P. Angelino Short wavelength ion temperature gradient mode and coupling with trapped electrons Phys. Plasmas 16, 082511 (2009)

[2] S. Jolliet, B.F. McMillan, T. Vernay, L. Villard, R. Hatzky, A. Bottino, P. Angelino Influence of the parallel nonlinearity on zonal flows and heat transport in global gyrokinetic particle-in-cell simulations Phys. Plasmas 16, 072309 (2009)

[3] S. Jolliet, B.F. McMillan, T. Vernay, L. Villard, A. Bottino, P. Angelino Quasisteady and steady states in global gyrokinetic particle-in-cell simulations Phys. Plasmas 16, 052307 (2009)

[4] J. Chowdhury, R. Ganesh, S. Brunner, J. Vaclavik, L. Villard, P. Angelino A comprehensive gyrokinetic description of global electrostatic microinstabilities in a tokamak Phys. Plasmas 16, 052507 (2009)

[5] P. Angelino, X. Garbet, L. Villard, A. Bottino, S. Jolliet, Ph. Ghendrih, V. Grandgirard, B.F. McMillan, Y. Sarazin, G. Dif-Pradalier, T.M. Tran The role of plasma elongation on turbulent transport in magnetically confined plasmas Phys. Rev. Lett. 102, 195002 (2009)

[6] S.H. Kim, M.M Cavinato, V. Dokuka, A.A. Ivanov, R.R. Khayrutdinov, P.T. Lang, J.B. Lister, V.E. Lukash, Y.R. Martin, S.Yu. Medvedev, L. Villard Comparing magnetic triggering of ELMs in TCV and ASDEX Upgrade Plasma Phys. Control. Fusion 51, 055021 (2009)

[7] A. Marinoni, S. Brunner, Y. Camenen, S. Coda, J.P. Graves, X. Lapillonne, A. Pochelon, O. Sauter, L. Villard and the TCV Team The effect of plasma triangularity on turbulent transport: modelling TCV experiments by linear and non-linear gyrokinetic simulations Plasma Phys. Control. Fusion 51, 055015 (2009)

[8] X. Lapillonne, S. Brunner, T. Dannert, S. Jolliet, A. Marinoni, L. Villard, T. Görler, F. Jenko, F. Merz Clarifications to the limitations of the s – alpha equilibrium model for gyrokinetic computations of turbulence Phys. Plasmas 16 032308 (2009)

[9] B.F. McMillan, S. Jolliet, T.M. Tran, L. Villard, A. Bottino, P. Angelino Avalanche-like bursts in global gyrokinetic simulations Phys. Plasmas 16, 022310 (2009)

Prof. Viola Vogel:

[1] Frédéric Saltel,Eva Mortier, Vesa P. Hytönen, Marie-Claude Jacquier, Pascale Zimmermann, ViolaVogel, Wei Liu, Bernhard Wehrle-Haller, New PI(4,5)P2- and integrin-binding motifs in the talin head that promote b3-integrin activation and clustering, J. Cell Biology, 187(2009) 715-31.

[2] Kristopher E. Kubow, Enrico Klotzsch, Michael L. Smith, Delphine Gourdon, William C. Little, and Viola Vogel, Crosslinking of cell-derived 3D matrices up-regulates the stretching and unfolding of new ECM assembled by reseeded fibroblasts, Integrative Biology , 1 (2009) 635-48.

[3] William Little, Ruth Schwartlander, 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.

[4] Eileen Puklin-Faucher, Viola Vogel, Integrin activation dynamics between the RGD-bunding site and the headpiece hinge, J Biol Chem, in press.

[5| Lara A. Touryan, Gretchen Baneyx, Viola Vogel, Exploiting fluorescence resonance energy transfer to probe structural changes in a macromolecule during adsorption and incorporation into a growing biomineral crystal, Colloids Surf B: Biointerfaces, 74 (2009) 401-409.

[6] Klotzsch E, Smith ML, Kubow KE, Muntwyler S, Little WC, Beyeler F, Gourdon D, Nelson BJ, Vogel V: Fibronectin forms the most extensible biological fibers displaying switchable force-exposed cryptic binding sites. Proc. Natl. Acad. Sci. 106 (2009) 18267-72.

[7] Smart dust biosensors powered by biomolecular motors, George D. Bachand, Henry Hess, Banahalli Ratna, Peter Satird, Viola Vogel, Lab on the Chip, 9 (2009) 1661 - 1666.

[8] Vogel, V. (2009). Nanomedicine: the next waves of medical innovations. Nanotechnology, Volume 5: Nanomedicine. V. Vogel (Editor) WILEY-VCH Verlag GmbH ISBN: 978-3-527-31736-3. pp. 1-16

[9] Vogel, V. and M. P. Sheetz (2009). Mechanical forces matter in health and disease: from cancer to tissue engineering. Nanotechnology, Volume 5: Nanomedicine. V. Vogel (Editor) WILEY-VCH Verlag GmbH ISBN: 978-3-527-31736-3. pp. 235-303.

[10] Viola Vogel (Editor), Nanotechnology, Volume 5: Nanomedicine. Copyright @ 2009 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim . ISBN: 978-3-527-31736-3. 425 pages.

[11] Vesa P. Hytönen, Michael L. Smith and Viola Vogel, Translating mechanical force into discrete biochemical signal changes: multimodularity imposes unique properties to mechanotransductive proteins, "Mechanotransduction" edited by Roger Kamm and Mohammad Reza Kaazempur Mofrad, Cambridge University Press, May 2009.

[12] Viola Vogel, Michael P. Sheetz, Cell Fate Regulation by Coupling Mechanical Cycles to Biochemical Signaling Pathways, Current Opinion Cell Biology 21 (2009) 1-9.

Dr. Tomasz Wesolowski:

[1] The cooperative effect of hydrogen-bonded chains in the environment of a p->p* chromophore Georgios Fradelos, Jakub W. Kaminski, Samuel Leutwyler, Tomasz A. Wesolowski Journal of Physical Chemistry A , 19 (2009) 9766-9771.

[2] Orbital-free embedding effective potential in analytically solvable cases Andreas Savin, Tomasz A. Wesolowski Progress in Theoretical Chemistry and Physics, 19 (2009) 327-339.

[3] Orbital-free effective embedding potential: Density-matrix functional theory case Katarzyna Pernal, Tomasz A. Wesolowski Intl. J. Quant. Chem. 109 (2009) 2520

[4] Linearized Orbital-Free Embedding Potential in Self-Consistent Calculations Marcin Dulak, Jakub W. Kaminski, and Tomasz A. Wesolowski, Intl. J. Quant. Chem. 109 (2009) 1886.

Dr. Laura Zoppi:

[1] L. Merz, M. Parschau, L. Zoppi, K.K. Baldridge, J.S. Siegel, K.H. Ernst Reversible phase transition in a Buckybowl monolayer Angew. Chem. Int. Engl. Ed. 48, 1966 (2009)

Papers published by CSCS employees in 2009

John Biddiscombe:

B. Schindler, R. Fuchs, J. Biddiscombe, R. Peikert, "Predictor-Corrector Schemes for Visualization of Smoothed Particle Hydrodynamics Data", IEEE Transactions on Visualization and Computer Graphics, Vol. 15, No. 6, 1243-1250, 2009.

Jean Favre:

Supersonically Turbulent, Shock Bound Interaction Zone/s, D. Folini, R. Walder, J. M. Favre, Numerical Modeling of Space Plasma Flows, ASTRONUM-2009, Proceedings of the 2nd International Conference, ASP Conference Series, Vol. 406, 2009

Recurrent Novae: Progenitors of SN Ia?/, D. Folini, R. Walder, J. M. Favre, S. N. Shore, Numerical Modeling of Space Plasma Flows, ASTRONUM-2009, Proceedings of the 2nd International Conference, ASP Conference Series, Vol. 406, 2009

Favre, J.M. – Swiss National Supercomputing Center, Switzerland, Parallel data visualization. Book Chapter in: High-Performance Computing of Industrial Flows, edited by J.-M. Buchlin, P. Rambaud, Ph. Planquart, VKI LS 2009-05

Fotis Georgatis:

"A Grid-enabled CPU scavenging architecture and a case study of its use in the Greek School Network", Georgatos F., Gkamas V., Ilias A., Kouretis G., Varvarigos E.; 2009, Springer Journal of Grid Computing. http://springerlink.com/openurl.asp?genre=article&id=doi:10.1007/s10723-009-9143-2

Maria Grazia Giuffreda:

Maria Grazia Giuffreda, Marco Bettelini, "La simulazione avanzata nelle scienze e nell'ingegneria", archi-rivista svizzera di architettura, ingegneria e urbanistica, vol. 3, pp. 56-60, 2009

Thomas Schulthess:

"Accuracy and performance of graphics processors: A Quantum Monte Carlo application case study", Meredith JS, Alvarez G, Maier TA, Schulthess TC and Vetter JS, PARALLEL COMPUTING, Volume: 35, Issue: 3, Special Issue: Sp. Iss. SI, Pages: 151-163, Published: MAR 2009

"Fast update algorithm for the quantum Monte Carlo simulation of the Hubbard model", Nukala PKVV, Maier TA, Summers MS, Alvarez G, and Schulthess TC, PHYSICAL REVIEW B, Volume: 80, Issue: 19, Article Number: 195111, Published: NOV 2009

"DCA++: a case for science driven application development for leadership computing platforms", Summers MS, Gonzalo A, Meredith J, Maier TA, and Schulthess TC, JOURNAL OF PHYSICS: CONFERENCE SERIES, Volume: 180, Article Number: 012077, Published: 2009

"A scalable method for ab initio computation of free energies in nanoscale systems", Eisenbach M, Zhou CG, Nicholson DM, Brown G, Larkin J, and Schulthess TC, International Conference for High Performance Computing, Networking, Storage and Analysis, NOV 14-20, 2009 Portland, OR, INTERNATIONAL CONFERENCE FOR HIGH PERFORMANCE COMPUTING, NETWORKING, STORAGE AND ANALYSIS, Pages: 22-31, Published: 2009

Tim Stitt:

N.S.Scott, M.P. Scott, P.G. Burke, T. Stitt, V. Faro-Maza, C. Denis and A. Maniopoulou. 2DRMP: a suite of two-dimensional R-matrix propagation codes, Computer Physics Communications (CPC), Volume 180, Issue 12, 2424-2449, December 2009

Mario Valle:

Y. Ma, M. Eremets, A. R. Oganov, Y. Xie, I. Trojan, S. Medvedev, A. O. Lyakhov, M. Valle, and V. Prakapenka, Transparent dense sodium, Nature, vol. 458, pp. 182-185, Mar. 14 2009.

A. R. Oganov and M. Valle, How to quantify energy landscapes of solids, The Journal of Chemical Physics, vol. 130, p. 104504, Mar. 14 2009.

A. O. Lyakhov, A. R. Oganov, Y. Ma, Y. Wang, and M. Valle, Crystal structure prediction, ch. Crystal structure prediction using evolutionary approach. Wiley-VCH, 2009.

M. Valle, Supercalcolatori e superbambini, Il Quaderno Montessori, vol. 100, pp. 9-15, 2009.

M. Valle, Vedere per capire, archi - rivista svizzera di architettura, ingegneria e urbanistica, vol. 3, pp. 65-68, June 2009.

Ugo Varetto:

Yun Jang, Ugo Varetto: Interactive Volume Rendering of Functional Representations in Quantum Chemistry. IEEE Transactions on Visualization and Computer Graphics (2009)

Invited talks and seminars

Jean Favre:

"Parallel Visualization tools", ENS Lyon, May 13-14, 2009; "ParaView: la visualization parallele pour les problemes de dynamique des fluides", Nouvelles Frontieres pour la simulation des Ecoulements, ONERA Paris, October 9, 2009

Fotis Georgatis:

Swiss Grid School 2009, SGS'09, Geneva, 7-8 May 2009, http://sgs2009.eig.ch/ "Grid laboratory: gLite middleware stack"

Maria Grazia Giuffreda and Ugo Varetto:

18.08.2009; "Molekel - A visualization tool for quantum chemistry data", M.G. Giuffreda (speaker), U. Varetto 238th ACS National Meeting, Washington, DC, August 16-20, 2009

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

Impressum

CSCS Swiss National Supercomputing Centre
Via Cantonale, Galleria 2
CH-6928 Manno
Switzerland
Tel +41 (0) 91 610 82 11
Fax +41 (0) 91 610 82 09
http://www.cscs.ch

Design, Production:
Dorothea Gerhardt

Printing:
Hürzeler AG, Regensdorf

Print-run:
500


Annu
An
Annual Re
Annual Report
Annual Report
Annual Report
Annual Report
Annual Report
Annual Report
Report
Annual Report
Annual Report
Annual Report
Annual Report
Annual Report
Annual Report
Annual Report