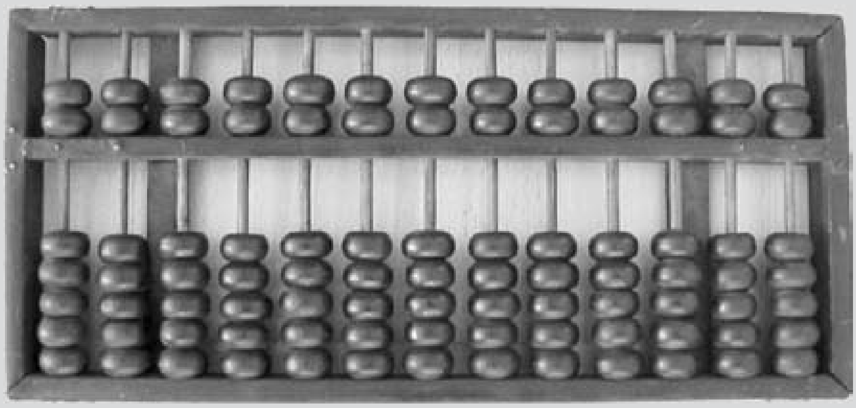
CSCS
Swiss National Supercomputing Centre



Annual Report 2008

CSCS

Swiss National Supercomputing Centre

Annual Report 2008

Content **Content**

Professore Piero Martinoli, presidente dell' Università della Svizzera Italiana, USI

Carte Blanche

I supercalcolatori di nuova generazione sono strumenti di ricerca rivoluzionari, autentici gioielli prodotti spingendo a limiti estremi le tecniche di miniaturizzazione e di integrazione. Con una potenza di calcolo che può raggiungere un milione di miliardi di operazioni matematiche al secondo essi operano come veri e propri laboratori virtuali, permettendo di accedere ad una conoscenza della realtà che, a causa della sua complessità, sfugge all'immaginazione del cervello umano.

Con una simile potenza di calcolo le scienze computazionali si stanno sviluppando vertiginosamente. Si possono infatti affrontare e risolvere, mediante la modellazione e la simulazione numerica, problemi ritenuti intrattabili fino a qualche anno fa, sia perché inaccessibili con metodi sperimentali tradizionali, troppo costosi e/o troppo lenti, o di difficile interpretazione. Ciò che distingue le scienze computazionali è il loro marcato carattere multi- e interdisciplinare: esse coprono un largo spettro di discipline, dalla fisica fino alle scienze economico-sociali, passando per la chimica, le scienze molecolari e dei materiali, le scienze della vita, la climatologia, la meteorologia. Inoltre, esse sono, e lo saranno sempre di più, di grande rilevanza per l'industria e il mondo economico.

È in questo contesto scientifico in piena effervescenza che si inserisce il Piano nazionale per il calcolo di grande potenza e la sua messa in rete (HPCN), un progetto d'avanguardia ora al vaglio delle Autorità federali. Con la sua implementazione, il CSCS potrà continuare il suo ruolo di leader nel supercalcolo a livello nazionale, permettendo alla Svizzera di non mancare l'appuntamento internazionale in un settore altamente competitivo. Un aspetto essenziale di HPCN è la creazione di una rete di competenze che, coinvolgendo università, istituti di ricerca e industria, intende promuovere la formazione di specialisti con spiccate competenze interdisciplinari. Auspico vivamente che HPCN riceva un convinto "sì" da parte delle Autorità federali, ricordando che la Città di Lugano e il Cantone Ticino hanno, dal canto loro, già fatto la loro parte: l'una accordando alla Confederazione i diritti di superfici sul terreno dove sorgerà il nuovo edificio del CSCS, l'altro sostenendone la costruzione con un credito di 5 milioni.

Conscia dell'importanza che il supercalcolo e il CSCS assumeranno in futuro, l'Università della Svizzera italiana ha creato in seno alla sua Facoltà di Scienze informatiche un Istituto di Scienze computazionali (ICS) che con il CSCS costituirà il nucleo centrale della rete nazionale di supercalcolo. Con l'arrivo del nuovo direttore del CSCS, il Prof. Thomas Schulthess, le premesse di una stretta e proficua collaborazione con l'ICS sono eccellenti: basti pensare che in tempi molto stretti si è potuto allestire, grazie al suo energico impegno, un progetto di cooperazione su scala nazionale che sta per essere avviato quale precursore di HPCN.

Auguro al CSCS e al suo staff un pieno successo nella sua fondamentale missione.

Piero Martinoli

Carte Blanche

New generation supercomputers are revolutionary research instruments, genuine jewels produced by pushing miniaturization and integration technologies to their limits. With a computing power that can reach a million billion mathematical operations per second, they operate like true virtual laboratories, enabling insight into a variety of phenomena that, due to their complexity, are beyond the imagination of the human brain.

Thanks to this huge computing power, computational sciences are developing at a dizzying speed. Today, modeling and numerical simulations make it possible to tackle and solve problems that were considered inaccessible just a few years ago either because they were out of reach of traditional experimental methods, too expensive and/or too slow, or difficult to interpret. A distinctive aspect of computational sciences is their prominent multi- and interdisciplinary character: they cover a wide spectrum of disciplines, from physics to socio-economic sciences, including chemistry, molecular sciences, material sciences, life sciences, climatology, and meteorology. Moreover, they are, and will be, increasingly important to industry and economy.

The National strategic plan for high-performance computing and networking (HPCN), now under close examination by the Federal authorities, fits in this exciting scientific context. Its implementation will allow CSCS to continue its role as the national leader in supercomputing, thus ensuring that Switzerland continues to be an internationally recognized player in this highly competitive field. An essential aspect of the HPCN strategy is the creation of a network of competences involving universities, research institutions and industry to promote the education of specialists with outstanding interdisciplinary know-how. I fervently hope that the HPCN strategy will soon be approved by the Federal authorities, thereby matching the support that it has already received from the city of Lugano and the canton of Ticino: the former by attributing the building rights to the land which will host the new CSCS building, the latter by supporting the construction with a contribution of 5 million francs.

The Univsrsità della Svizzera Italiana is well aware of the importance that supercomputing and CSCS willl have in the future. For this reason it has created an Institute of Computational Sciences (ICS) within its Faculty of Informatics. This institute, together with CSCS, will form the core of the national supercomputing network. With the arrival of the new CSCS director, Professor Thomas Schulthess, the prerequisites for a tight and successful collaboration with the ICS are excellent. Within an extremely short time it has in fact been possible, thanks to his energetic commitment, to set up a collaboration project at the national scale that will shorty kick-off as the precursore of the HPCN strategy.

I wish CSCS and its staff a very successful accomplishment of their fundamental mission.

Piero Martinoli

Prof. Thomas Schulthess, Director CSCS
(Foto S.Ulmer, ETH Zürich)

Introduction

The year 2008 was a landmark year for high-performance computing (HPC) in general, and for CSCS in particular.

In June 2008 Roadrunner, a supercomputer based on the Cell Broadband Engine and built at Los Alamos National Laboratory by IBM, was the first computer ever to deliver a petaflop/s performance running the Linpack benchmark. In early November two scientific applications for the first time surpassed one petaflop/s of sustained performance under production conditions on Jaguar, a Cray XT5 supercomputer at Oak Ridge National Laboratory (ORNL). Even more significant from a scientific point of view is that the machines at ORNL belong to the Leadership Computing Facility (LCF), a user program that is openly accessible to scientists from around the world. The two codes that first passed the petaflop/s barrier implement well-known methods for studying challenging problems in nano- and materials science. With appropriate access to knowhow in computing at scale, these codes could have been written anywhere in the world, and used to study scientific problems with unprecedented performance.

In autumn 2009, the petaflop/s scale supercomputer Jaguar, will be integrated into the INCITE program. This will mark the completion of the LCF project started in 2004 as the US Department of Energy's (DoE) response to the Earth Simulator, a supercomputer built in Japan in 2002. With the Japanese Earth Simulator and the LCF project at ORNL, leadership in high-performance computing is no longer limited to the weapons labs of the US DoE – Los Alamos, Sandia, and Lawrence Livermore National Laboratories – but rather, is now established at large-scale user facilities for open science. These developments present huge opportunities, and of course challenges as well, for scientific simulations in particular and open science in general.

In 2008, CSCS consolidated its organizational structure under the leadership of Prof. Marco Baggiolini, the acting director who was called in to lead the center through challenging times. Thanks to Marco's excellent managerial skills and hard work of the new management team he supported, CSCS is now a vital institution with a lean but very competent crew, ready to take on the leading role for HPC in Switzerland. On October 1, 2008, I was given the opportunity to lead the CSCS as its director.
In the coming year, CSCS will focus its activities in three areas that are essential to enabling an initiative for high-performance and high-productivity computing in Switzerland.

1. In order to prepare for the Petascale installation in 2012 CSCS will progressively upgrade its Cray XT system to the maximum capacity of the current building. In the 2nd half of May 2009 CSCS will thus upgrade to an XT5 system named Rosa with 14'752 AMD Opteron cores for a total of 141Tflop/s. In November 2009 this system will be further upgraded to 22'128 cores for 212 Tflop/s. A final upgrade is foreseen for 2010/11 that will boost the number of cores even further. These upgrades will allow CSCS to accommodate the growing user community and permit the users to gradually adapt to working with an increasing number of cores.

2. Planning for the new building that will host the petascale/s scale computers from 2012 onwards is well underway. The canton of Ticino and the city of Lugano have already pledged their strong support for the project. For 2009 we expect the final decision on the funding of the building project as part of the national HPCN-Strategy.

3. Jointly with the USI, CSCS will lead the development of a platform for high performance and high productivity computing (HP2C) in Switzerland. This platform will have a core group of computational scientists in Lugano - consisting primarily of computational mathematicians and problem oriented computer scientists - that will interact with a network of computational scientists throughout Switzerland. Initially this network will consist of a small number of projects that are focused development of high-risk / high-impact applications for petaflop/s scale computing platforms. These projects will be lead by domain scientists at Swiss Universities and supported by staff from the core program in Lugano. In the longer term, we plan on working with the Swiss institutions of higher education, in order to incorporate high-performance computing into their computational science and engineering teaching and research curricula.

I very much look forward to working with CSCS, its users, and computational scientists at academic institutions throughout Switzerland, to develop high performance and high productivity scientific computing in Switzerland. I believe that the Swiss academic landscape, with its high density of internationally recognized users of HPC, will prove to be a very fertile ground for the future development of computing, and I am certain that our scientific community will increase its international impact in high-end scientific computing in the coming years.

Professor Thomas Schulthess
Director of CSCS

Research Digest

Prof. Marcella Carollo

Interview
with Prof. Marcella Carollo
by David Bradley, Science Base, UK

Marcella Carollo of ETH Zurich is involved in research into universal mysteries: the dark side of matter and energy, galaxy formation and supermassive black holes. As such, she leads the Extragalactic Astrophysics Group conducting both observational and computational work dedicated to improving our understanding of the history of the universe.

What is involved in large observational astronomical surveys?

Today's astronomy is, like every other branch of science, a big operation. While we nurture our pet programs, making big discoveries necessitates (many) big telescopes on earth or in space, and coverage of huge sky patches with exquisite resolution at fantastic depths. This can only mean large international collaborations.

What do such studies reveal about the universe?

With the cosmological framework rather well-constrained (assuming 'dark energy' is correct!), we use astrophysical data provided by these large surveys to map star formation and mass assembly histories in structures at different mass scales, and to understand how these histories depend on the surrounding small- and large-scale dark matter filamentary structure, and how supermassive black holes, a million or a billion times more massive than the Sun, grow in the centres of galaxies like the Milky Way.

Can you tell us what projects you are currently involved in?

My group is a key node in the COSMOS project, the largest survey of the distant universe conducted with Hubble. COSMOS is a collaboration of more than a hundred astronomers in Europe, Japan, and North America and focuses on the evolution of galaxies, structures and black holes from about 2 to about 10 billion years ago. To push back the explored frontier, we have developed a program of observations of the very distant universe, the Hubble Ultra Deep Field 2005 (UDF05), which has allowed us to probe the galaxy population out to when the Universe was just a billion years old.

UDF05 gives us the credentials to be granted a new allocation of ~200 orbits on the Hubble with its new Wide Field Camera 3, being installed in May 2009. This extension involves us, the University of California Santa Cruz, Leiden Observatory, and the Space Telescope Science Institute. At the other extreme, part of my group is developing the Zurich ENvironmental Survey (ZENS), to pin down how galactic properties depend on their local environment at the current time, 13.5 billion years after the Big Bang.

How does CSCS work mesh with observations?
My use of state-of-the-art numerical simulations is in total synergy with my observational programs. I use simulations to interpret the results provided by the observational studies and the simulations then shape the observational studies; numerical simulations are a fundamental ingredient of my research programs.

Why is simulating galaxy formation important?

What we observe are spots of light. With effort we can learn about their astrophysical properties. But understanding our universe and its development requires theory. Theory tells us what the composition of the universe is, how structure should form, and how it should develop over billions of years. This is not something that we can directly observe. The simulations are the natural link between the theoretical principles and the observational facts, a third pillar which stabilizes our understanding of what we see and what we believe it means.

How do studies of dark energy and dark matter fit into the work?

Our current working hypothesis is that galaxy evolution takes place in a universe made of more than 70% dark energy, and in which most of the matter eludes our telescopes. This is the framework within which we ask ourselves 'what does what we see mean?' Of course, at times, we may end up seeing something that perturbs this assumed cosmological framework! Either way, the dark universe and the luminous one cannot be disembodied from each other. The CSCS simulations are crucial to inter-relate the luminous sources we study with the dark matter that develops in a universe mostly made of dark energy.

What is EUCLID and how is the CSCS work relevant to its development?

EUCLID should launch in 2017, under the European Space Agency to take images of about half of the sky and spectra of a hundred million galaxies. This will help us understand dark energy or reveal that there is no dark energy and rather it is simply gravity on very large scales.

The CSCS simulations are important in understanding what systematics we should expect, on physical grounds, in the data that we will obtain with EUCLID in order to avoid interpreting as dark energy (or gravity) features signals which are produced by the filamentary structure of the universe.

Tell me about ETH BRUTUS Cluster and the CSCS Cray?

Our use of the ETH Brutus cluster and CSCS resources is fully complementary: we need Brutus to run our resolution tests (never trust a simulation without those), and to explore parameter space in simulations of lower resolution than the CSCS ones. We use CSCS for a few, ultra-high-resolution runs, which allow us to reach down to size and mass scales which are totally unexplored.

How are you studying large-scale structure?

Intrinsic galaxy alignments - produced by the development of galaxies in the filamentary dark matter backbones, through anisotropic gas streams, etc - are one of those systematics which we are assessing in order to prepare for the interpretation of the EUCLID-like data. We have conducted baryonic cosmological simulations at a spatial resolution that permits us to measure the alignment of thousands and thousands of galaxies within a dark matter filament. The analysis and visualization of these simulations is a daunting job, but we are on our way - not least thanks to the help of the CSCS staff, whom we are very grateful to not only for their outstanding professionalism, but also for their friendly 24-7 availability and willingness to help. We are eager to see our results.

Presentation of Three Large User Projects
by David Bradley, Science Base, UK

We propose here a special insight into the work of three scientists, who carried out their research using computing resources from CSCS. The reader can find the list of all the 2008 projects on page 18.

Ab initio study of LiAl alloy: a prototype for superionic conduction and hydrogen storage

Dr. Clotilde Cuccinotta, ETH Zurich USI campus, Switzerland

Metal alloy is a hydrogen storage alloy

Researchers in Switzerland and Italy are investigating the properties of superionic alloys of the metals lithium and aluminium. Their theoretical studies carried out on CSCS computers are not only providing new insights into the fundamental behaviour of these novel materials but could open up new possibilities for high-density batteries and hydrogen storage for fuel cells.

Computational scientist Clotilde Cucinotta working in the research group of Michele Parrinello of the Department of Chemistry and Applied Biosciences, at ETH Zurich, USI-Campus, in Lugano, Switzerland, and her colleagues there and in the Department of Materials Science at the University of Milano-Bicocca, Italy, hope to reveal the atomic-level secrets of LiAl alloys as having enormous technological potential.

Lithium has become an important element, technologically speaking, the conductivity and high-speed mobility of its ions make it a vital component of the rechargeable batteries that power all kinds of portable electronic devices from notebook computers and PDAs to cell phones and media players. Lightweight, low density alloys of this soft metal formed with aluminium are even more intriguing.

Such LiAl alloys have so-called superionic properties, which makes them ideal candidates for a range of electrical applications but also of interest from the perspective of purely fundamental materials science.

The superionic properties of this alloy are fully expressed when it is sub-stoichiometric, which means there are fewer lithium atoms than aluminium atoms in the crystal lattice, explains Cucinotta.

The US Department of Energy has set a target for onboard hydrogen storage materials for vehicles of 9.5% hydrogen by weight before the year 2015. Hydrogen storage materials will lie at the heart of devices known as fuel cells, basically gas-powered batteries, that could power electric vehicles and countless electronic gadgets, and even providing electrical power for hospitals and industrial plants.

Fuel cells are destined to form the basis of the hydrogen economy and could ultimately displace power plants and internal combustion engines that burn fossil fuels. Because fuel cells convert the chemical energy of a gas, such as hydrogen into electrical energy, they need a constant supply of the chemical feedstock. Gas cylinders are intrinsically unsafe, but porous materials within which huge volumes of gas can be locked avoid hydrogen's explosive tendencies.

In the search for possible strategies to meet the US DOE target for hydrogen storage, new systems have been developed by testing reactive mixtures of single salts. One focus of that work has been so-called reactive hydride composites. LiAl alloy, is also the ultimate decomposition product of the lithium alanate, which is considered, together with sodium aluminium hydride ($NaAlH_4$) to be archetypical among all these complex hydrides.

Indeed, this material has emerged as one of the most promising for hydrogen storage. "The microscopic understanding of the processes underlying

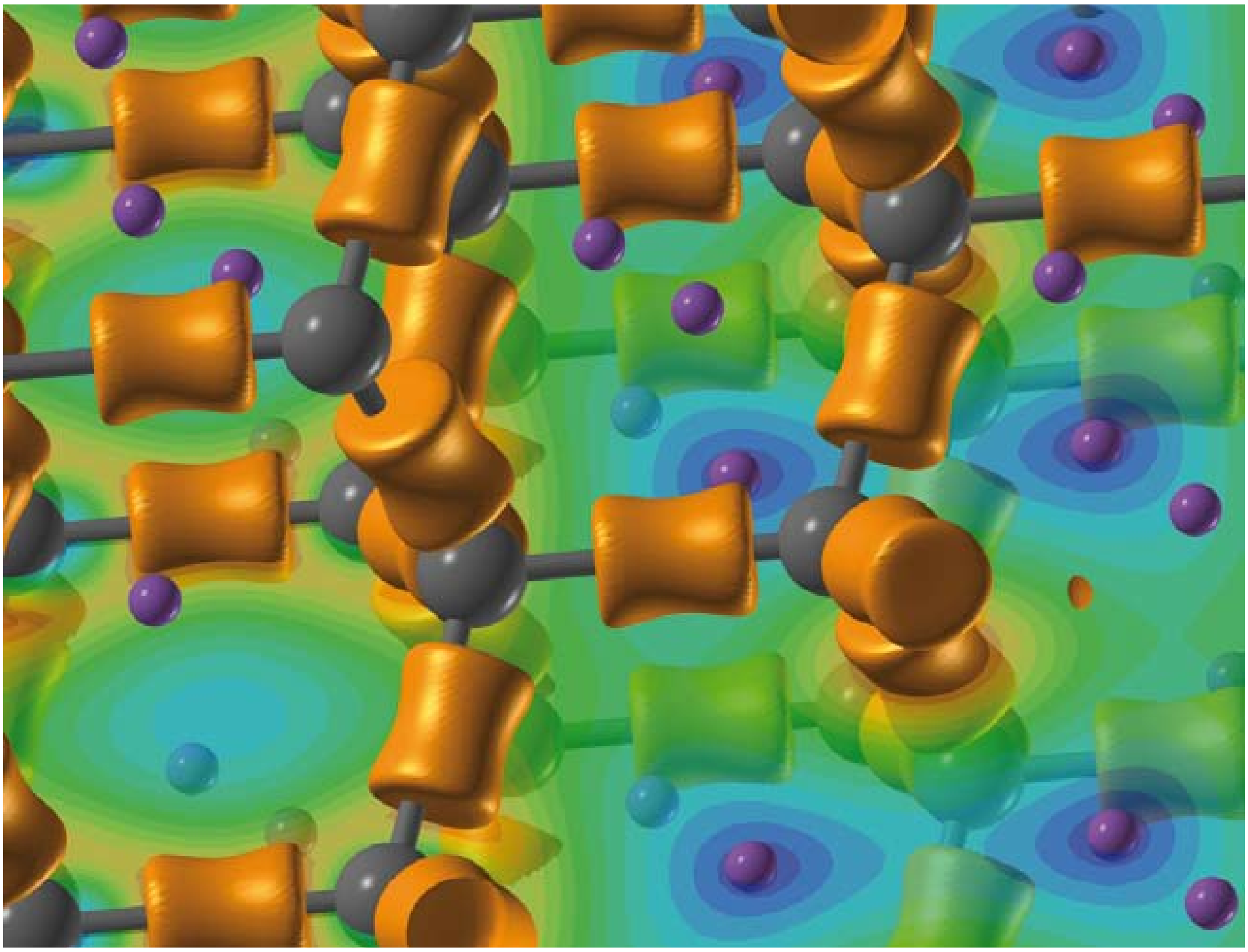


Figure 1: Study of diffusion of vacancies in solid LiAl alloys.

lithium ion conduction in lightweight alloys can help us to gain a better knowledge of the microscopic mechanism leading to hydrogen release than currently exists," says Cucinotta.

The LiAl alloys have the generic chemical structure Li1-xAl. At compositions where the value of x is between -0.1 and 0.2 Li(1-x)Al crystallizes in a structure corresponding to the Zintl crystal phase.

Cucinotta and colleagues have now explained one puzzling aspect of these materials and how they behave when the alloy is substoichiometric (x is less than 0). Electrochemical measurements of the lithium chemical diffusion coefficient reveal that lithium diffusivity is weakly dependent on the materials composition for x greater than 0 (that is, an excess of lithium).

In contrast, it rises steeply when the lithium content decreases (that is, x falls below 0) down to the stability boundary Li0.88Al, where the diffusivity becomes independent of temperature. At this point, no matter how much extra energy is added, the number of lithium ion vacancies does not rise substantially. Since lithium diffusion is mediated by lithium ion vacancies the diffusion dependence on temperature disappears.

The team's calculations, based on a hypothetical fragment of LiAl crystal lattice of just 128 atoms, allowed them to model the pathways taken by lithium ions for low lithium composition and at different temperatures. The work revealed minimum electronic charge corridors along which the lithium ions can move irrespective of temperature if the Li to Al ratio is just right.

The formation of disk galaxies in a cold dark matter Universe

Prof. Lucio Massimiliano Mayer. Universty of Zurich and ETH Zurich, Switzerland

Galactic heritage

One billion years after the Big Bang the Universe was very different. Until then, it was composed of nothing but highly energetic plasma. Stars and galaxies were only just beginning to form. How these first galaxies emerged from the plasma is not entirely clear, so researchers are running computer simulations of the early Universe on CSCS equipment to help cosmologists get a clearer picture.

”Understanding the origin of galaxies is one of the key goals of modern cosmology and astrophysics,” says Lucio Mayer of the University of Zurich, ”Over the last decade the study of the large-scale structure of the Universe and of the relic radiation from the Big Bang, known as the cosmic microwave background, has allowed scientists to construct the standard cosmological model.”

In this model, there is eight times as much cold dark matter in the Universe as there is ordinary baryonic matter from which stars, planets, and galaxies are made. Dark matter is invisible because it does not interact through the electromagnetic or nuclear forces that control the ordinary matter of atoms and molecules. However, it is thought to be composed of massive but incredibly small subatomic particles that do interact through gravity.

”Since cold dark matter provides most of the mass, hence most of the gravity in the Universe, galaxies form when ordinary baryonic matter collapses into the potential energy wells of dark matter clumps (called dark matter halos),” explains Mayer, ”In order to study galaxy formation one has to solve the equations for dark matter and baryonic matter together.”

These complex equations need adaptive algorithms. Mayer explains the problem further: ”Since the motion and thermal energy evolution of millions of mass elements have to be integrated simultaneously one needs massively parallel algorithms to

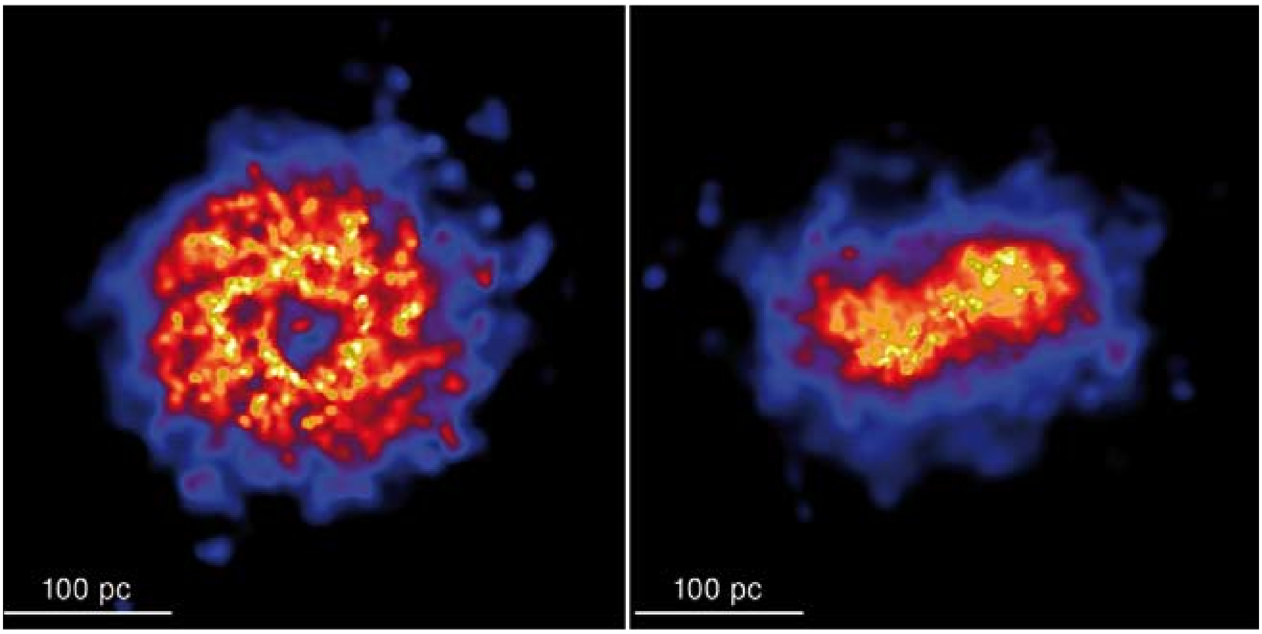


Figure 1: 1.3 billion years after the Big Bang, simulations show, face-on and edge-on gas density, colour-coded from blue (low) to yellow (high), of the first rotating structure that forms in our simulation. This proto-disk is already forming stars, and will accrete material from the surrounding medium and satellite galaxies, ending up at the centre of the final galaxy.

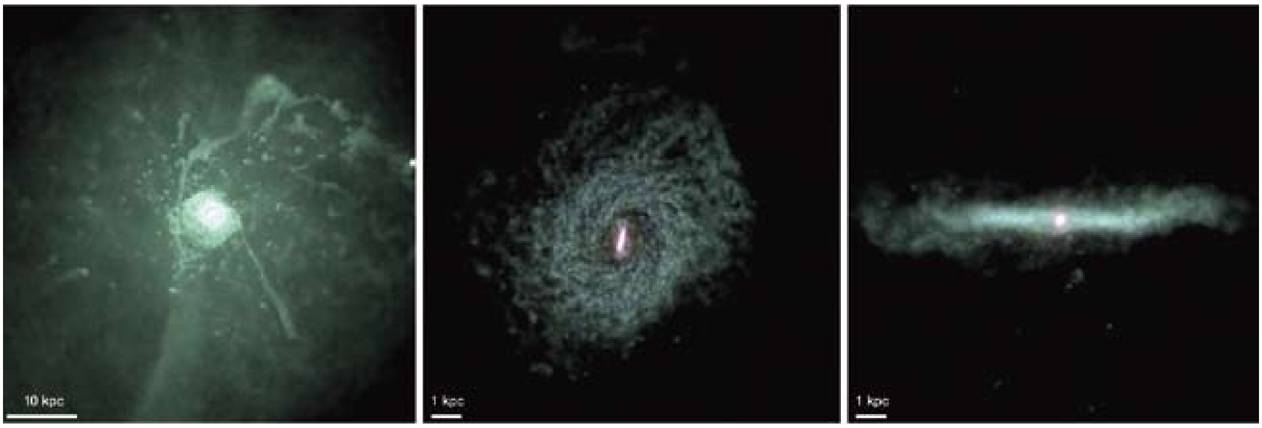


Figure 2: The "final" disk galaxy at a lower resolution, taken 6 billion years after the Big Bang, (almost half the age of the Universe). Gas is shown in gray-green, while red and blue are old and young stars, respectively.

evolve the relevant differential equations." Parallel algorithms allow the team to divide the heavy computation among hundreds or thousands of processing units rather than just one. "Smoothed particle hydrodynamics codes are one kind of such advanced algorithms, and GASOLINE, the code employed for the galaxy formation simulations run at CSCS, is state-of-the-art in the field," says Mayer.

Simulations performed using GASOLINE by Mayer and collaborators at the University of Washington, USA, were the first to show that a galactic disk of gas and stars similar to our Milky Way galaxy could be formed within the standard cosmological model. Unfortunately, the resolution of images and the simulations from just a few billion years after the Big Bang was not good enough to support these simulations because the expanding Universe was so much smaller and denser at this time.

The new generation of ground-based and space-born telescopes, among them the infra-red James Webb Space Telescope (JWST), will probe the first few billion years of galaxy formation with much higher resolution, which will allow Mayer and others to test the current cosmological paradigm.

PhD student Simone Callegari and Mayer have now performed new galaxy formation simulations at CSCS; so far using 700 000 CPU hours. For the first time, they have enough spatial and temporal resolution to study the galaxy formation process all the way from a billion years after the Big Bang to the present epoch. In other words, spanning 12 billion years of cosmic history.

"At a couple of billion years after the Big Bang our best simulation has unprecedented detail," explains Mayer. Indeed, resolution for these ancient galaxies is on a par with what was achieved by previous work only for present-day stage of galaxy evolution.

One of their most striking results is that at around two billion years after the Big Bang, the galaxy, which is ten times smaller and less massive than at the present epoch, will already have assembled a disk of gas and stars not very different from present-day disks. This is in contrast to the earlier assumption that disks form late while the spheroidal components of galaxies form much earlier. This finding suggests earlier results were spurious because of a lack of resolution.

"Our results can be translated into important and unprecedented predictions of what the new space telescope JWST will see when it probes the far reaches of the Universe," enthuses Mayer.

Molecular Modeling of Artificial Multifunctional Pores and their Catalytic Properties

Dr. Jiri Mareda, University of Geneva, Switzerland

Natural mimics

(Mimicking nature with computational chemistry)

Nature has solved countless chemical problems. Enzymes, for instance, accelerate otherwise tardy reactions, transport molecules control the flow of chemicals in and out of cells, and protein receptors act as exquisite and selective detectors for other molecules.

For decades mimicking nature's sensors and receptors effectively has been a dream of chemists working at the biological interface. The promise of exploiting the incredible sensitivity and selectivity of biosensors is enormous, but efforts have not yet achieved the ultimate goal.

Jiri Mareda and colleagues Stefan Matile, Guillaume Bollot, Danil Emery, Shinya Hagihara, Virginie Gorteau, and Ludovic Gremaud of the Department of Organic Chemistry, at the University of Geneva, Switzerland, are taking their lead from nature to build laboratory versions of protein receptors and transport supramolecular assemblies. By using the power of CSCS they are able, for example, to build computational models of their synthetic ion channels. They can then determine what chemical tweaks to make to improve selectivity for target molecules. Ultimately, they hope to exploit molecular modelling to garner insights into how to build supramolecular assemblies for specific tasks.

The protein receptors and transport channels found in nature recognise and detect charged particles through electrostatic interactions, ion pairing, metal coordination, anion-dipole interactions, or so-called hydrogen bonds.

The Geneva team was inspired by how positive particles, cations, interact fleetingly with the clouds of negatively charged pi-electrons around aromatic chemical groups in biomolecules. Anions, of course, being negatively charged, are excluded from this kind of interaction. Therefore, Mareda and Matile have carried out experimental and computational work to investigate the possibility of simulating nature's receptors using the concept of interactions between anions and acidic pi-surfaces, which are rare in nature as well as in chemistry.

The team reasoned that locking together pi-acidic aromatic groups would form a rigid framework for anion-pi interactions. By embedding this framework in a lipid bilayer to mimic a cell membrane, their aim was to transport anions. They recently published details in ”Chemistry: A European Journal” and the journal ”Organic & Biomolecular Chemistry”, which underscores the interface between modelling, chemistry, and biology of the work.

The alignment of multiple anion-pi sites in the embedded framework leads to ”anion slide” in which the anions are transported across the bilayer in an ion-hopping mechanism. The researchers can design the framework to be selective for almost any anion so it could be used to separate different anions from a mixture. It might also be coupled to a sensing molecule inside a spherical bilayer that glows, or fluoresces, when hit by the transported anion, thus acting as a sensitive and specific detector for that anion.

In related work, published in Nature Materials, and more recently in Journal of the American Chemical Society, the team has also demonstrated a method for finding synthetic aromatic receptors to be used as sensors that could also amplify the chemical signal. They are looking for pi-basic molecules such as modified naphthalenes and anthracenes that would grab any target molecule present in a sample and draw them into the synthetic pore decorated with pi-acidic framework and would generate at the same time an amplified signal (Figure 1).

Much of the work relies on advanced computational modelling and molecular dynamics simulations based on density functional theory and ab initio methods counting up to 80'000 atoms, hence the need for the powerful CSCS computer platforms.

New approaches to building channels to mimic natural proteins as well as the pioneering work of Mareda's and Matile's team on amplifier molecules is bringing the dream of biomimetic sensors closer.

"Overall, this is an adventurous concept that builds on scarce and mostly indirect experimental evidence," they say. Future developments in the laboratory and on the modelling front are now needed. That work will reveal whether these artificial sensor molecules will be useful in working as sensors for medical diagnostics, pharmaceutical applications, environmental science, and other areas.

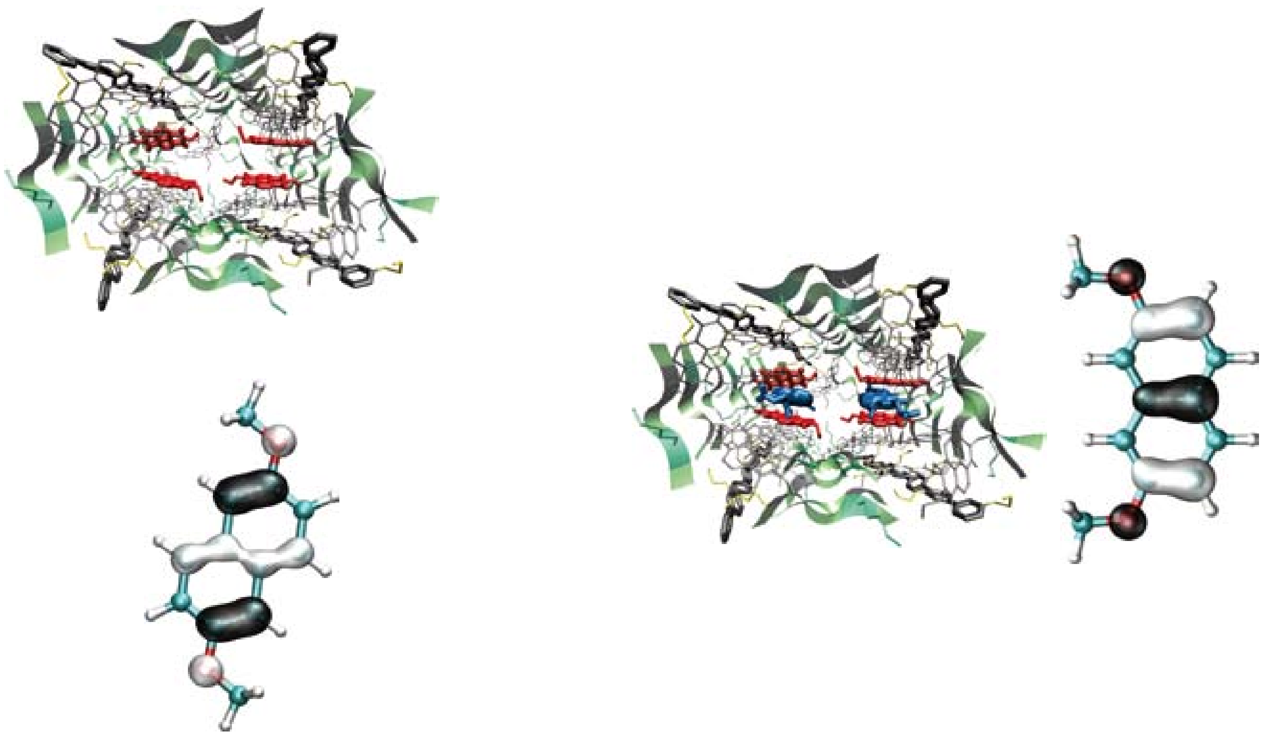


Figure 1: Molecular model of an active pore–amplifier–analyte complex used for modelling of the successful laboratory sensing of several organic substrates.

List of Production Projects 2008

Name	Organisation	Project Title
Arbenz P.	ETH Zurich	Multi-level Micro-Finite Element Analysis for Human Bone Structures
Baiker A.	ETH Zurich	Surface Chemistry of Transition Metals and Catalysis for CO2 Fixation
Bakowies D.	ETH Zurich	Atomization energies from ab initio calculations without empirical corrections
Baldereschi A.	EPF Lausanne	Solid surfaces and interfaces
Boley A.	University Zurich	The Accretion Mechanism of T Tauri Stars
Bürgi T.	University Neuchatel	Structure and enantiospecificity of chiral nanoparticles and interfaces
Carollo M.	ETH Zurich	Galaxy Formation in the Cosmic Web (and its Impact on Measurements of the EoS of Dark Energy)
Carollo M.	ETH Zurich	The Role of Environment in the Formation and Evolution of Galaxies
Cooper W. A.	EPF Lausanne	Computation of Stellarator Coils, Equilibrium, Stability and Transport
Cucinotta C.	ETH Zurich	Ab initio study of LiAL alloy: a prototype for superionic conduction and hydrogen storage
Deubel D.	ETH Zurich	Quantum Chemical Studies of Tansition Metal Anticacer Drugs
Fichtner W.	ETH Zurich	Computational Science and Engineering in Nanoelectronics
Folini D.	EMPA	Inverse modeling to monitor source regions of air
Fouchet L.	ETH Zurich	Dust in protoplanetary disks
Gervasio F.	ETH Zurich	New computational approaches to study large-scale protein conformational transitions
Gervasio F.	ETH Zurich	Folding mechanism of HIV1 protease in explicit solvent
Goedecker S.	University Basel	Atomistic simulations and electronic structure
Hauser A.	University Geneva	Photophysics and photochemistry of transition metal compounds: theoretical approaches
Hutter J.	University Zurich	Development and Applications of ab initio Molecular Dynamics Methods
Iannuzzi M.	PSI	Transport properties and microstructural changes in uranium dioxide
Jackson A.	ETH Zurich	Models of Convection and Magnetic Field Generation in Earth
Jackson A.	ETH Zurich	Thermal Convection in Giant Planets: The effect of an oblate spheroidal geometry
Joos F.	University Bern	Modelling CARBOn Cycle CLIMate Feedbacks (CARBOCLIM)
Khaliullin R.	ETH Zurich	A molecular dynamics study of the phase diagram of carbon employing a neural network potential

Name	Organisation	Project Title
Kleiser L.	ETH Zurich	Numerical Simulation of Transitional, Turbulent and Multiphase Flows
Koumoutsakos P.	ETH Zurich	Aircraft Wake Evolutionary Optimization
Koumoutsakos P.	ETH Zurich	Multiphysics Simulations using Multiscale Particle Methods
Kröger M.	ETH Zurich	Computer-Aided Design of Nanostructured Interfaces for Biological Sensors
Lake G.	University Zurich	Galaxy Formation (even dwarfs) in Full Cosmological Context
Läuchli A.	EPF Lausanne	Simulating Quantum States of Matter
Leyland P.	EPF Lausanne	Study of flight characteristics of a generic reentry launcher vehicle
Liebendörfer M.	University Basel	Three-dimensional modelling of Core-collapse Supernovae
Lodziana Z.	EMPA	Computational investigation of complex hydrides for hydrogen storage
Maddocks J.	EPF Lausanne	Atomistic molecular dynamics simulations of DNA minicircles
Man H.-K.	ETH Zurich	Investigation of 3D Size Effects in Numerical Concrete Containing Realistic Aggregate Shapes
Mapelli M.	University Zurich	Formation of massive stars in the Galactic Centre
Mareda J.	University Geneva	Molecular Modeling of Artificial Multifunctional Pores and their Catalytic Properties
Mayer L.	University Zurich	The formation of disk galaxies in a cold dark matter Universe
Meher A.	ETH Zurich	Metadynamics study of large-scale pH-induced conformational changes in dengue virus envelope protein
Meuwly M.	University Basel	Influence of Dimerization on Allostery of Multidomain Proteins
Meuwly M.	University Basel	Electronic Structure Calculations for Chemical Reactions involving Transition Metals
Miniati F.	ETH Zurich	Turbulence in Clusters of Galaxies: code testing
Oganov A.	ETH Zurich	Computational Crystallography: crystal structure prediction and simulation of planetary materials
Parrinello M.	ETH Zurich	Advanced computational methods
Parrinello M.	ETH Zurich	Ab-initio study of GeSbTe phase change alloys
Pasquarello A.	EPF Lausanne	Atomic-Scale Modelling at Semiconductor-Oxide Interfaces (2)
Passerone D.	EMPA	Atomistic simulation of surface-supported molecular nanostructures and of quasicrystal surfaces
Pfaendtner J.	ETH Zurich	Metadynamics Investigation of the Dynamics of the Actin Cytoskeleton
Porciani C.	ETH Zurich	The physics of baryons, dark matter and dark energy
Poulikakos D.	ETH Zurich	Biothermofluidics for Cerebrospinal Fluid Diagn.
Raible C.	University Bern	Modelling and Reconstruction of North Atlantic Climate System Variability (MONALISA II)

Name	Organisation	Project Title
Roethlisberger U.	EPF Lausanne	Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Studies of Systems of Biological Interest
Sbalzarini I.	ETH Zurich	Simulations of biological systems and development of a parallelization framework
Schär C.	ETH Zurich	Modeling Weather and Climate on European and Alpin Scales
Seneviratne S.	ETH Zurich	Land-climate interactions: Modelling and analysis
Van Lenthe H.	ETH Zurich	What genetic loci are involved in the regulation of bone strength?
Van Swygenhoven H.	PSI	The atomistic modeling of size effects in plastic
Walder R.	ETH Zurich	Stellar Cosmic Engines in Galaxies
Wesolowski T.	University Geneva	Multi-level computer simulations of electronic structure in condensed matter
Zoppi L./Baldridge K.	University Zurich	Corannulene-copper systems by a multilevel theoretical approach

List of Advanced Large Projects in Supercomputing (ALPS)

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

Activity Report

Collaboration Projects and Partnerships

CSCS entertains several bilateral partnerships, such as the collaboration with the Swiss Federal Meteorological Service MeteoSwiss and the Swiss Institute for Particle Physics CHIPP, but also our relationship with the Paul-Scherrer-Institute (PSI). In 2008, we institutionalised our staff exchange programme with the US American supercomputing centre NERSC at Lawrence Berkeley National Laboratories. The success of these partnerships is shown by the wish of our partners to continue the collaboration with CSCS for the long term.

Several other institutions approached CSCS in 2008 on the subject of potential collaborations as well as for dedicated HPC services. This interest, for example, leads us to run a successful test suite with the Swiss defence institution armasuisse and its subcontractor MeteoTest. As soon as computational and human resource capacities permit, CSCS will intensify its activities and broaden its offer in this sector.

Besides such contractual bi-lateral partnerships, CSCS is engaged in several collaboration projects. In 2008, two major collaboration projects funded by the European Union started, PRACE and LinkSCEEM. The PRACE project, which involves 13 European countries, runs over two years and aims to create the foundation for future pan-European HPC infrastructure. CSCS leads one of the eight work packages of the project and has contributed to some of the major deliverables and results in 2008. CSCS staff members are main authors of a survey report on HPC training and education in Europe, which received highest remarks by the European Commission. CSCS also wrote a survey on European supercomputer centre building infrastructures and organised the first workshop meeting on this topic on the continent. Due to the success of this workshop, we will continue this event as an annual meeting series organised by CSCS.

The second EU-funded project, LinkSCEEM, will help to create a regional HPC centre for the Eastern Mediterranean region at the Cyprus Institute. The project is targeted at the creation of a user community for this new centre. CSCS' main contribution is the organisation of an international conference on Cyprus in 2009, which will bring together potential users from the region, international HPC experts and HPC industry. Furthermore, CSCS consults on the construction of the facilities for the new supercomputing centre.

HPC Services and Scientific Computing

During the early part of 2008 the head count of the HPC Services group increased from three to six people, and improved the level of expertise in the areas of chemistry, climate modelling, compiler optimisation, numerical libraries and advanced parallel programming paradigms.

The MeteoSwiss high resolution forecast suite went into full production at the end of February 2008, with the full suite including the HPC simulations and the post-processing of the results all being carried out on the Cray XT4. The tight integration of the full suite on one machine also enabled a complete failover solution to be implemented on the Cray XT3, providing an enhanced level of availability and reliability for MeteoSwiss to deliver products to its customers.

Within the PRACE project, the HPC Services group's commitments were primarily in the areas of training and education and in the analysis and preparation of strategic applications for the forthcoming Petascale systems. A highlight of CSCS contribution to the PRACE project was the Survey on "HPC Training Needs and Education" which surveyed the top 10 most active users at each of the main HPC centres belonging to the PRACE initiative. The survey received a high recommendation from the European Commission reviewers and forms the basis for the training and education programmes which will be developed across Europe as part of PRACE. Furthermore, the survey has gone on to form the template for a similar study in North East Asia, and more recently within the United States TeraGrid.

With an array of compilers, tools and numerical libraries available on CSCS systems, the selection of the correct combinations of these can deliver a dramatic improvement in application performance. With the new expertise within the group able to provide up-to-date and informed recommendations on the most appropriate selection of compiler flags and libraries, dramatic speedups are now possible for some codes, with a twenty-fold improvement having been achieved for one user application running on hundreds of processors.

In order to prepare the CSCS user community for future systems, which will typically be composed of a large number of multi-core nodes, the HPC Services group has begun to investigate alternative programming paradigms to the pure MPI model. Initially this has involved the development of a course on the Global Arrays Toolkit which provides an approach similar to “Shared Memory” programming for distributed memory computers. The investigation of these alternative paradigms is continuing with work on MPI/OpenMP hybrid programming and partitioned global address space languages (PGAS), with all work being carried out in the context of real user applications.

With the arrival of the new Director of CSCS, the direction and priorities of the HPC Services team were realigned and this is reflected in a change of name as of 2009 to the Scientific Computing group.

Technical Services

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

The center-wide parallel filesystem, first announced during 2007, has been extended to reach the current capacity of 180 TB and will be further extended during 2009.

Together with the ”project” filesystem, another center-wide filesystem project has started, this time for storing home directories. This new filesystem, available on all HPC systems, will allow easy access to files stored on the home directory of varius HPC system from any machine.

After a trial period of some weeks, the pre- and post-processing cluster RIGI was moved to full production at the beginning of July. This small cluster allows users to run some pre- and post-processing jobs on data produced on the HPC systems. This new facility is complementary to the large Supercomputers and is intended for running jobs in preparation of large simulations or to process data produced in large simulation runs.

August saw the installation of a SUN SL8500, a tape library that can hold up to 11’000 tapes. This new library allows CSCS to use widely used LTO tapes, reducing costs for future capacity increase. With the currently installed tape technology CSCS’ tape library can hold up to 4PB of data. Data growth during 2008 was in the order of 50%.

With the installation of a 10Gbit network in 2007, network bandwith proved to be very important. Following users need for internet bandwith, CSCS upgraded its internet connection and from August 2008 various computers in our HPC farm were equipped with a 10Gbit connection to the external world.

Resources provided by the Phoenix computing cluster, a cluster specially built for the Swiss Institute of Particle Physics (CHIPP), were increased by 100% by replacing the installed dual core CPUs with quad core ones. The storage capacity was also doubled.

The number of available computing cores is 960 and the storage capacity is 530 TB.

Infrastructure

Following the intense upgrade and extension phases of the infrastructure in 2006 and 2007 most of 2008 was spent on consolidating the changes and updating documentation and procedures accordingly.

In the 1st quarter of the year we installed the water-cooled system for the LCG SUN cluster. Following this, the 17-year old building automation system was retired and replaced by a Siemens solution. During the night of July 18th there was a fire incident on one UPS machine that also affected the battery unit. This did not affect the operations of CSCS. The incident was rapidly dealt with and all necessary functions restored. As the UPS system operates with sufficient redundancy the loss of one machine posed no risk to reliability. A new UPS unit was installed during the 4th quarter.
An additional pre-cooling unit was added to improve the temperatures on the XT4 and two additional cooling units were added in the transformer room to cope with the summer temperatures.

During the early months of the year the administrative offices were updated with a fresh coat of paint and new parquet flooring to replace the carpeting. Beyond this all regular building and infrastructure maintenance work was carried out.

As the project team for the national HPCN-Strategy continued its work, plans for a new CSCS building began to take shape. During the July meeting the project management selected the site in Lugano Cornaredo as the preferred site for the new building. CSCS continues to work closely with the buildings department of ETH Zurich in the planning of this building.

Outreach

CSCS User Events
On April 4th the User Assembly took place in the KKL in Luzern. During the event users received an update and status report on CSCS activities as well as a presentation on the resource allocation process and upcoming courses and events.
Based on the positive feedback on the selection of Luzern as a venue in spring, we decided to return there for the User Day on September 12th. Dr. D. Obrist and Prof. L. Kleiser (ETH Zurich), Dr. Chr.

The fire incident of July 18th 2008 affected the battery unit.

Impression of the User Day 08

Raible (University of Bern), Dr. B. Sahli (ETH Zurich), Dr. J. VandeVondele (University of Zurich) and Dr. M. Liebendoerfer (University of Basel) gave scientific presentations. Prof. U. Suter, ETH Zurich, presented the National HPCN-Strategy project. CSCS outlined its HW & SW roadmap, data storage policy and gave information on the upcoming call for proposals. For the first time a competition for the best poster was held and the winning vote went to the poster “The formation of disk galaxies in a cold dark matter universe” by Simone Callegari.

Courses and workshops

Based on its success in previous years, the Parallel Programming Workshop by Rolf Rabenseifner was held on August 12-14th. CSCS also offered a course on Global Array programming languages that unfortunately had to be cancelled.

Within the framework of the European PRACE project, CSCS was tasked with the analysis of existing and planned data centre infrastructures of partner sites. This led to the organization of the first European Workshop on Data Centre Infrastructure that was hosted at CSCS on October 2-3rd. Attendance for this first edition of the event was restricted to PRACE partner sites. Given the success of the event a 2nd edition will be held in the fall of 2009 in Lugano and will be open to a wider attendance.

Conferences, inaugurations and events

On January 30th CSCS celebrated its 15th anniversary. Celebrations began with a tour of CSCS facilities for the invited guests. The attendees were then addressed by the Director of CSCS, the State Secretary for Research and Education, Prof. Viola Vogel of ETH Zurich, Dr. Frederica Darema of the National Science Foundation of the USA, and Dr. Stephan Bieri former President of ETH Board. After a festive aperitif the doors were opened for the members of the public who enjoyed tours of the facility, visualization demonstrations and poster presentations on the various units and achievements of CSCS.

On May 30th the inauguration of the LCG Tier-2 CHIPP cluster took place. Presentations were given by Dave Barney, CMS Outreach Coordinator of CERN; Prof. Allan Clark, department Director of Particle Physics of the University of Geneva and Dr. Les Roberston, Leader of the LHC Computing Grid Project of CERN.

From October 22-25th CSCS was present at the annual Ticino Informatica tradeshow in Lugano where it shared a stand with the University of Lugano and the technical college (SUPSI).

Public Seminars

In 2008 CSCS launched a series of public seminars. During this first year CSCS hosted seminars by: Howard Walter, Division Deputy of NERSC on "Designing the next generation NERSC Computing Building"; David Skinner, Group Leader for the Open Software and Programming group at NERSC on "Monitoring the performance of scientific computation through passive profiling"; Sadaf Alam, member of the Computer Science and Mathematics Division of Oak Ridge National Laboratory on "Molecular Dynamics Simulations on Teraflops-scale Systems and Emerging Architectures: Opportunities and Challenges"; Tony Drummond, member of the Scientific Computing Group of NERSC on "The U.S. DOE Advanced CompuTational Software Collection(ACTS)"; Charles Ramin-Wright and Adrian Honegger of ETH Zurich on "Drug Candidates against Viral Infections" or "Computational Analysis and Data Management of Image-Based siRNA HCS"; William E. Johnston, ESnet Department Head of Lawrence Berkeley National Laboratory on "The Evolution of Research and Education Networks and their Essential Role in Modern Science".

We look forward to sharing another eventful year with you in 2009!

Impressions of the inauguration of the LCG Tier-2 CHIPP cluster

CSCS' 15th anniversary celebration

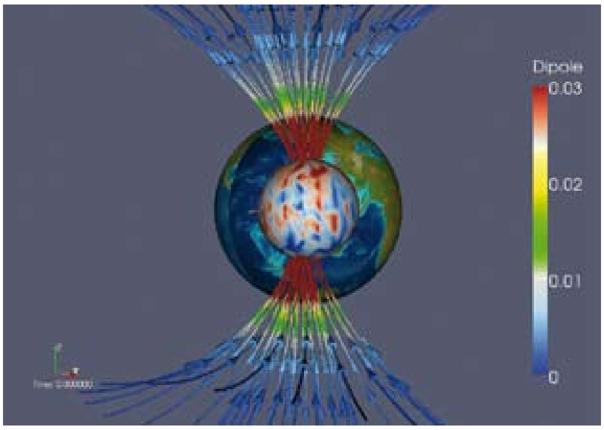


Figure 1: Magnetic Field Lines of the Earth, J. Rotvig, Dept. of Geophysics ETH Zurich.

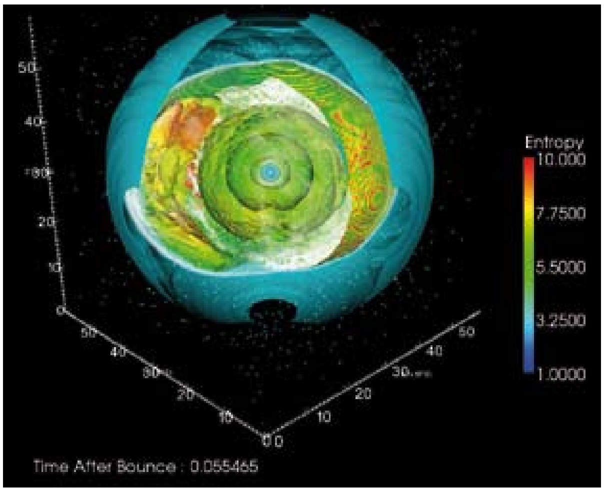


Figure 2: Visualization of Stellar Core Collapse, Simon Scheidegger, Matthias Liebendoerfer, Stuart Whitehouse, University Basel.

Data Management, Analysis and Visualisation

This year is marked by many advances in hardware, software and algorithms. We had the pleasure to host the internship of an ETH Zurich student, Alessandro Rigazzi, who participated for 8 months in building up our expertise in advanced rendering techniques such as GPU instancing, geometry shaders, and order independent transparency. Usage of the GPU as a custom execution engine has also increased with our work in volume rendering advanced 2D transfer functions and Non-Photorealistic Rendering (NPR) techniques.

We integrated the horus visualization cluster with the global file system of CSCS, enabling the user community to compute, and later analyse data without copying files across networks.

Our group contributed directly to a European Fellowship Exchange project (ESPHI) with visits at Andritz VaTech Hydro and Electricite de France (EDF) where we have developed a post processing tool for turbomachinery using conventional CFD and particle based methods and SPH post processing tools for large datasets integrated in our pv-meshless tool.

Visualisation Tools and Toolkits
pv-meshless is a customized version of the parallel visualization package ParaView maintained at CSCS. During 2008 we added a new library of Probing tools which enables users to directly compare the results of meshed or meshless (particle based) simulations in a uniform way.

The molecular visualization toolkit STM4 was upgraded to AVS/Express 7.2 and to run on more platforms. Also the range of modules provided has expanded with the addition of Fermi Surfaces and Bands visualization, a new Crystal Symmetries Finder, and more formats readers. STM4 also provides an interface for the crystal structures analysis and classification library CrystalFp. To ease the extraction of unique and potentially interesting structures from computationally defined sets of crystal structures, we applied usual high-dimensional classification concepts to the unusual field of crystallography. The result is the CrystalFp library that, not only has already accelerated the analysis at these datasets by at least one order of magnitude, promoting some new crystallographic insight and discovery, but is also contributing to new insight into the highly abstract space of crystal structures, visualizing unexpected correlations and structures.

Crystal Viewer is a multi-platform (Linux, Windows, Mac OS) program to visualize large chemical datasets with support for unit cell replication and mapping of atom colors to scalar values.

The rendering algorithm can scale from low to high end graphics cards allowing high-quality real-time rendering of 100’000 to 6’000’000+ atoms with bonds. The current version supports a custom file format in addition to all the formats supported by OpenBabel. New features currently in development will allow support for multiple per-atom scalar values, change the color map and perform queries to visualize only atoms associated with specific ranges of the scalar values.

A new version of Molekel (5.3) was released in February 2008. A new system for collecting usage statistics and improve user support has been put in place. According to the gathered statistics, in 2008 Molekel was downloaded about 10’000 times and we have answered 150 direct support requests. Some Molekel code has been contributed to the OpenBabel project and has been included in the official OpenBabel 2.2 distribution.

Figure 3: Illustrative volume rendering of negative high potential protein molecule, Y Jang, CSCS.

Facts & Figures

Income & Expenditure Flow (1.1.2008-31.12.2008)

Expenditures		Income	
Investments	**2’044’641.43**	**Basic Budget**	**12’000’000.00**
		Contribution ETH Zurich	12’000’000.00
Personnel	**5’347’691.86**		
Payroll	4’175’294.65	**Third-party contributions**	**2’344’909.82**
Employer’s contributions	589’942.65	Project PRACE	363’641.93
Other (education, travel etc.)	582’454.56	Project EGEE II	56’220.12
		Project LINKSCEEM	48’779.76
Other material expenses	**4’395’150.49**	HPCN Project CHIPP	1’205’876.90
Floor space	189’672.42	Meteo Swiss	616’475.80
Maintenance	733’861.71	Project ESF	25’705.68
Energy & media	1’275’079.95		
Administrative expenses	151’482.48	Other contributions	28’209.63
Hardware, software, services	1’972’183.45		
Services & remunerations	71’092.70		
Other	1’777.78		
Extraordinary incom/expenditures	**12’263.29**		
Extraordinary income	-297.59		
Overhead	12’560.88		
Expenses total	**11’799’747.07**	**Income total**	**14’344’909.82**
Balance			**2’545’162.75**

– The balance is rolled over to the 2009 budget.

Cost Distribution

Cost element	Q1	Q2	Q3	Q4	Total
Salaries	*932.26*	*947.78*	*1’096.57*	*1’199.68*	*4’175.29*
Contribution social insurances	*136.85*	*112.41*	*156.33*	*184.35*	*589.94*
Other personnel costs	*116.27*	*108.07*	*211.81*	*146.31*	*582.45*
Total costs of personnel	**1’185.38**	**1’168.26**	**1’464.71**	**1’529.34**	**5’347.69**
Floor space	*34.53*	*40.76*	*73.57*	*40.81*	*189.67*
Maintenance	*70.69*	*456.99*	*44.54*	*161.64*	*733.86*
Energy & media	*364.80*	*366.61*	*269.06*	*274.67*	*1’275.16*
Adminstrative expenses	*13.26*	*11.55*	*58.18*	*68.48*	*151.48*
Hardware, Software, Services	*565.32*	*502.48*	*362.23*	*542.08*	*1’972.10*
Services & remunerations	*30.44*	*15.23*	*51.05*	*-25.63*	*71.09*
Other costs	*1.28*	*0.42*	*0.59*	*-0.51*	*1.78*
Depreciation of investments	*1’929.58*	*1’932.29*	*1’587.84*	*1’014.40*	*6’464.12*
Total costs of materials	**3’009.92**	**3’326.34**	**2’447.05**	**2’075.97**	**10’859.27**
Extraordinary costs	**0.89**	**0.11**	**0.00**	**5.87**	**6.88**
Total costs	**4’196.19**	**4’494.71**	**3’911.76**	**3’611.17**	**16’213.84**

Cost Analysis

Breakdown of costs per customer

Customer	ETHZ	PSI	Uni Zürich	Uni Basel	EPFL	Uni Genf	Meto CH	EMPA	CHIPP	PRACE	EGEE II/III	CSCS	Other	TOTAL
Income federal base funding	**12’000**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**12’000**
Income third party funds	**0**	**0**	**0**	**0**	**0**	**0**	**611**	**0**	**1’206**	**364**	**56**	**17**	**91**	**2’345**
Distribution direct costs														
IT Depreciation Total	**3’560**	**774**	**560**	**229**	**322**	**109**	**348**	**67**	**357**	**0**	**0**	**68**	**70**	**6’464**
Technical services	*3’542*	*772*	*559*	*229*	*321*	*108*	*347*	*67*	*327*	*0*	*0*	*29*	*70*	*6’371*
Frontline desk	*6*	*1*	*1*	*0*	*1*	*0*	*1*	*0*	*0*	*0*	*0*	*0*	*0*	*10*
Data mgmt. & visualisation	*12*	*0*	*0*	*0*	*0*	*1*	*0*	*0*	*0*	*0*	*0*	*38*	*0*	*51*
Distr. hight-throughput comp.	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*30*	*0*	*0*	*0*	*0*	*30*
High-performance comp.	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
Personnel Payroll Total	**848**	**106**	**158**	**102**	**85**	**62**	**237**	**69**	**172**	**191**	**117**	**824**	**368**	**3’339**
Technical services	*433*	*76*	*79*	*42*	*63*	*40*	*116*	*33*	*172*	*0*	*0*	*114*	*155*	*1’324*
Frontline desk	*24*	*18*	*12*	*6*	*12*	*6*	*6*	*2*	*0*	*0*	*0*	*24*	*14*	*124*
Data mgmt. & visualisation	*263*	*0*	*26*	*39*	*6*	*13*	*0*	*30*	*0*	*0*	*0*	*165*	*128*	*671*
Distr. hight-throughput comp.	*41*	*0*	*17*	*0*	*0*	*0*	*17*	*0*	*0*	*108*	*117*	*93*	*66*	*458*
High-performance comp.	*86*	*12*	*24*	*15*	*3*	*3*	*99*	*3*	*0*	*83*	*0*	*428*	*4*	*762*
Personnel other costs Total	**55**	**8**	**12**	**6**	**5**	**5**	**14**	**5**	**0**	**31**	**7**	**84**	**33**	**266**
Technical services	*31*	*7*	*5*	*3*	*4*	*3*	*8*	*2*	*0*	*1*	*0*	*17*	*16*	*97*
Frontline desk	*0.3*	*0.3*	*0.2*	*0.1*	*0.2*	*0.1*	*0.1*	*0*	*0*	*0*	*0*	*0.3*	*0.1*	*1.7*
Data mgmt. & visualisation	*12*	*0*	*1*	*2*	*0*	*1*	*0*	*3*	*0*	*0*	*0*	*15*	*7*	*41*
Distr. hight-throughput comp.	*5*	*0*	*3*	*0*	*0*	*0*	*1*	*0*	*0*	*21*	*7*	*19*	*10*	*66*
High-performance comp.	*6*	*1*	*2*	*1*	*0*	*1*	*6*	*0*	*0*	*9*	*0*	*33*	*0*	*61*
IT expenses and maintenance Total	**1’021**	**223**	**161**	**66**	**93**	**31**	**100**	**19**	**73**	**0**	**0**	**8**	**32**	**1’815**
Technical services	*940*	*205*	*148*	*61*	*85*	*29*	*92*	*18*	*0*	*0*	*0*	*8*	*19*	*1’604*
Frontline desk	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*
Data mgmt. & visualisation	*39*	*9*	*6*	*3*	*4*	*1*	*4*	*1*	*0*	*0*	*0*	*0*	*1*	*67*
Distr. hight-throughput comp.	*26*	*6*	*4*	*2*	*2*	*1*	*3*	*1*	*73*	*0*	*0*	*0*	*1*	*119*
High-performance comp.	*14.5*	*3.2*	*2.3*	*1*	*1.3*	*0.4*	*1.4*	*0.3*	*0*	*0*	*0*	*0.1*	*0.3*	*25*
Building, Infrastructure Total	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**83**	**0**	**0**	**0**	**0**	**83**
Total direct costs	5’484	1’110	890	404	505	207	700	160	685	222	124	984	601	12’065
Overhead Total	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**0**	**5**	**11**	**4’231**	**0**	**4’247**
CSCS	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*11*	*60*	*0*	*71*
Facility management	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*2*	*0*	*334*	*0*	*336*
Administration	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*4*	*0*	*1’483*	*0*	*1’486*
Building and energy	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*2’175*	*0*	*2’175*
Technical services	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*0*	*180*	*0*	*180*
Total costs	**8’484**	**1’110**	**890**	**404**	**505**	**207**	**700**	**160**	**685**	**228**	**135**	**5’215**	**601**	**16’312**

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

Compute Infrastructure

Vendor & Model	CPU Type	No. of Processors	No. of Nodes	Inter-connect type	Interconnect bandwidth (MB/s)	Total memory size (GB)	Year of installation	Peak Performance (Tflop/s)	LINPACK Performance (Tflop/s)	TOP500 position Nov. 07	Millions of produced CPU hours	Average Utilisation (%)	Annual direct costs in 2006 (kCHF)
Cray XT3	AMD Opteron 2.6 GHz	3328	1664	Cray XT3	7600 (per router) 2’000’000 (total)	3’328	2005	17	0,014	414	27.07	92.6	4’254
IBM P5 p575	Power-5 1.5 GHz	768	48	Infiniband 4X DDR	1’000	1’650	2006	4.6			5.46	80.94	1’939
Cray XT4	AMD Opteron 2.6 GHz	896	448	Cray XT4	7600(per router)	896	2007	4.7			3.71	47.12	1’386
HP-XC Cluster	AMD Opteron	34	16	Infininband 4X SDR	20 GB	128	2007	0.16			0.16	10.73	150
SUN Cluster	AMD Opteron dual core 2.6 GHz	104	26	Infiniband 4X SDR	10 GB	208	2007	0.54			0.66	14.43	153

Usage Statistics

Usage by research fields

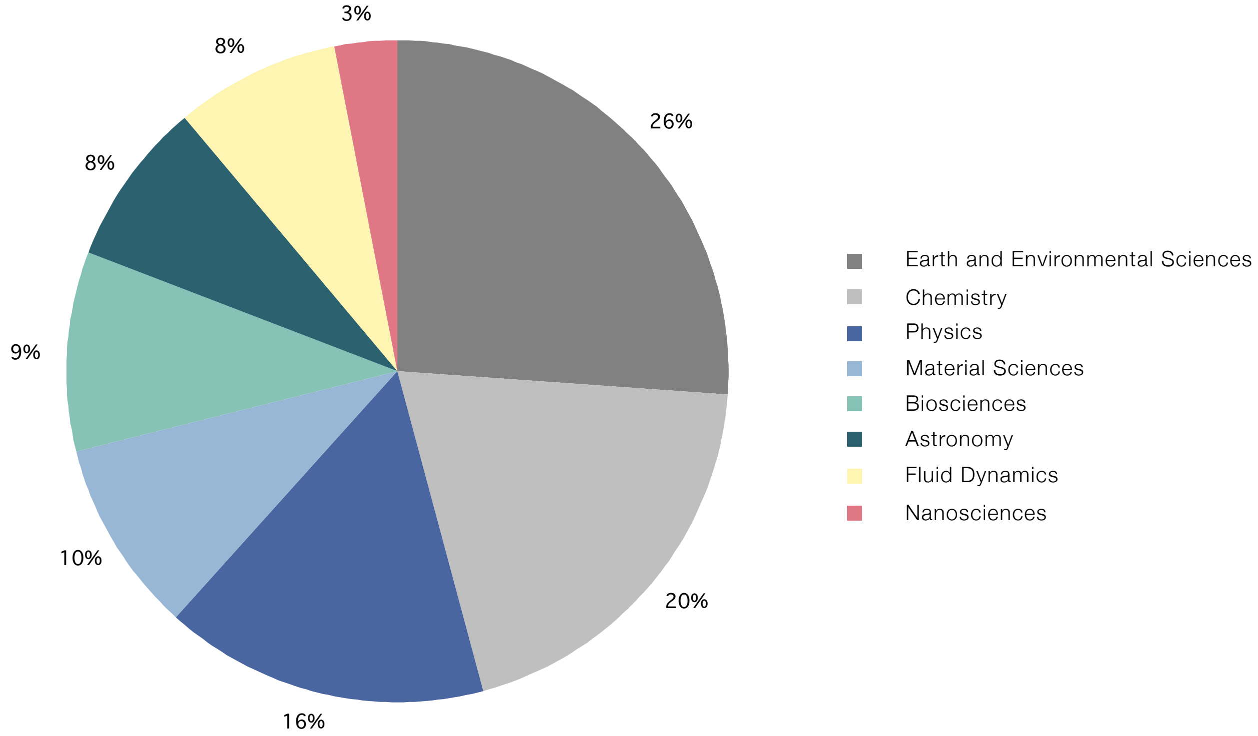
	Earth and Environmental Sciences	Chemistry	Physics	Material Sciences	Biosciences	Others	Internal
Cray XT3	23.90%	15.13%	18.86%	7.15%	12.33%	22.41%	0.21%
IBM p5-575	16.27%	30.94%	10.44%	25.11%	0.73%	15.34%	1.16%
Cray XT4	54.20%	35.54%	0.95%	4.60%	0.84%	2.78%	1.09%
HP Cluster	3.36%	1.82%	0.00%	0.00%	12.00%	7.97%	74.85%
SUN Cluster	31.59%	0.00%	0.95%	0.00%	56.18%	11.01%	0.27%

Usage by customer

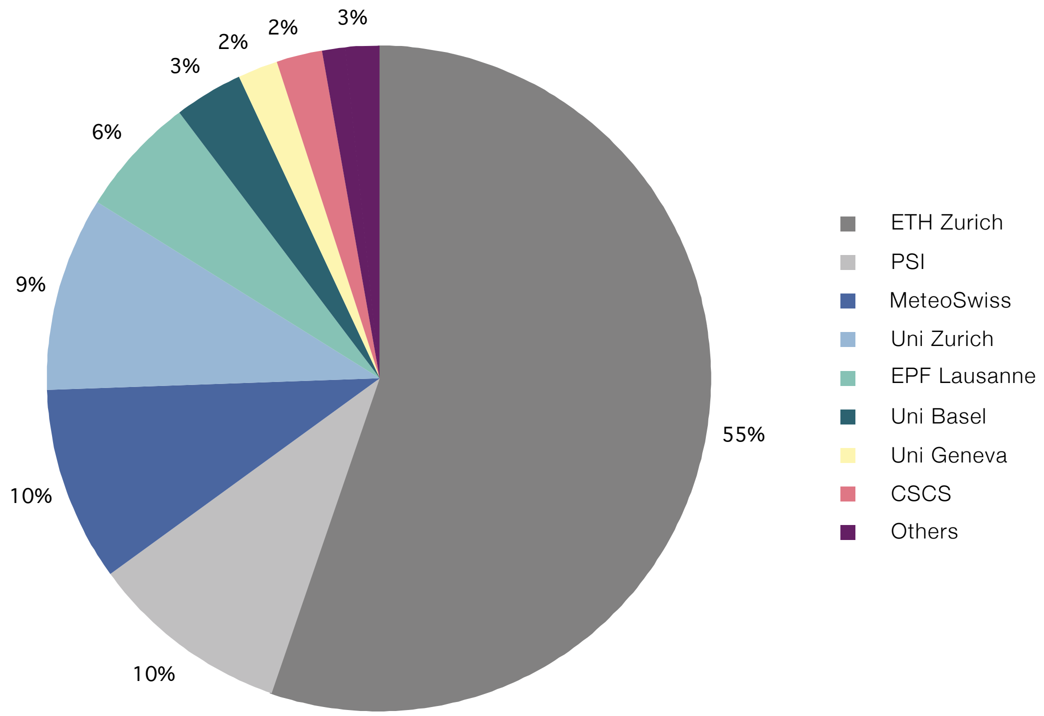
	ETH Zurich	PSI	Meteo Schweiz	Uni Zurich	EPFL	Uni Basel	Others	CSCS
Cray XT3	62.03%	16.52%	0.94%	8.63%	4.00%	4.61%	6.14%	0.21%
IBM p5-575	50.29%	2.44%	0.00%	18.21%	15.56%	2.33%	9.96%	1.21%
Cray XT4	46.74%	0.95%	49.07%	0.76%	0.00%	0.00%	0.00%	1.09%
HP Cluster	23.33%	0.00%	0.00%	0.00%	0.00%	0.00%	1.82%	74.85%
SUN Cluster	13.08%	0.00%	18.51%	0.00%	0.00%	0.95%	67.19%*	0.27%

* IRB was the principal user in 2008 on the SUN Cluster with 56.18%

CPU Usage per Research Field



Direct costs of machines per Institution



FIDIREVISA

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

Lugano, den 13. Februar 2009/GZW/NZA

Sehr geehrte Damen und Herren

Auftragsgemäss haben wir das Financial Reporting (4. Quartal 2008/Jahresabschluss) des CSCS SWISS NATIONAL SUPERCOMPUTING CENTRE für das am 31. Dezember 2008 abgeschlossene Geschäftsjahr geprüft.

Für das Financial Reporting (4. Quartal 2008/Jahresabschluss) ist der Vorstand (Steering Board) verantwortlich, während unsere Aufgabe darin besteht, dieses zu prüfen und zu beurteilen. Wir bestätigen, dass wir die gesetzlichen Anforderungen hinsichtlich Befähigung und Unabhängigkeit erfüllen.

Wir haben unsere Prüfung in Übereinstimmung mit den Schweizer Prüfungsstandards vorgenommen. Nach diesen Standards haben wir die Prüfung so zu planen und durchzuführen, dass wir hinreichende Sicherheit gewinnen, ob das Financial Reporting (4. Quartal 2008/Jahresabschluss) frei von wesentlichen falschen Angaben ist. Wir prüften die Posten und Angaben des Financial Reporting (4. Quartal 2008/Jahresabschluss) mittels Analysen und Erhebungen auf der Basis von Stichproben. Ferner beurteilten wir die Anwendung der massgebenden Rechnungslegungsgrundsätze, die wesentlichen Bewertungsentscheide sowie die Darstellung des Financial Reporting (4. Quartal 2008/Jahresabschluss) als Ganzes. Wir sind der Auffassung, dass unsere Prüfung eine ausreichende Grundlage für unser Urteil bildet.

Wir empfehlen, das vorliegende Financial Reporting (4. Quartal 2008/Jahresabschluss) zu genehmigen.

FIDIREVISA SA

G. Zwahlen
Leitender Revisor
Dipl. Wirtschaftsprüfer
Zugelassener Revisionsexperte

ppa. N. Zanetti

Beilagen:
- Financial Reporting (4.Quartal 2008/Jahresabschluss)

Fidirevisa SA
Via G. B. Pioda 14
C. P. 5935
CH-6901 Lugano
Tel. +41 (0)91 913 32 00
Fax +41 (0)91 913 32 60
info@fidirevisa.com
www.fidirevisa.com

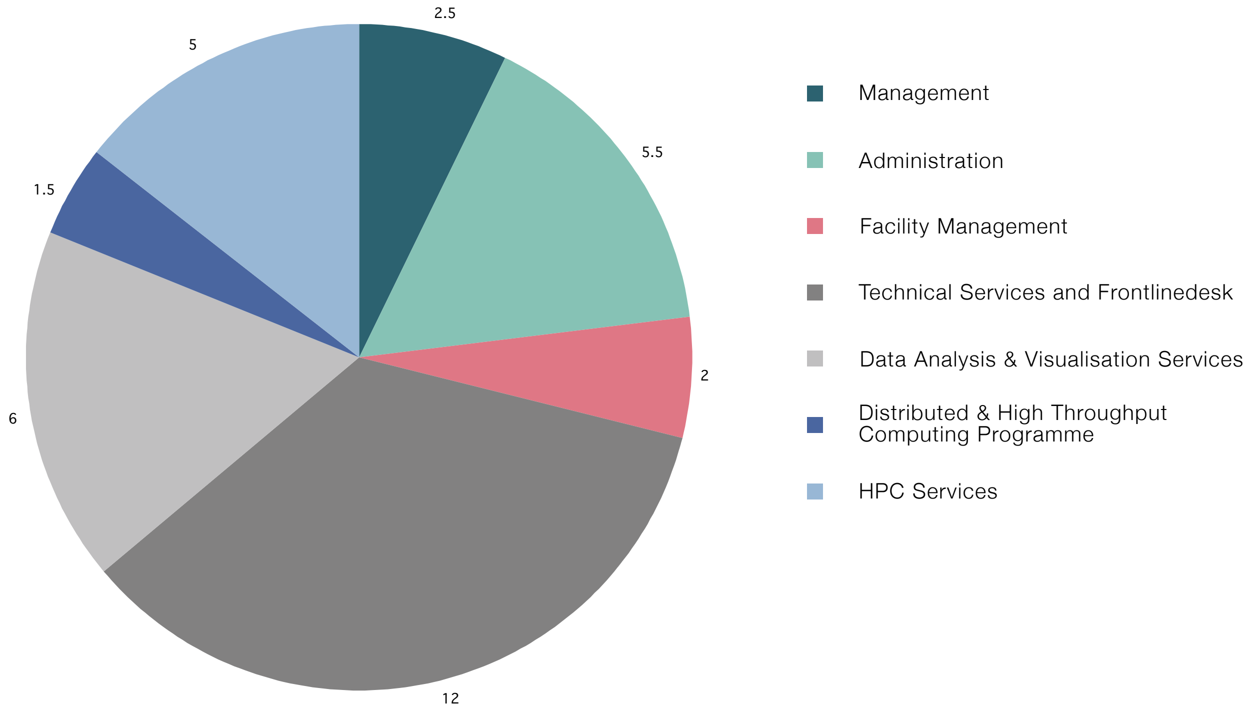
Journal Impact Factor for Papers Listed in the 2007 Annual Report

Publication	Impact factor	Principal investigator	Application field
Mallat T, Orglmeister E, Baiker A ; Asymmetric catalysis at chiral metal surfaces; Chem.Rev. 107 (11), 4863-4890 (2007)	22.757	A. Baiker	Nanosciences
Litvinchuk S, Tanaka H, Miyatake T, et al.; Synthetic pores with reactive signal amplifiers as artificial tongues;Nature Materials, 6 (8), 576-580 (2007)	19.782	J. Mareda	Chemistry
Vogel P, Turks M, Bouchez L, et al.; New organic chemistry of sulfur dioxide; Accounts of Chemical Research, 40 (10),931-942 (2007)	16.214	P. Vogel	Chemistry
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)	10.031	M. Parrinello	Material Sciences
Vargas A, Ferri D, Bonalumi N, et al.; Controlling the sense of enantioselection on surfaces by conformational changes of adsorbed modifiers; Angewandte Chemie-International Edition, 46 (21),3905-3908 (2007)	10.031	A. Baiker	Nanosciences
Markert C, Neuburger M, Kulicke K, et al.; Palladium-catalyzed allylic substitution: Reversible formation of allyl-bridged dinuclear palladium(I) complexes; Angewandte Chemie-International Edition,46 (31), 5892-5895 (2007)	10.031	M. Meuwly	Chemistry
Krivokapic I, Zerara M, Daku ML, et al.; Spin-crossover in cobalt(II) imine complexes; Coord.Chem.Rev.,251 (3-4) 364, (2007)	8.568	A. Hauser	Chemistry
Bussi G, Gervasio FL, Laio A, et al.; Free-energy landscape for beta hairpin folding from combined parallel tempering and metadynamics, J.Am.Chem.Soc., 128 (41),13435-13441 (2006)	7.885	M. Parrinello	Biosciences
Deubel DV ; Mechanism and control of rare tautomer trapping at a metal-metal bond: Adenine binding to dirhodium antitumor agents; J.Am.Chem.Soc.,130 (2) , 665-675 (2008)	7.885	D. Deubel	Chemistry
Gossens C, Tavernelli I, Rothlisberger U; DNA structural distortions induced by ruthenium-arene anticancer compounds; J. Am.Chem.Soc.,130 (33),10921-10928 (2008)	7.885	U. Röthlisberger	Chemistry
Hoxha F, Konigsmann L, Vargas A, et al.; Role of guiding groups in cinchona-modified platinum for controlling the sense of enantiodifferentiation in the hydrogenation of ketones Record contains structures; J.Am.Chem.Soc., 129 (34),10582-10590 (2007)	7.885	A. Baiker	Nanosciences
Markovic D, Varela-Alvarez A, Sordo JA, et al.; Mechanism of the diphenyldisulfone-catalyzed isomerization of alkenes. Origin of the chemoselectivity: Experimental and quantum chemistry studies; J.Am.Chem.Soc., 128 (24),7782-7795 (2006)	7.885	P. Vogel	Chemistry
Xiao W, Passerone D, Ruffieux P, et al.; C-60/corannulene on Cu(110): A surface-supported bistable buckybowl-buckyball host-guest system; J.Am.Chem.Soc.,130 (14), 4767-4771 (2008)	7.885	D. Passerone	Chemistry

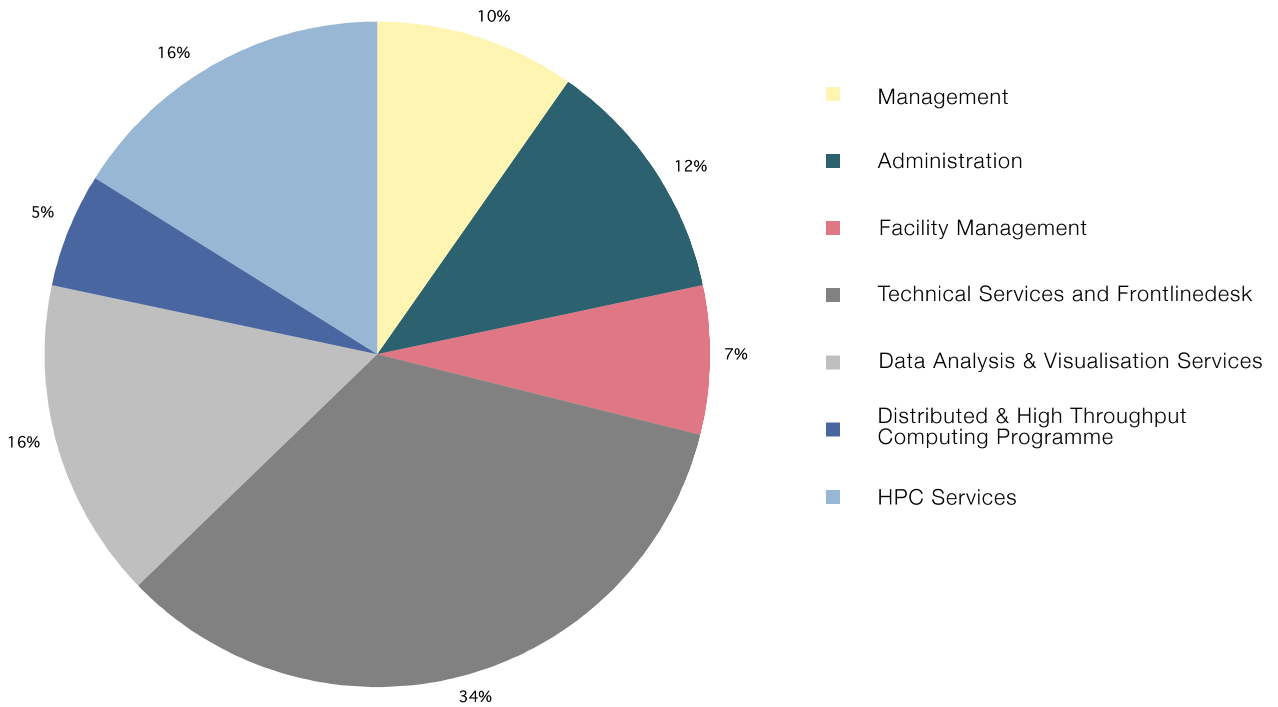
Source: ISI Web of Knowledge [SM]

Personnel

Average FTE per Unit

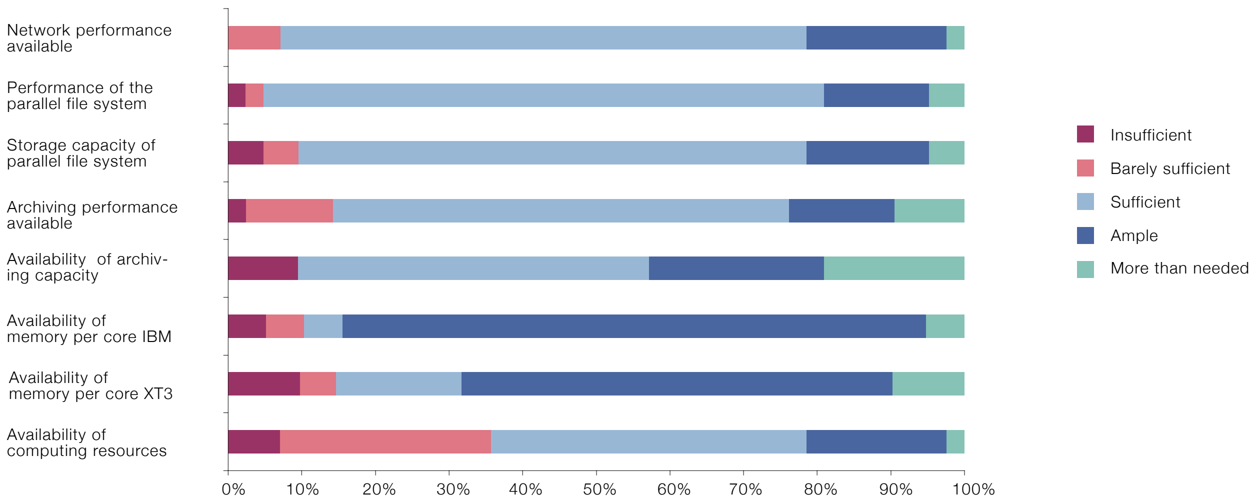


Staffing costs

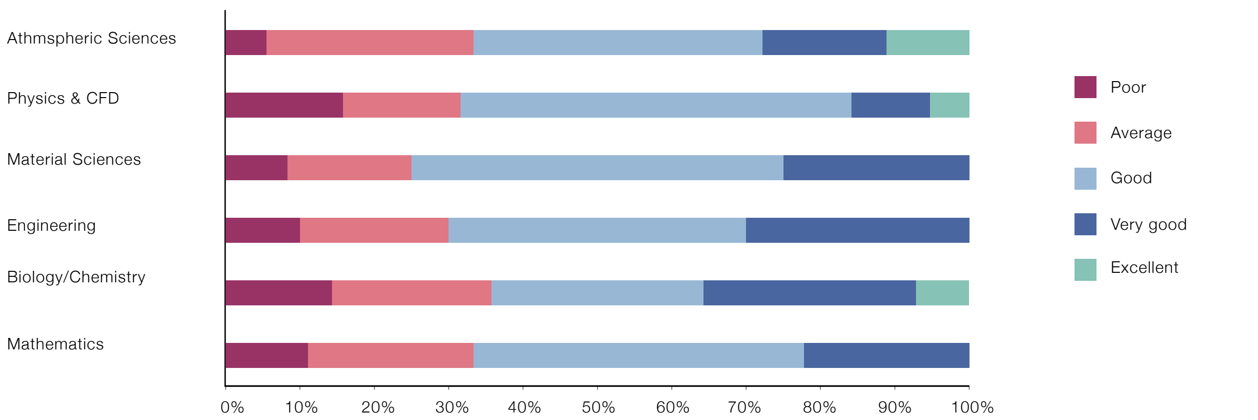


Customer satisaction

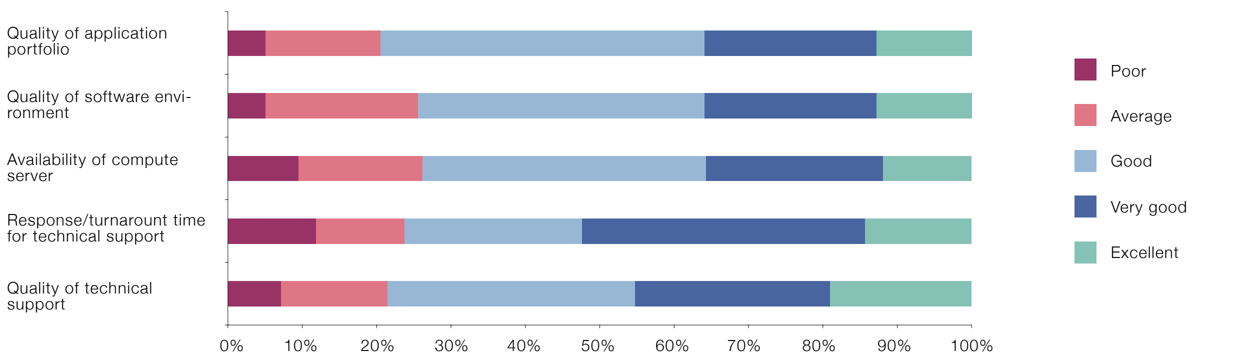
CSCS services portfolio



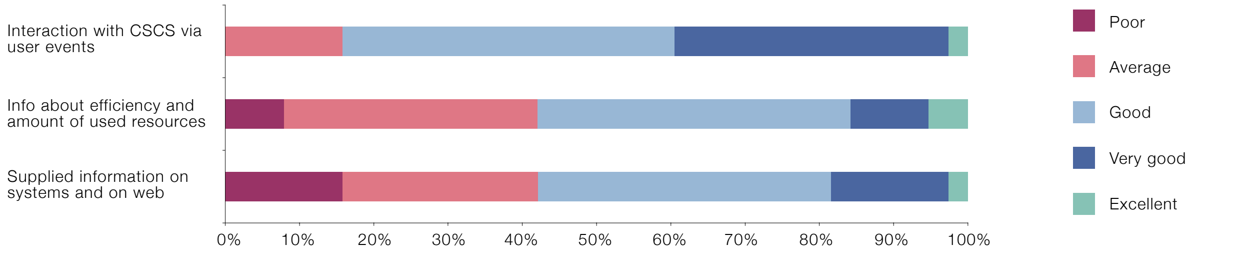
Quality of user support in the following fields

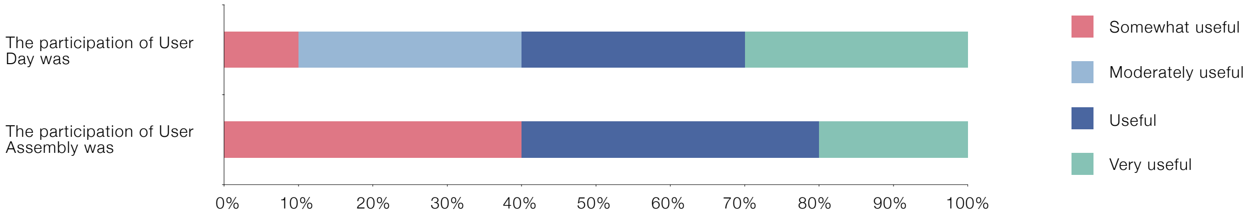


Application and user support

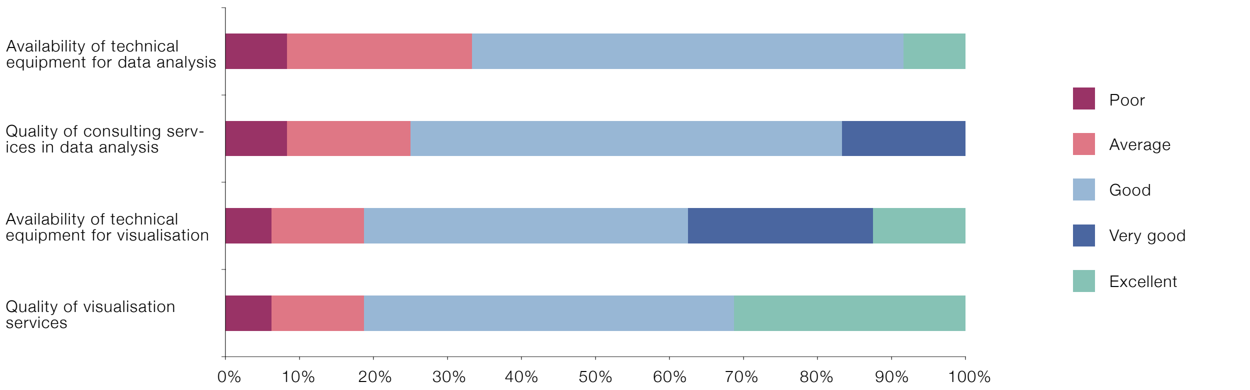


Information services

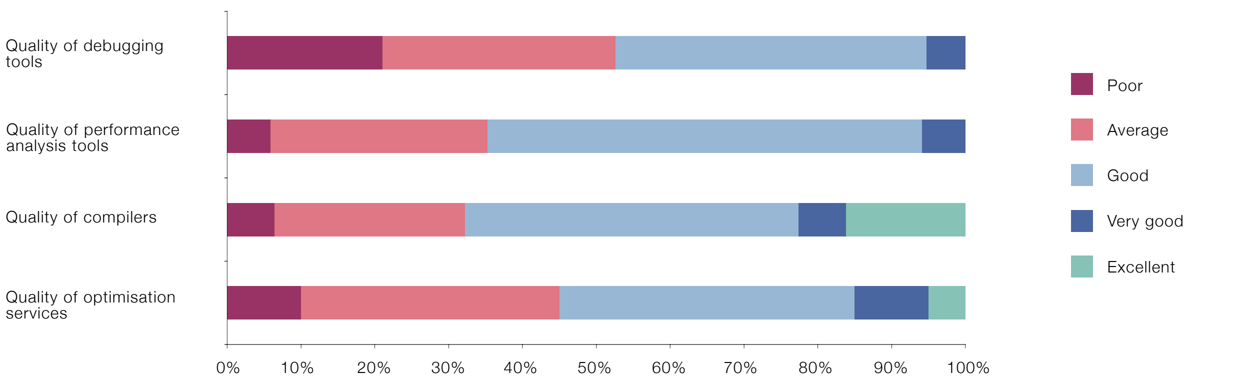




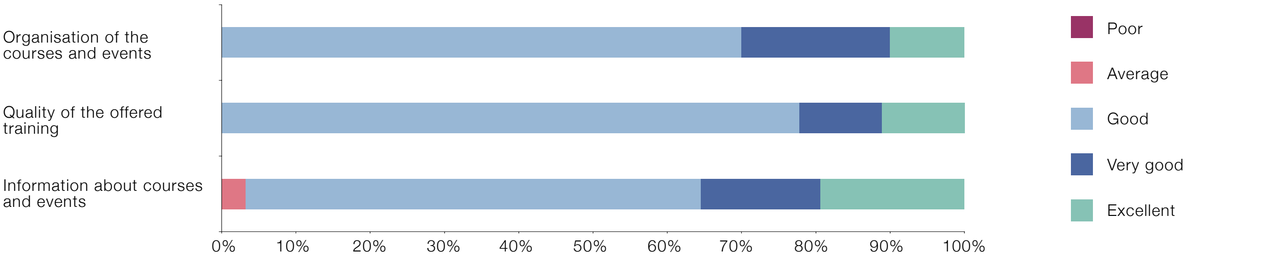
Data analysis and visualisation



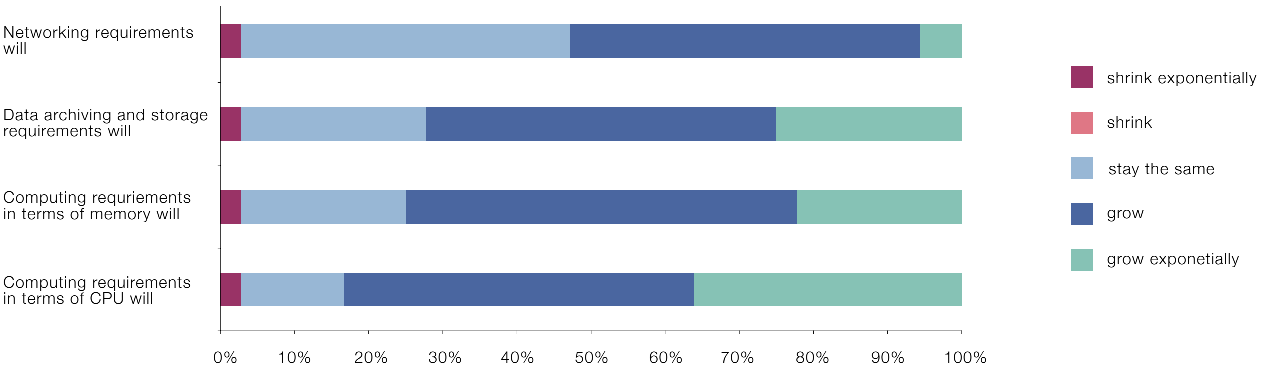
Data analysis and visualisation



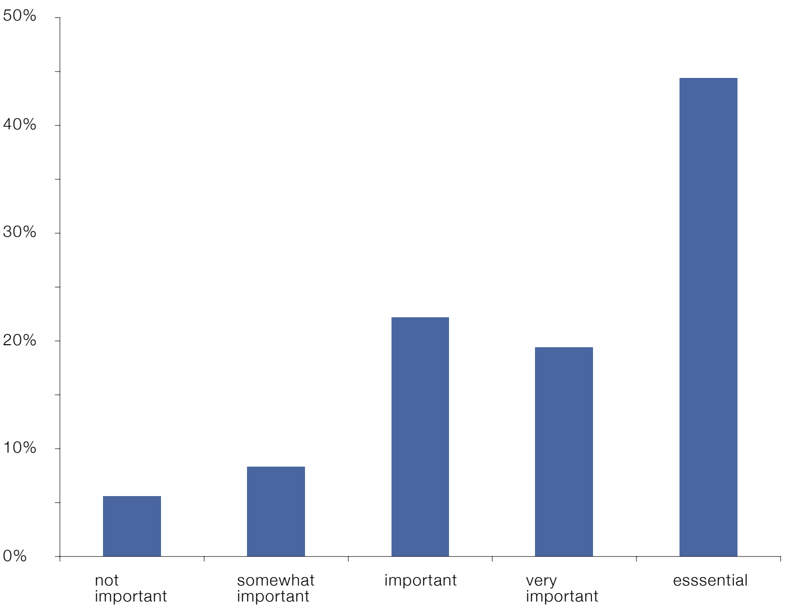
Training course and events



Future expectations and wishes



For achieving the scientific results the contribution of CSCS was:



Publications

Papers published by users of CSCS

Alkauskas A. , P. Broqvist, and A. Pasquarello; Defect energy levels in density functional calculations: Alignment and band gap problem; A. Physical Review Letters 101, 046405 (2008).

Abedijaberi A., J. Soulages, M. Kröger, B. Khomami; Flow of branched polymer melts in a lubricated cross-slot channel: A combined computational and experimental study; Rheol. Acta 48 (2008) 97-108.

Ahrens, B. and A. Walser, 2008: Information based skill scores for probabilistic forecasts. Mon. Wea. Rev., 136, 352-363.

Akurati K.K., A. Vital, J.P. Dellemann, K. Michalow, T. Graule, D. Ferri, and A. Baiker; Flame-Made WO_x/TiO_2 Nanoparticles: Relation between Acidity, Structure and Photocatalytic Activity; Appl. Catal. B, 79. 53 (2008).

Alkauskas A., P. Broqvist, and A. Pasquarello, Charge state of the O_2 molecule during silicon oxidation through hybrid functional calculations; Physical Review B – Rapid Communications 78, 161305(R) (2008).

Alkauskas A., P. Broqvist, F. Devynck, and A. Pasquarello; Band offsets at semiconductor- oxide interfaces from hybrid density functional calculations; Physical Review Letters 101, 106802 (2008).

Arbenz P. and O. Chinellato: On solving Complex-Symmetric Eigenvalue Problems Arising in the Design of Axisymmetric VCSEL Devices" Appl. Numer. Math. 58 (4): 381-394 (2008).

Arbenz P., G.H. van Lenthe, U. Mennel, Müller R. and M. Sala (2008): A scalable multi-level preconditioner for matrix-free µ-finite element analysis of human bone structures; Int. J. for Numerical Methods in Engineering 73 (7): 927-947.

Arbenz P., S.D. Margenov, and Y. Vutov: "Parallel MIC(0) Preconditioning of 3D Ellipticc Problems Discretized by Rannacher-Turek Finite Elements". Comput. Math. Appl. 55 (10): 2197-2211 (2008).

Bakowies D.; Ab initio thermochemistry using optimal-balance models with isodesmic corrections: The ATOMIC protocol; submitted to: J. Chem. Phys. 01, 2008.

Barducci A., G. Bussi, M. Parrinello; Well-Tempered Metadynamics: A Smoothly Converging and Tunable Free-Energy Method; Phys. Rev. Lett. 2008, 100, 020603.

Bayati B., Chatelain P., Koumoutsakos P., Multiresolution stochastic simulations of reaction-diffusion processes, Physical Chemistry Chemical Physics, 10, 39, 5963-5966, 2008.

Behler J., R. Martonak, D. Donadio, M. Parrinello; Metadynamics simulations of the high-pressure phases of Silicon employing a high-dimensional neural network potential; Phys. Rev. Lett. 2008, 100, 185501.

Behler J., R. Martonak, D. Donadio, M. Parrinello; Pressure-induced phase transitions in silicon studied by neural network-based metadynamics simulations; Phys. Stat. Sol. (b) 2008, 245 (12), 2618-2629.

Bernard Y.A., M. Dulak, J.W. Kaminski, and T. A. Wesolowski;The energy-differences based exact criterion for testing approximations to the functional for the kinetic energy of non-interacting electrons; J. Phys. A. 41 (2008) 055302.

Bernet M.L., F. Miniati, S.J. Lilly, P.P. Kronberg, M. Dessauges-Zavadsky; Strong magnetic fields in normal galaxies at high redshift; Nature, 454 (7202) 302-304 (2008).

Bitzek E., C. Brandl, P.M. Derlet, H. Van Swygenhoven; Dislocation cross-slip in nanocrystalline fcc metals; Phys. Rev. Lett. 100 (23)235501 (2008).

Bitzek E., P.M. Derlet, P.M. Anderson, H. Van Swygenhoven; The Stress-Strain Response of Nanocrystalline Metals: A Statistical Analysis of Atomistic Simulations; Acta Materalia 56 (17): 4846-4857.

Bonomi M., D. Branduardi, F.L. Gervasio, M. Parrinello; The unfolded ensemble and folding mechanism of the C-terminal GB1 beta-hairpin; J. Am. Chem. Soc. 2008, 130, 13938-13944.

Bovshuk V. R., W. A. Cooper, M. I. Mikhailov, J. Nührenberg and V. D. Shafranov; Search for Very-High-β MHD Stable Quasi-Isodynamic Configurations, ; Plasma and Fusion Research 3 (2008) S1046-1-5.

Braun J., A. Fouqueau, R. J. Bemish and M. Meuwly; Solvent Structures of Mixed Water/Acetonitrile Mixtures at Chromatographic Interfaces from Computer Simulations; PCCP, 10, 4765 (2008).

Brockhaus P., D. Lüthi and C. Schär, 2008. Aspects of the Diurnal Cycle in a Regional Climate Model; Meteorol. Z., 17 (4), 433-443.

Broqvist P., A. Alkauskas, and A. Pasquarello; Band alignments and defect levels in Si-HfO_2 gate stacks: Oxygen vacancy and Fermi-level pinning; Applied Physics Letters 92, 132911 (2008).

Broqvist P. , A. Alkauskas, and A. Pasquarello; Defect levels of dangling bonds in silicon and germanium through hybrid functionals; Physical Review B 78, 075203 (2008).

Buch V., A. Dubrovskiy, F. Mohamed, M. Parrinello, J. Sadlej, A.D. Hammerich, J.P. Devlin; HCl Hydrates as model systems for protonated water; J. Phys. Chem. A 2008, 112, 2144-2161.

Buchter F., Z. Lodziana, A. Remhof, O. Friedrichs, A. Borgschulte, Ph. Mauron, A. Zuttel, D. Sheptyakov, G. Barkhordarian, R. Bormann, K. Chłopek, M. Fichtner, M. Sørby, M. Riktor, B. Hauback, and S. Orimo; Structure of $Ca(BD_4)(2)$ beta-phase from combined neutron and synchrotron X-ray powder diffraction data and density functional calculations; J. Phys. Chem. B 112, 8042 (2008).

Buchter F., Z. Lodziana, Ph. Mauron, A. Remhof, O. Friedrichs, A. Borgschulte, A. Züttel, D. Sheptyakov, Th. Strässle, and A. J. Ramirez-Cuesta; Dynamical properties and temperature induced molecular disordering of $LiBH_4$ and $LiBD_4$; Phys. Rev. B 78, 094302 (2008).

Buffa G., L. Dore, F. Tinti and M. Meuwly; Experimental and theoretical study of Helium broadening and shift of HCO^+ rotational lines; Chem. Phys. Chem, 9, 2237 (2008).

Buehler, T., "Atmospheric blocking events and extreme temperatures in climate simulations and data", Diploma thesis, 2008.

Bussi G., M. Parrinello; Stochastic thermostats: comparison of local and global schemes; Comp. Phys. Comm. 2008, 179, 26-29.

Callegari S., L. Mayer, S.Kazantzidis; Pairing of supermassive black holes in unequal-mass mergers; 2008 MmSAI.79.1302C.

Caputi K., ..., C.M. Carollo, et al; The Optical Spectra of 24 m Galaxies in the COSMOS Field. I. Spitzer MIPS Bright Sources in the zCOSMOS-Bright 10k Catalog; ApJ, 680, 939, 2008.

Casapu M., J.D. Grunwaldt, M. Maciejewski, A. Baiker, R. Hoyer, and S. Eckhoff, Enhancement of Activity and Self-Reactivation of NSR Catalysts by Temporary Formation of $BaPtO_3$-Perovskite, Catal. Lett., 120, 1 (2008).

Casapu M., J.D. Grunwaldt, M. Maciejewski, F. Krumeich, A. Baiker, S. Eckhoff, and M. Wittrock , Comparative Study of Structural Properties and NO_X Storage-Reduction Behavior of $Pt/Ba/CeO_2$ and $Pt/Ba/Al_2O_3$, Appl. Catal. B, 78, 288 (2008).

Ceriotti M., T.D. Kühne, M. Parrinello; An efficient and accurate decomposition of the Fermi operator; J. Chem. Phys. 2008, 129, 024707.

Chatelain P., Curioni A., Bergdorf M., Rossinelli D., Andreoni W., Koumoutsakos P., Billion Vortex Particle Direct Numerical Simulations of Aircraft Wakes, Computer Methods in Applied Mechanics and Engineering, 197, 13-16, 1296-1304, 2008.

Chatelain P., Curioni A., Bergdorf M., Rossinelli D., Andreoni W., Koumoutsakos P.; Vortex Methods for Massively Parallel Computer Architectures; Lecture Notes in Computer Science, 5336, 479-489, 2008.

Colombo M., J. VandeVondele, A. Laio, L. Guidoni and U. Rothlisberger; Hybrid QM/MM molecular dynamics study of copper binding sites in the C-terminal domain of mouse prion protein; Proteins-Structure, Function, and Bioinformatics, 70, 1084-1098 (2008).

Cucinotta C. S., A. Ruini, E. Molinari, C. A. Pignedoli, A. Catellani, M. J. Caldas; Competitive chemisorption of bifunctional carboxylic acids on H:Si(100): a first-principles study; J. Phys. Chem. C. 112(27); 10167-10175 (2008).

D'Onghia E., M. Mapelli, B. Moore; Merger and ring galaxy formation rates at z <= 2; 2008, MNRAS, 389, 1275.

Danielsson J. and M. Meuwly; Atomistic Simulation of Adiabatic Reactive Processes Based on Multi-State Potential Energy Surfaces; J. Chem. Theory Computing, 4, 1083 (2008).

Debattista V. P., B. Moore, T. Quinn, S. Kazantzidis, R. Maas, L. Mayer, J. Read, J. Stadel; The Causes of Halo Shape Changes Induced by Cooling Baryons: Disks versus Substructures; 2008 ApJ. 681.1076D.

Del Gado E., P. Ilg, M. Kröger, H.C. Öttinger; Non-affine deformations of inherent structure as signature of cooperativity in supercooled liquids; Phys. Rev. Lett. 101 (2008) 095501 (4 pages).

Devynck F. and A. Pasquarello; Band gap opening at the 6H-SiC(0001) surface pas- sivated by an epitaxial silicon oxynitride layer: a first-principles investigation; Surface Science 602, 2989 (2008).

Dolamic I., C. Gautier, J. Boudon, N. Shalkevich and T. Bürgi; Adsorption of Thiol-Protected Gold Nanoparticles on TiO_2 and Their Behavior under UV Light Irradiation; J. Phys. Chem. C 2008, 112 (15), 5816-5824.

Domene C., M.L. Klein, D. Branduardi, F.L. Gervasio, M. Parrinello; Conformational changes and gating at the selectivity filter of Potassium channels; J. Am. Chem. Soc.2008, 130, 9474-9480.

Donadio D., R. Martonak, P. Raiteri, M. Parrinello; Influence of temperature and anisotropic pressure on the phase transitions in alpha-Cristobalite; Phys. Rev. Lett. 2008, 100, 165502.

Dongmei Jiang, T. Mallat, F. Krumeich, and A. Baiker; Copper-Based Metal-Organic Framework for the Facile Ring-Opening of Epoxides; J. Catal., 257, 390 (2008).

Dotti M., M. Colpi, F. Haardt, L. Mayer; Massive black hole binaries in gaseous nuclear discs; 2008 MmSAI.79.1294D.

Dotti M., M. Colpi, F. Haardt, L. Mayer; Simulating the dynamics of binary black holes in nuclear gaseous discs; 2008 IAUS.245.241D.

Dupuis A., Chatelain P., Koumoutsakos P., An Immersed Boundary-Lattice Boltzmann Method for the Simulation of the Flow Past an Impulsively Started Cylinder, J. Computational Physics, 227, 9, 4486-4498, 2008.

Elsener A., O. Politano, P. M. Derlet, and H. Van Swygenhoven; Modelling and Simulation in Materials; Science and Engineering 16, 025006 (2008).

El-Turk F., M. Cascella, H. Ouertatani-Sakouhi, R.L. Narayanan, L. Leng, R. Bucala, M. Zweckstetter, U. Röthlisberger and H.A. Lashuel; The conformational flexibility of the carboxy terminal residues 105-114 is a key modulator of the catalytic activity and stability of Macrophage Migration Inhibition Factor (MIF); Biochemistry, 47(40), 10740 (2008).

Errea I., Martinez-Canales M., Oganov A.R., et al.; Fermi surface nesting and phonon instabilities in simple cubic calcium; HIGH PRESSURE RESEARCH 28 (4), 443-448, (2008).

Ertl G., H. Knözinger, F. Schüth, J. Weitkamp, Eds.,Metallic Glasses by A. Baiker and A. Molnar, in Handbook of Heterogeneous Catalysis, 2nd Ed., Vol. 3, VCH, Weinheim, 2008, pp. 1285-1298.

Eshet H., F. Bruneval, M. Parrinello; New Lennard-Jones metastable phase; J. Chem. Phys. 2008, 129, 026101.

Evonuk M.; The role of density-stratification in generating zonal flow structures in a rotating fluid. Astrophys; J. 673, 1154-1159, 2008.

Feldmann R., L. Mayer, C.M. Carollo; Tidal Debris in Elliptical Galaxies as Tracers of Mergers with Disks; 2008 ApJ. 684.1062F.

Feldmann R., L. Mayer, C.M. Carollo;Tidal Debris in Elliptical Galaxies as Tracers of Mergers with Disks; The Astrophysical Journal, ApJ, 684, 1062, 2008.

Ferguson S.J., J.D. Langhoff, K. Voelter, B. von Rechenberg, D. Scharnweber, S. Bierbaum, M. Schnabelrauch, A.R. Kautz, V. Frauchiger, T.L. Mueller, G.H. van Lenthe and F. Schlottig (2008): Biomechanical comparison of different surface modifications for dental implants; International Journal of Oral and Maxillofacial Implants 23 (6): 1037-1046.

Fichtner W.; Overview of Technology Computer-Aided Design Tools and Applications in Technology Development, Manufacturing and Design; Journal of Computational and Theoretical Nanoscience 5, 1089 - 1105 (2008).

Fischer E.M. and C. Schär, 2008: Future changes in daily summer temperature variability: driving processes and role for temperature extremes; Clim. Dyn., in press, DOI 10.1007/s00382-008-0473-8.

Fischer T., P. Goegelein, M. Liebendörfer, A. Mezzacappa, F.- K. Thielemann; The accretion phase of core collapse supernovae; AIP Conf. Proc. 1016: 277 [5 p.] (2008).

Fischer T., S. C. Whitehouse, A. Mezzacappa, F.-K. Thielemann, M. Liebendörfer; The neutrino signal from protoneutron star accretion and black hole formation; submitted to A&A, arXiv:08095129 (2008).

Folini D., S. Ubl, P. Kaufmann; Lagrangian particle dispersion modeling for the high Alpine site Jungfraujoch; J. Geophys. Res., 113, D18111, 2008.

Foteinopoulou K., N.C. Karayiannis, M. Laso, M. Kröger, M.L. Mansfield; Universal scaling, entanglements, and knots of model chain molecules; Phys. Rev. Lett. 101 (2008) 265702.

Frein S., J. Boudon, M.Vonlanthen, T. Scharf, J. Barberá, G. Süss-Fink, T. Bürgi and R.Deschenaux; Liquid-Crystalline Thiol- and Disulfide-Based Dendrimers for the Functionalization of Gold Nanoparticles; Helv. Chim. Acta 2008, 91 (12), 2321-2337.

Fröhlich C., T. Fischer, M. Liebendörfer, F.-K. Thielemann, J. W. Truran; Detailed nucleosynthesis yields from the explosion of massive stars; Proc. IAU Symp. 250: 401 [6 p.] (2008).

Fukagata K., Kern S., Chatelain P., Koumoutsakos P., Kasagi N., Evolutionary optimization of an anisotropic compliant surface for turbulent friction drag reduction, J. Turbulence, 9, 35, 1-17, 2008.

Gangsto R., M. Gehlen, B. Schneider, L. Bopp, O. Aumont, and F. Joos; Modeling the marine aragonite cycle: changes under rising carbon dioxide and its role in shallow water $CaCO_3$ dissolution; Biogeosciences, 5, 1057-1072, 2008.

Gao G., Oganov A.R., Bergara A., Martinez-Canalez M., Cui T., Iitaka T., Ma Y., Zou G.; Superconducting high pressure phase of germane; Phys. Rev. Lett. 101, 107002, (2008).

Garcia Lastra J.-M., J.W. Kaminski, and T.A. Wesolowski; Orbital-free effective embedding potential at nuclear cusps; J. Chem. Phys. 129 (2008) 074107.

Gautier C. and T. Bürgi; Chiral Inversion of Gold Nanoparticles; J. Am. Chem. Soc. 2008, 130 (22), 7077-7084.

Gautier C., R. Taras, S. Gladiali and T. Bürgi; Chiral 1,1'-binaphthyl-2,2'-dithiol-stabilized gold clusters: Size separation and optical activity in the UV-vis; Chirality 2008, 20 (3-4), 486-49.

Gellé A., A. Läuchli, B. Kumar, and F. Mila; A 2D quantum antiferromagnet with a four-fold degenerate valence-bond-solid ground state; Phys. Rev. B 77, 014419 (2008).

Genovese L., A. Neelov, S. Goedecker, T. Deutsch, A. Ghasemi, O. Zilberberg, A. Bergman, M. Rayson and R. Schneider; Daubechies wavelets as a basis set for density functional pseudopotential calculations; J. Chem. Phys. 129, 014109 (2008).

Ghasemi S. A., S. Goedecker, A. Baratoff, T. Lenosky, E. Meyer, and H. J. Hug; Ubiquitous Mechanisms of Energy Dissipation in Noncontact Atomic Force Microscopy; Phys. Rev. Lett. 100, 236106 (2008).

Ghosh K.K., M. Mapelli; UGC 7069: the largest ring galaxy; 2008, MNRAS Letters, 386, 38.

Giustino F. and A. Pasquarello; First-principles theory of infrared absorption spectra at surfaces and interfaces: Application to the Si(100):H2O surface; Physical Review B 78, 075307 (2008).

Gossens C., I. Tavernelli and U. Rothlisberger; DNA structural distortions induced by ruthenium-arene anticancer compounds; Journal of the American Chemical Society, 130, 10921-10928 (2008).

Governato F., L. Mayer, C. Brook; The Formation of Galaxy Disks; 2008 ASPC..396..453G.

Goze C., E. Beitler, N. Dupont, C. Leiggener, H. Jia, P. Monbaron, S.-X. Liu, A. Neels, A. Hauser and S. Decurtins; Ruthenium(II) Coordination Chemistry of a Fused Donor-Acceptor Ligand: Synthesis, Characterization and Photoinduced Electron Transfer Reactions of $[\{Ru(bpy)_2\}_n(TTF\text{-}ppb)](PF6)_{2n}$ (n = 1, 2); Inorganic Chemistry, 47 (23) , 2008 , p11010-11017.

Goze C., S.-X. Liu, C. Leiggener, L. Sanguinet, E. Levillain, A. Hauser and S. Decurtins; Synthesis of new ethynylbipyridine-linked mono- and bis-tetrathiafulvalenes: electrochemical, spectroscopic, and Ru(II)-binding studies; Tetrahedron, 64 (7) , 2008 , p1345 -1350.

Guedes J., J. Diemand, M. Zemp, M. Kuhlen, P. Madau, L. Mayer; Massive Black Hole recoil in high resolution hosts; 2008 AN 329.1004G.

Guidon M., F. Schiffmann, J. Hutter, J. VandeVondele; Ab initio molecular dynamics using hybrid density functionals; J. Chem. Phys. 128 Art. No. 214104 (2008).

Hagemann H., M. Longhini , J.W. Kaminski, T.A. Wesolowski, R. Cerny, N. Penin, M.H. Sorby, B.C. Hauback, G. Severa, and C.M. Jensen ; $LiSc(BH_4)_4$: a novel salt of Li^+ and discrete $Sc(BH_4)^{4-}$ complex anions; J. Phys. Chem. A 112 (2008) 7551-7555.

Haider P., B. Kimmerle, F. Krumeich, W. Kleist, J.D. Grunwaldt, and A. Baiker; Gold-Catalyzed Aerobic Oxidation of Benzyl Alcohol: Effect of Gold Particle Size on Catalytic Behavior in Different Solvents; Catal. Lett.,125, 169 (2008).

Hansen N, Niederberger ASR, Guzzella L, Koumoutsakos, P., Evolutionary optimization of feedback controllers for thermoacoustic instabilities IUTAM Bookseries, Volume: 7 Pages: 311-317, 2008.

Hieber S.E., Koumoutsakos P., A Lagrangian particle method for the simulation of linear and nonlinear elastic model of soft tissue, J. Computational Physics, 227, 9195-9215, 2008.

Hieber S.E., Koumoutsakos P., An immersed boundary method for smoothed particle hydrodynamics of self-propelled swimmers, J. of Computational Physics, 227, 19, 8636-8654, 2008.

Hohenegger C., A. Walser, W. Langhans and C. Schär, 2008: Cloud-resolving ensemble simulations of the August 2005 Alpine flood; Quart. J. Roy. Meteorol. Soc., 134 (633), 889-904.

Hohenegger C., P. Brockhaus and C. Schär, 2008: Towards climate simulations at cloud-resolving scales; Meteorol. Z., 17 (4), 383-394.

Hu C.H., Oganov A.R., Wang Y.M., et al.; Crystal structure prediction of $LiBeH_3$ using ab initio total-energy calculations and evolutionary simulations: JOURNAL OF CHEMICAL PHYSICS 12 (23), 234105, 2008.

Jaun, S., B. Ahrens, A. Walser, T. Ewen and C. Schär, 2008: A probabilistic view on the August 2005 floods in the upper Rhine catchment. Nat. Hazards Earth Syst. Sci., 8, 281-291.

Jaeger E.B., I. Anders, D. Lüthi, B. Rockel, C. Schär, and S.I. Seneviratne, 2008: Analysis of ERA40-driven CLM simulations for Europe; Meteor. Z., 17 (4), 349-367. (CLM special issue).

Jaeger E.B., I. Anders, D. Lüthi, B. Rockel, C. Schär, S. I. Seneviratne, 2008: Analysis of ERA40-driven CLM simulations for Europe; Meteorol. Z., submitted.

Jocksch A. and L. Kleiser; Growth of turbulent spots in high-speed boundary layers on a flat plate; Int. J. Heat and Fluid Flow, 29(6), 1543-1557, 2008.

Joos F. and R. Spahni; Rates of change in natural and anthropogenic radiative forcing over the past 20'000 years; Proceedings of the National Academy of Sciences USA (PNAS) , 105, 1425-1430, 2008.

Jucker M., J. P. Graves, G. A. Cooper and W. A. Cooper; Impact of pressure anisotropy on tokamak equilibria and the toroidal magnetic precession; Plasma Phys. Control. Fusion 50 (2008) 065009-1-16.

Jutz F., J.D. Grunwaldt, and A. Baiker, Mn(III)(salen)-Catalyzed Synthesis of Cyclic Organic Carbonates from Propylene and Styrene Oxide in Supercritical CO_2, J. Mol. Catal. A., 279, 94, (2008).

Karamertzanis P.G., P. Raiteri, M. Parrinello, M. Leslie, S.L. Price; The thermal stability of lattice-energy minima of 5-Fluorouracil: metadynamics as an aid to polymorph prediction; J. Phys. Chem. B 2008, 112, 4298-4308.

Karlin I.V., M. Colangeli, M. Kröger; Exact linear hydrodynamics from the Boltzmann equation; Phys. Rev. Lett. 100 (2008) 214503.

Kern S, Chatelain P, Koumoutsakos P Modeling, simulation and optimization of anguilliform swimmers BIO-MECHANISMS OF SWIMMING AND FLYING: FLUID DYNAMICS, BIOMIMETIC ROBOTS, AND SPORTS SCIENCE,Pages: 167-178, 2008.

Khaliullin R.Z., A.T. Bell, M. Head-Gordon; Analysis of charge transfer effects in molecular complexes based on absolutely localized molecular orbitals; J. Chem. Phys., 2008, 128(18), 184112.

Kiebach R., W. Bensch, J.D. Grunwaldt, A. Michailovski, A. Baiker, T. Fox, Y. Zhou, and G.R. Patzke, Hydrothermal Formation of W/Mo-Oxides: A Comprehensive Approach; Chem. Mat., 20, 3022 (2008).

Kim J.M., D.J. Keffer, M. Kröger, B.J. Edwards; Rheological and entanglement characteristics of linear chain polyethylene liquids in planar Couette and planar elongational flows; J. Non-Newtonian Fluid Mech. 152 (2008) 168-183.

Kleppek S., V. Muccione, C. C. Raible, D. N. Bresch, P. Koellner-Heck, T. F. Stocker, 2008: Tropical cyclones in ERA-40 - a detection and tracking method; Geophys. Res. Lett., 35, L10705, doi:10.1029/2008GL033880.

Klimentowski J., E.L. Łokas, S. Kazantzidis, F. Prada, L. Mayer, G.A. Mamon; Mass Modelling of dwarf Spheroidal Galaxies; 2008 IAUS. 244. 321K.

Koci L., Ma Y., Oganov A.R., et al.; Elasticity of the superconducting metals V, Nb, Ta, Mo, and W at high pressure; PHYSICAL REVIEW B 77 (21), 214101 (2008).

Kosa M., M. Krack, A.K. Cheetham, M. Parrinello; Modeling the hydrogen storage materials with Exposed M^{2+} Coordination sites; J. Phys. Chem. C 2008, 112 (42), 16171-16173.

Kotsalis E.M., Koumoutsakos P., A Control Algorithm for Multiscale Simulations of Liquid Water, Lecture Notes in Computer Science, 5102, 234-241, Springer Berlin, 2008.

Krivokapic I., C. Enachescu, R. Bronisz and A. Hauser; Spin transition and relaxation dynamics coupled to a crystallographic phase transition in a polymeric iron(II) spin-crossover system; Chemical Physics Letters, 455 (4-6) , 2008 , p192 -196.

Krivokapic I., C. Enachescu, R. Bronisz and A. Hauser; The interaction between the spin transition and a crystallographic phase transition in the spin-crossover compound $[Fe(bbtr)_3](ClO_4)_2$: Nucleation, formation of domains and fluctuations; Inorganica Chimica Acta, 361 (12-13) , 2008 , p3616 -3622.

Kröger M., A. Ammar, F. Chinesta; Consistent closure schemes for statistical models of anisotropic fluids; J. Non-Newtonian Fluid Mech. 149 (2008) 40-55.

Kröger M., O. Peleg, Y. Ding, Y. Rabin; Formation of double helical and filamentous structures in models of physical and chemical gels; Soft Matter 4 (2008) 18-28.

Kronberg P.P., M.L. Bernet, F. Miniati, S.J. Lilly, M.B. Short, D.M. Higdon; A Global Probe of Cosmic Magnetic Fields to High Redshifts; Astrophysical Journal, 676, (1), 70-79, (2008).

Kukula P., V. Matoušek, T. Mallat, A. Baiker, Enantioselective Decarboxylation of ß-Ketoesters with Pdamino Alcohol Systems: Successive Metal- and Organocatalysis, Chem. Eur. J., 14, 2699 (2008).

Lammers S., S. Lutz and M. Meuwly; Reactive Force Fields for Proton Transfer Dynamics; J. Comp. Chem., 29, 1048 (2008).

Läuchli A. and C. Kollath; Spreading of correlations and entanglement after a quench in the Bose-Hubbard model; J. Stat. Mech. (2008) P05018.

Läuchli A., S. Capponi, and F.F. Assaad; Dynamical dimer correlations at bipartite and non-bipartite Rokhsar-Kivelson points; J. Stat. Mech. (2008) P01010.

Legreid G., D. Folini, J. Staehelin et al.; Measurements of organic trace gases including oxygenated volatile organic compounds at the high alpine site Jungfraujoch (Switzerland): Seasonal variation and source allocations; J. Geophys. Res., 113, D05307, 2008.

Lemercier G., A. Bonne, M. Four and L.M. Lawson Daku; 3MLCT excited states in Ru(II) complexes: Reactivity and related two-photon absorption applications in the near-infrared spectral range; Comptes Rendus Chimie, 11 (6-7) , 2008 , p709-715.

Liebendörfer M., T. Fischer, C. Fröhlich, F.-K. Thielemann, S. C. Whitehouse; Nuclear physics with spherically symmetric supernova models; J. of Phys. G 35: 014056 [8 p.] (2008).

Liebendörfer M., T. Fischer, C. Fröhlich, W. R. Hix, K. Langanke, G. Martínez-Pinedo, A. Mezzacappa, S. Scheidegger, F.-K. Thielemann, S. C. Whitehouse; Nuclear physics in core-collapse supernovae; New Astronomy Reviews 52: 373 [4 p.] (2008).

Lin I.-C. and U. Rothlisberger; Atom-centered potentials for describing dispersion forces in density functional theory; CHIMIA, 62, 231-234 (2008).

Lin I.C. and U. Rothlisberger; Describing weak interactions of biomolecules with dispersion-corrected density functional theory; Physical Chemistry Chemical Physics, 10, 1-5 (2008).

Lochan R.C., R.Z. Khaliullin, M. Head-Gordon; The interaction of molecular hydrogen with open transition metal centers for enhanced binding in metal oxide frameworks: a computational study; Inorg. Chem., 2008, 47(10), 4032-4044.

Lodziana Z., A. Züttel and P. Zielinski; Titanium and native defects in LiBH4 and NaAlH4; J. Phys. Cond. Matter, 20, 465210 (2008).

Łokas E.L., J. Klimentowski, S. Kazantzidis, L. Mayer; The anatomy of Leo I: how tidal tails affect the kinematics; 2008 MNRAS.390..625L.

Luisier M., A. Schenk, W. Fichtner, T. Boykin and G. Klimeck; A Parallel Sparse Linear Solver for Nearest-Neighbor Tight-binding Problems; submitted to Europar 2008, Gran Canaria, Spain, August 2008.

Lüscher A., R.M. Noack, and A. Läuchli; The FFLO state in the one-dimensional attractive Hubbard model and its fingerprint in the spatial noise correlations; Phys. Rev. A 78, 013637 (2008).

Ma Y.-M., Oganov A.R., Xie Y.; High pressure structures of lithium, potassium, and rubidium predicted by ab initio evolutionary algorithm; Phys. Rev. B78, 014102 (2008).

Maciejewski M., T.J. Brunner, S.F. Loher, A. Baiker, and W.J. Stark; Phase Transitions in Flame-Made Calcium Phosphates; Thermochim. A., 468, 75 (2008).

Mallat T. and A. Baiker; Oxidations of Alcohols with Molecular Oxygen in Handbook of Heterogeneous Catalysis, (G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp, Eds.), 2nd Ed., Vol. 7, VCH, Weinheim, 2008, pp. 3521-3538.

Mallat T., A. Baiker, W. Kleist and K. Köhler, Catalytic Aminations in Handbook of Heterogeneous Catalysis, (G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp, Eds.), 2nd Ed., Vol. 7, VCH, Weinheim, 2008, pp. 3584-3564.

Mallat T., S. Diezi and A. Baiker; Chiral Surfaces and Enantioselective Catalysis in Handbook of Heterogeneous Catalysis, (G. Ertl, H. Knözinger, F. Schüth, J. Weitkamp, Eds.), 2nd Ed., Vol. 7, VCH, Weinheim, 2008, pp. 3603-3626.

Man H.-K. and J.G.M van Mier; Size effect on strength and fracture energy for numerical concrete with realistic aggregate shapes; International Journal of Fracture, 154(1):61–72, 11 2008. doi:10.1007/s10704-008-9270-y.

Man H.-K. and J.G.M. van Mier (2008b); Influence of Particle Density on 3D Size Effects in Numerical Concrete; Mechanics of Materials, 40:470-486.

Mandelbaum R., ..., C.M. Carollo, et al; Precision Photometric Redshift Calibration for Galaxy-Galaxy Weak Lensing MNRAS, 386, 781, 2008.

Mapelli M., B. Moore, E. Ripamonti, L. Mayer, M. Colpi, L. Giordano; Are ring galaxies the ancestors of giant low surface brightness galaxies?; 2008 MNRAS.383.1223M.

Mapelli M., B. Moore, J. Bland-Hawthorn; Lopsided galaxies: the case of NGC 891; 2008, MNRAS, 388, 697.

Mapelli M., B. Moore, L. Giordano, L. Mayer, M. Colpi, E. Ripamonti, S. Callegari; Intermediate-mass black holes and ultraluminous X-ray sources in the Cartwheel ring galaxy; 2008, MNRAS, 383, 230.

Mapelli M., B. Moore; Are ring galaxies the ancestors of giant low surface brightness galaxies?; 2008, Astronomische Nachrichten, 329, 948.

Marlon J. R., P. J. Bartlein, C. Carcaillet, D. G. Gavin, S. P. Harrison, P. E. Higuera, F. Joos, M. J. Power, and I. C. Prentice; A climate-driven decline in global biomass burning during the past two millennia; Nature Geoscience, doi:10.1038/ngeo313, 2008.

Masson F., T. Laino, I. Tavernelli, U. Rothlisberger, and J. Hutter; Computational Study of Thymine Dimer Radical Anion Splitting in the Self-Repair Process of Duplex DNA; J. Am. Chem. Soc., 130 (11), pp 3443–3450 (2008).

Masson F., T. Laino, I. Tavernelli, U. Rothlisberger and J. Hutter; Computational Study of Thymine Dimer Radical Anion Splitting in the Self-Repair Process of Duplex DNA; CHIMIA, 62, 439 (2008).

Masson F., T. Laino, I. Tavernelli, U. Rothlisberger and J. Hutter; Computational Study of Thymine Dimer Radical Anion Splitting in the Self-Repair Process of Duplex DNA; J. Am. Chem. Soc., 130(11), 3443-3450 (2008).

Mayer L., A.J. Gawryszczak; Protoplanetary Disk Fragmentation with Varying Radiative Physics, Initial Conditions and Numerical Techniques; 2008 ASPC. 398. 243M.

Mayer L., F. Governato, & T. Kaufmann; The formation of disk galaxies in computer simulations; 2008, Advanced Science Letters, 1, 1.

Mayer L., S. Kazantzidis, P. Madau, M. Colpi, T. Quinn, J. Wadsley; Multi-Scale Simulations of Merging Galaxies with Supermassive Black Holes; 2008 ralc.conf.152M.

Mayer L., S. Kazantzidis; Formation of Nuclear Disks and Supermassive Black Hole Binaries in Galaxy Mergers; 2008 MmSAI.79.1284M.

Meier D. M., A. Urakawa, N. Turrà, H. Rüegger, and A. Baiker; Spectroscopic and Theoretical Investigation of Hydrogen Bonding Interactions in Cinchonidine - 2-Methyl-2-Hexenoic Acid Complexes; J. Phys. Chem. A, 112, 6150 (2008).

Milde F., Bergdorf M., Koumoutsakos P., A Hybrid Model for 3D Simulations of Sprouting Angiogenesis, Biophysical J., 95, 7, 3146–3160, 2008.

Milde F., Bergdorf M., Koumoutsakos P., A Hybrid Model of Sprouting Angiogenesis, Lecture Notes in Computer Science, 5102, 167-176, Springer Berlin, 2008.

Milos M., S. Kairouani, S. Rabaste and A. Hauser; Energy migration within the 2E state of Cr3+; Coordination Chemistry Reviews, 252 (23-24) , 2008, p2540 -2551.

Mobian P., C. Nicolas, E. Francotte, T. Bürgi and J. Lacour; Synthesis, Resolution, and VCD Analysis of an Enantiopure Diazaoxatricornan Derivative; J. Am. Chem. Soc. 2008, 130 (20), 6507-6514.

Molina-Montes E., D. Donadio, A. Hernandez-Laguna, C.I. Saint-Diaz, M. Parrinello; DFT research on the Dehydroxylation reaction of Pyrophyllite 1. first-principle molecular dynamics simulations; J. Phys. Chem. B 2008, 112, 7051-7060.

Mondelli C., D.Ferri and A. Baiker; Ru at Work in Ru-Hydroxyapatite during the Aerobic Oxidation of Benzyl Alcohol: An in situ ATR-IR Spectroscopy Study; J. Catal., 258, 170 (2008).

Müller S. A., F. Joos, N. R. Edwards, and T. F. Stocker; Modeled natural and excess radiocarbon: Sensitivities to the gas exchange formulation and ocean transport strength; Global Biogeochemical Cycles , 22, GB3011, doi:10.1029/2007GB003065, 2008.

Müller S. B. and L. Kleiser; Viscous and inviscid spatial stability analysis of compressible swirling mixing layers; Phys. Fluids,20:114103, 2008.

Muolo M. L., F. Valenza, A. Passerone and D. Passerone; Oxygen Influence on ceramics wettability by liquid metals Ag-aAl_2O_3. Experiments and modeling Materials Science and engineering A, 495, 153 (2008).

Nielsen G.J., H.M. Ronnow, A.M. Läuchli, F.P.A. Fabbiani, J. Sanchez-Benitez, K.V. Kamenev, and A. Harrison; A new realisation of the S=1/2 frustrated chain antiferromagnet; Chem. Mater. 20, 8 (2008).

Obrist D. and L. Kleiser; Localization of acoustic sources in subsonic jets; Proc. Appl. Math. Mech., 8(1), 10693-10694, 2008.

Obrist D. and S. Hegemann; Fluid-particle dynamics in canalithiasis; Roy. Soc. Interface, 5(27), 2008. DOI: 10.1098/rsif.2008.0047.

Oganov A.R., Glass C.W.; Evolutionary crystal structure prediction as a tool in materials design; JOURNAL OF PHYSICS-CONDENSED MATTER 20 (6), 064210 (2008).

Oganov A.R., Ono S., Ma Y.M, et al.; Novel high-pressure structures of $MgCO_3$, $CaCO_3$ and CO_2 and their role in Earth's lower mantle; EARTH AND PLANETARY SCIENCE LETTERS 273 (1-2) , 38-47, (2008).

Ono S., Oganov A.R., Brodholt J.P., et al.; High-pressure phase transformations of FeS: Novel phases at conditions of planetary cores; EARTH AND PLANETARY SCIENCE LETTERS 272 (1-2), 481-487 (2008).

Pagliai M., C. Cavazzoni, G. Cardini, G. Erbacci, M. Parrinello, V. Schettino; Anharmonic infrared and Raman spectra in Car-Parrinello molecular dynamics simulations; J. Chem. Phys. 2008, 128, 224514.

Parekh P., F. Joos, and S. A. Müller; A modeling assessment of the interplay between aeolian iron fluxes and iron-binding ligands in controlling carbon dioxide fluctuations during Antarctic warm events; Paleoceanography , 23, doi:10.1029/2007PA001531, 2008.

Peleg O., M. Kröger, Y. Rabin; Model of microphase separation in two-dimensional gels; Macromolecules 41 (2008) 3267-3275.

Petraglio G., M. Bartolini, D. Branduardi, V. Andrisano, M. Recanatini, F.L. Gervasio, A. Cavalli, M. Parrinello; The role of Li^+, Na^+, and K^+ in the ligand binding inside the human acetylcholinesterase gorge; Proteins 2008, 70, 779-785.

Pfaendtner J. and L. J. Broadbelt; Mechanistic Modeling of Lubricant Degradation. 1. Structure-Reactivity Relationships for Free-Radical Oxidation; Ind. Eng. Chem. Res., 2008, 47 (9), 2886-2896.

Pfaendtner J. and L. J. Broadbelt; Mechanistic Modeling of Lubricant Degradation. 2. The Autoxidation of Octane and Decane; Ind. Eng. Chem. Res., 2008, 47 (9), 2897- 2904.

Pfrändtner J., G.A. Voth; Molecular Dynamics Simulation and Coarse-Grained Analysis of the Arp2/3 Complex; Biophysical Journal 95 (11), 5324-5333, 2008.

Pietrucci F., M. Bernasconi, A. Laio, M. Parrinello; Vacancy-vacancy interaction and oxygen diffusion in stabilized cubic ZrO_2 from first principles; Phys. Rev. B 2008, 78, 094301.

Plattner G.-K., R. Knutti, F. Joos, T. F. Stocker, W. von Bloh, V. Brovkin, D. Cameron, E. Driesschaert, S. Dutkiewicz, M. Eby, N. R. Edwards, T. Fichefet, J. C. Hargreaves, C. D. Jones, M. F. Loutre, H. D. Matthews, A. Mouchet, S. A. Müller, S. Nawrath, A. Price, A. Sokolov, K. M. Strassmann, and A. J. Weaver. Long-term climate commitments projected with climate - carbon cycle models; Journal of Climate , 21, 2721-2751, 2008.

Plattner N. and M. Meuwly; Atomistic Simulations of CO Vibrations in Ices Relevant to Astrochemistry; ChemPhysChem, 9, 1271 (2008).

Plattner N. and M. Meuwly; The Role of Higher CO-Multipole Moments in Understanding the Dynamics of Photodissociated Carbonmonoxide in Myoglobin; Biophys. J., 94, 2505 (2008).

Plattner N., T. Bandi, J. D. Doll, D. L. Freeman and M. Meuwly; MD Simulations using Distributed Multipole Electrostatics: Structural and Spectroscopic Properties of CO^- and Methane-Containing Clathrates; Mol. Phys., 106, 1675 (2008).

Poncet Ph., Hildebrand R., Cottet G.H., Koumoutsakos P., Spatially distributed control for optimal drag reduction of the flow past a circular cylinder, J. Fluid Mechanics, 599, 111-120, 2008.

Prakash M. K. and R. A. Marcus; Dielectric dispersion interpretation of single enzyme dynamic disorder, spectral diffusion and radiative fluorescence lifetime; accepted to J. Phys. Chem. B, 112, 399-404 (2008).

Racu A.-M., J. Schoenes, Z. Lodziana, A. Borgschulte, A. Züttel; High-Resolution Raman Spectroscopy Study of Phonon Modes in $LiBH_4$ and LiBD4; J. Phys. Chem. A.; 112, 9716 (2008).

Raderschall, N., M. Lehning and C. Schär, 2008: Fine-scale modeling of the boundary-layer wind field over steep topography. Water Resour. Res., 44, Art. No. W09425.

Raible C.C., P. Della-Marta, C. Schwierz, H. Wernli, and R. Blender, 2008: Northern Hemisphere extratropical cyclones: A comparison of detection and tracking methods and different reanalyses; Mon. Wea. Rev., 136 880-897.

Raible, C. C., R. De Jong, T. F. Stocker, M. Yoshimori, "Maunder Minimum climate variability from wind and moisture-sensitive proxies and model simulations", /Pages Newsletter, 16/2/, 10-11, 2008.

Raiteri P., G. Bussi, C. S. Cucinotta, A. Credi, J. F. Stoddart, M. Parrinello; Unravelling the Shuttling Mechanism in a Photoswitchable Multicomponent Bistable Rotatane; Angew. Chem. Int. Ed. 47, 3536 –3539 (2008).

Rakhmatullina E., A. Mantion, T. Bürgi, V. Malinova, W. Meier; Solid-supported amphiphilic triblock copolymer membranes grafted from gold surface; J. Polymer Sci. Polymer Chem. 2008, 47 (1), 1-13.

Reimann S., M. K. Vollmer, D. Folini et al.; Observations of long-lived anthropogenic halocarbons at the high-Alpine site of Jungfraujoch (Switzerland) for assesement of trends and European sources; Sci. Tot. Env., 391, 2-3, 224-231, 2008.

Reimann S., T. Mallat, and A. Baiker; A New Efficient Heterogeneous Pd Catalyst for Enantioselective Allylic Substitution; J. Catal., 254, 79 (2008).

Reimann S., T. Mallat, and A. Baiker; Phosphine-Modified Pd/Al2O3 for Asymmetric Allylic Substitution, Chim. Oggi, 26 (Suppl.1) 23 (2008).

Riis-Johannessen T., N. Dupont, G. Canard, G. Bernardinelli, A. Hauser and C. Piguet; Towards inert and pre-organized d-block-containing receptors for trivalent lanthanides: The synthesis and characterization of triple-helical monometallic OsII and bimetallic OsII-LnIII complexes; Dalton Transactions, 28 , 2008 , p3661-3677.

Ripamonti E., M. Mapelli, S. Zaroubi: Radiation from early black holes - I. Effects on the neutral intergalactic medium; 2008, MNRAS, 387, 158.

Roedel E., A. Urakawa, S. Kureti, and A. Baiker; On the Local Sensitivity of Different IR Techniques: Ba Species Relevant in NO_x Storage-Reduction; Phys. Chem. Chem. Phys., 10, 6190 (2008).

Roesch A., E.B. Jaeger, D. Lüthi, and S.I. Seneviratne, 2008: The analysis of CLM model biases in relation to intra-ensemble model variability; Meteor. Z., 17 (4), 369-382. (CLM special issue).

Rossinelli D., Bayati B., Koumoutsakos P., Accelerated Stochastic and Hybrid Methods for Spatial Simulations of Reaction-Diffusion Systems, Chemical Physics Letters, 451, 1-3, 136-140, 2008.

Rossinelli D., Koumoutsakos P., Vortex Methods for incompressible Flow Simulations on the GPU, Visual Computer, 24, 7-9, 699-708, 2008.

Rousochatzakis I., A. Läuchli, and F. Mila; Highly Frustrated Magnetic Clusters: The kagomé on a sphere; Phys. Rev. B 77, 094420 (2008).

Roy S., S. Goedecker, and V. Hellmann; Bell-Evans-Polanyi principle for molecular dynamics trajectories and its implications for global optimization; Phys. Rev. E 77, 056707 (2008).

Sabo D., M. Meuwly, D. L. Freeman and J. D. Doll; A constant entropy increase model for the selection of parallel tempering ensembles; J. Chem. Phys., 128, 174109 (2008).

Sague J. L., M. Meuwly and K. M. Fromm; Counterion effect on the formation of coordination polymer networks between AgNO3 and L(2,2'-oxybis(ethane-2,1-diyl)diisonicotinate). Part 2" Cryst. Eng. Comm, 10, 1542 (2008).

Santarossa G., A. Vargas, M. Iannuzzi, et al.; Modeling bulk and surface Pt using the "Gaussian and plane wave" density functional theory formalism: Validation and comparison to k-point plane wave calculations; Journal of Chemical Physics, 129 (23), 234703 (2008).

Santarossa G., M. Iannuzzi, A. Vargas, and A. Baiker, Adsorption of Quinoline and Naphthalene on Pt, Pd and Rh: a DFT Study, Phys. Chem. Phys., 9, 401 (2008).

Scheidegger S., T. Fischer, S. C. Whitehouse, M. Liebendörfer; Gravitational waves from 3D MHD core collapse simulations; A&A 490: 231 [11 p.] (2008).

Schiemann R., D. Lüthi, P.L. Vidale, and C. Schär, 2008: The Precipitation Climate of Central Asia – Intercomparison of Observational and Numerical Data Sources in a Remote Semiarid Region; Int. J. Climatol., 28, 295–314.

Schiffmann F., J. Hutter, J. VandeVondele; Atomistic simulations of a solid/liquid interface: a combined force field and first principles approach to the structure and dynamics of acetonitrile near an anatase surface; J. Phys.-Condensed Matter 20 Art. No. 064206 (2008).

Schimmoeller B., H. Schulz, A. Ritter, A. Reitzmann, B. Kraushaar-Czarnetzki, A. Baiker, S. E. Pratsinis; Structure of Flame-Made V2O5/TiO2 and Catalytic Behavior in the Partial Oxidation of o-Xylene J. Catal., 256, 74 (2008).

Schmid F.-F. and M. Meuwly; Direct Comparison of Experimental and Calculated NMR-Scalar Coupling Constants for Force Field Validation and Adaptation; JCTC, 4, 1949 (2008).

Schmidt E., D. Ferri, A. Vargas, and A. Baiker, Chiral Modification of Rh and Pt Surfaces: Effect of Rotational Flexibility of Cinchona Type Modifiers on their Adsorption Behavior, J. Phys. Chem. C, 112, 3866 (2008).

Schmidt K.P., J. Dorier, A. Läuchli, and F. Mila; Supersolid phase induced by correlated hopping in spin-1/2 frustrated quantum magnets; Phys. Rev. Lett. 100, 090401 (2008).

Schmidt K.P., J. Dorier, and A. Läuchli; Solids and supersolids of three-body interacting polar molecules in an optical lattice; Phys. Rev. Lett. 101, 150405 (2008).

Schneider B., L. Bopp, M. Gehlen, J. Segschneider, T. L. Frölicher, P. Cadule, P. Friedlingstein, S. Doney, M. J. Behrenfels, and F. Joos; Climate-induced interannual variability of marine primary and export production in three global coupled climate carbon cycle models; Biogeosciences , 5, 597-614, 2008.

Seki T., J.D. Grunwaldt and A. Baiker, Palladium Supported on an Acidic Resin: A Unique Bifunctional Catalyst for the Continuous Catalytic Hydrogenation of Organic Compounds in Supercritical CO_2, Adv. Synth. Catal., 350, 691 (2008).

Seki T., J.D. Grunwaldt, and A. Baiker; Heterogeneous Catalytic Hydrogenation in Supercritical Fluids: Potential and Limitations; Ind. Eng. Chem. Res, 47, 4561 (2008).

Seneviratne S.I., and R. Stöckli, 2008: The role of land-atmosphere interactions for climate variability in Europe. In: Climate Variability and Extremes during the Past 100 years, Brönnimann et al. (eds.); Springer Verlag, (Book chapter).

Sheth K., ..., C.M. Carollo, et al; Evolution of the Bar Fraction in COSMOS: Quantifying the Assembly of the Hubble Sequence; ApJ, 675, 1141, 2008.

Solozhenko V, Kurakevych O, Oganov A; On the hardness of a new boron phase, orthorhombic gamma-B-28; JOURNAL OF SUPERHARD MATERIALS 30 (6), 428-429 2008.

Soulages J., T. Schweizer, D.C. Venerus, J. Hostettler, F. Mettler, M. Kröger, H.C. Öttinger; Lubricated optical rheometer for the study of two-dimensional complex flows of polymer melts; J. Non-Newtonian Fluid Mech. 150 (2008) 43-55.

Soulages J., T. Schweizer, D.C. Venerus, M. Kröger, H.C. Öttinger; Lubricated cross-slot flow of a low density polyethylene melt; J. Non-Newtonian Fluid Mech. 154 (2008) 52-64.

Spiegel K., A. Magistrato, P. Maurer, P. Ruggerone, U. Rothlisberger, P. Carloni, J. Reedijk and M.L. Klein; Parameterization of novel azole-bridged diplatinum anticancer drugs via a QM/MM force matching procedure; J. Comput. Chem., 29, 38-49 (2008).

Steinacher M., F. Joos, T. L. Frölicher, G.-K. Plattner, and S. C. Doney; Imminent ocean acidification projected with the NCAR global coupled carbon cycle-climate model; Biogeosciences Discuss., 5, 4353-4393, 2008.

Strassmann K. M.; F. Joos and G. Fischer; Simulating effects of land use changes on carbon fluxes: past contributions to atmospheric CO_2 increases and future commitments due to losses of terrestrial sink capacity; Tellus B, 60B, 583-603, 2008.

Tapavicza E., I. Tavernelli, U. Rothlisberger, C. Filippi and M.E. Casida; Mixed Time-Dependent Density-Functional/Classical Trajectory Study of Oxirane Photochemistry; Journal of Chemical Physics, 129, 124108 (2008).

Teuling A.J., and S.I. Seneviratne, 2008: Contrasting spectral changes limit albedo impact on land-atmosphere coupling during the 2003 European heat wave; Geophys. Res. Lett., 35, L03401, doi:10.1029/2007GL032778.

Torcasio A., G.H. van Lenthe and H. Van Oosterwyck (2008): The importance of loading frequency, rate and vibration for enhancing bone adaptation and implant osseointegration; European Cells and Materials 16: 56-68.

Tsai W.F., H. Yao, A. Läuchli, and S.A. Kivelson; The Optimal Inhomogeneity for Superconductivity: Finite Size Studies; Phys. Rev. B 77, 214502 (2008).

Tschumi T., F. Joos, and P. Parekh.How important are Southern Hemisphere wind changes for low glacial carbon dioxide? A model study; Paleoceanography , 23, PA4208 doi:10.1029/2008PA001592, 2008.

Turco A., D. Passerone and F. Cardin; Tonelli Principle: finite reduction and fixed energy molecular dynamics trajectories Multiscale modeling and simulation, 7, 1161 (2008).

Urakawa A., D. M. Meier, H. Rüegger, and A. Baiker; Conformational Behavior of Cinchonidine Revisited: A Combined Experimental and Theoretical Study; J. Phys. Chem. A, 112, 7250 (2008).

Urakawa A., F. Trachsel, P.R. von Rohr, and Alfons Baiker; On-Chip Raman Analysis of Heterogeneous Catalytic Reaction in Supercritical CO_2: Phase Behavior Monitoring and Activity Profiling, The Analyst, 133, 1352 (2008).

Urakawa A., N. Maeda, and A. Baiker; Space- and Time-Resolved Combined DRIFT and Raman Spectroscopy: Monitoring Dynamic Surface and Bulk Processes during NO_x Storage-Reduction; Angew. Chem., Int. Ed., 47, 9256 (2008).

Urakawa A., T. Bürgi, and A. Baiker; Sensitivity Enhancement and Dynamic Behavior Analysis by Modulation Excitation Spectroscopy: Principle and Application in Heterogeneous Catalysis; Chem. Eng. Sci., 63, 4902 (2008).

Van Lenthe G.H. and R. Müller (2008): CT-based visualization and quantification of bone microstructure in vivo; IBMS BoneKEy 5 (11): 410-425.

Van Lenthe G.H., R. Voide, S.K. Boyd and R. Müller (2008): Tissue modulus derived from beam theory is biased by bone size and geometry: implications for the use of three-point bending tests to determine bone tissue modulus; Bone 43: 717-723.

Van Lenthe G.H., T.L. Mueller, A.J. Wirth and R. Müller (2008): Quantification of bone structural parameters and mechanical competence at the distal radius; J. Orthop. Trauma 22 (8 Suppl.): S66-S72.

Van Mier J.G.M., D. Meyer and H.-K. Man; Fracture of Quasi-Brittle Materials like Concrete under Compressive Loading; Advanced Materials Research. 41-42:207-214. 2008.

Van Vuuren D. P., M. Meinshausen, G.-K. Plattner, F. Joos, K. M. Strassmann, S. J. Smith, T. M. L. Wigley, S. C. B. Raper, K. Riahi, F. de la Chesnaye, M. den Elzen, J. Fujino, K. Jiang, N. Nakicenovic, S. Paltsev, and J. M. Reilly; Temperature increase of 21st century mitigation scenarios; Proceedings of the National Academy of Sciences USA (PNAS), 105, 15258-15268, 2008.

Vargas A., G. Santarossa, M. Iannuzzi, and A. Baiker; Chiral Recognition on Catalytic Surfaces: Insight in a Biomimetic Heterogeneous Catalytic System; J. Phys. Chem. C, 112, 10200 (2008).

Vargas A., S. Reimannn, S. Diezi, T. Mallat, and A. Baiker; Adsorption Modes of Aromatic Ketones on Platinum and their Reactivity Towards Hydrogenation; J. Mol. Catal. A., 282, 1 (2008).

Voide R., G.H. van Lenthe and Müller R. (2008): Bone morphometry strongly predicts cortical bone stiffness and strength, but not toughness, in inbred mouse models of high and low bone mass; J Bone Miner Res 23 (8): 1194-1203.

Voide R., G.H. van Lenthe and Müller R. (2008): Differential effects of bone structural and material properties on bone competence in C57BL/6 and C3H/He inbred strains of mice; Calcified Tissue International 83: 61–69.

Voide R., G.H. van Lenthe and R. Müller (2008): Femoral stiffness and strength critically depend on loading angle: a parametric study in a mouse-inbred strain; Biomedizinische Technik/Biomedical engineering 53: 122-129.

Voide R., G.H. van Lenthe, M. Stauber, P. Schneider, P. Thurner, P. Wyss, M. Stampanoni and R. Müller (2008): Functional microimaging: a hierarchical investigation of bone failure behavior; Journal of the Japanese Society of Bone Morphometry 18: 9-21.

Volonteri M., S. Callegari, M. Colpi, M. Dotti, L. Mayer; Massive black holes and their hosts; 2008 MmSAI. 79.1231V.

Walder R., D. Folini, and S.N. Shore; 3D simulations of RS Oph: from accretion to nova blast. Astronomy and Astrophysics Letters, 484, L9--L12, 2008.

Walder R., D. Folini, S. N. Shore; 3D simulations of RS Ophiuchi: from accretion to nova blast; Astronomy & Astrophysics, 484, 2008.

Wanner H., J. Beer, J. Bütikofer, T. J. Crowley, U. Cubasch, J. Flückiger, H. Goosse, M. Grosjean, F. Joos, J O. Kaplan, M. Küttel, S. Müller,C. Prentice, O. Solomina, T. F. Stocker, P. Tarasov, M. Wagner, M. Widmann; Mid- to late Holocene climate change - an overview; Quaternary Science Reviews , 27, 1791-1828, 2008.

Weber V. and J. Hutter; A smooth [script-l]1-norm sparseness function for orbital based linear scaling total energy minimization; J. Chem. Phys. 128, 064107 (2008).

Weber V., J. VandeVondele, J. Hutter, and A. M. N. Niklasson; Direct energy functional minimization under orthogonality constraints; J. Chem. Phys. 128, 084113 (2008).

Webster D.J., P. Morley, G.H. van Lenthe and R. Müller (2008): A novel in vivo model for mechanically stimulated bone adaptation - a combined experimental and computational study; Comp. Meth. Biomech. and Biomed. Eng. 11 (5): 435-441.

Wesolowski T.A.; Embedding a multi-determinantal wavefunction in orbital-free environment; Phys. Rev.A. 77 (2008) 012504.

Whitehouse S.C., M. Liebendörfer; A new approach to neutrino transport in 3D simulations of core collapse supernovae; submitted to Proceedings of Science (2008).

Wild M., Grieser, J. and Schär, C., 2008, Combined surface solar brightening and increasing greenhouse effect favor recent intensification of the hydrological cycle; Geophys. Res. Letters, 35, Art. No. L17706.

Wirth A. J., C. Flaig, Th. L. Mueller, R. Müller, P. Arbenz, G. H. van Lenthe "Fast Smooth-Surface Micro-Finite Element Analysis of Large-Scale Bone Models". Journal of Biomechanics 41, p. S100, July 2008, doi:10.1016/S0021-9290(08)70100-3.

Wirz R., D. Ferri, and A. Baiker; Enantioselective Interactions at the Solid-Liquid Interface of an HPLC Column under Working Conditions, Anal. Chem., 80, 3572 (2008).

Wodrich M.D., A. Vargas, P.-Y. Morgantini, G. Merino and C. Corminboeuf; What governs nitrogen configuration in substituted aminophosphines?; Journal of Physical Organic Chemistry, 22 (2) , 2008 , p101-109.

Xiao W., D. Passerone, P. Ruffieux, K. Aït-Mansour, O. Gröning, E. Tosatti, J. S. Siegel, and R. Fasel, C60/Corannulene on Cu(110): A surface-supported bistable buckybowl-buckyball host-guest system; Journal of the American Chemical Society, 130, 4767 (2008).

Yazyev O. V. and A. Pasquarello; Carbon diffusion in CVD growth of carbon nanotubes on metal nanoparticles; Physica Status Solidi (b) 245, 2185 (2008).

Yazyev O. V. and A. Pasquarello; Effect of metal elements in catalytic growth of carbon nanotubes; Physical Review Letters 100, 156102 (2008).

Yu M., Isaev, K. Y. Watanabe, M. Yokoyama, N. Ohyabu, C. D. Beidler, H. Maassberg, W. A. Cooper, T. M. Tran and M. I. Mikhailov; LHD Bootstrap Current Coefficient Calculations with the VENUS+ δf code; Plasma and Fusion Research 3 (2008) 036-1-7.

Yu X., J. Pfaendtner, and L. J. Broadbelt, "Ab Initio Study of Acrylate Polymerization Reactions: Methyl Methacrylate and Methyl Acrylate Propagation"; J. Phys. Chem. A, 2008, 112 (29), 6772-6782.

Zappa, A., M.W. Rotach, A. Arpagaus, M. Dorninger, C. Hegg, A. Montani, R. Ranzi, F. Ament, U. Germann, G. Grossi, S. Jaun, A. Rossa, S. Vogt, A. Walser, C. Wunram, 2008: MAP D-PHASE: Real-time demonstration of hydrological ensemble prediction systems. Atmos. Sci. Letters, 9 (2), 80-87.

Zemp M., B. Moore, J. Stadel, M.C. Carollo, P. Madau; Multimass Spherical Structure Models for N-body Simulations; MNRAS, 386, 1543, 2008.

Zhang Z.Y.; L.Y. Lu; W.G. Noid, et al.; A Systematic Methodology for Defining Coarse-Grained Sites in Large Biomolecules; Biophysical Journal 95 (11), 5073-5083, 2008.

Zhuang W., E. Kasemi, Y. Ding, M. Kröger, A.D. Schlüter, J.P. Rabe; Self-folding of charged single dendronized polymers; Adv. Mater. 20 (2008) 3204-3210.

Ziefle J. and L. Kleiser; Assessment of a film-cooling flow structure by large-eddy simulation; J. Turbulence, 9(N 29), 2008.

Ziefle J., S. Stolz, and L. Kleiser; Large-eddy simulation of separated flow in a channel with streamwise-periodic constrictions; AIAA J., 46(7):1705-1718, 2008.

Zimmerli U., Koumoutsakos P., Simulations of Electrophoretic RNA Transport through Transmembrane Carbon Nanotubes, Biophysical J. , 94, 7, 2546-2557, 2008.

Zoppi L., A. Calzolari. A. Ruini, M. J. Caldas; Defect induced effects on carrier migration through one-dimensional poly(paraphenylenevinylene) chains; Phys. Rev B 78, 165204 (2008).

Zykova-Timan T., P. Raiteri, M. Parrinello; Investigating the polymorphism in PR179: a combined crystal structure prediction and metadynamics study; J. Phys. Chem. B 2008, 112, 13231-13237.

Paper published by collaborators CSCS

Abdennadher N, Engel P, Feichtinger D, Flanders D, Flury P, Jermini P, Maffioletti S, Pautasso C, Stockinger H, Sudholt W, Thiemard M, Williams N, and Witzig C; Initialising a National Grid Infrastructure - Lessons Learned from the Swiss National Grid Association Seed Project; CCGrid2008.

Balle T and Stringfellow N; "Implementing the Operational Weather Forecast Model of MeteoSwiss on a Cray XT3"; CUG 2007, Seattle, USA.

Biddiscombe J, Geveci B, Martin K, Moreland K and Thompson D; "Time Dependent Processing in a Parallel Pipeline Architecture," IEEE Transactions on Visualisation and Computer Graphics, vol. 13, no. 6, pp. 1376-1383, Nov/Dec, 2007.

Biddiscombe J, Graham D, Maruzewski P, "Interactive Visualisation And Exploration Of SPH Data" 2nd International SPHERIC SPH Workshop, Madrid, May 2007.

Biddiscombe J, Geveci B, Martin K, "A Pipeline Architecture for Parallel Processing of Time-Dependent Data within a VTK Framework", Short Paper, Eurographics Symposium on Parallel Graphics and Visualisation 2007.

Cheesman M and Stringfellow N; "Cray XT3 I/O Performance on Real Applications"; CUG 2007, Seattle, USA.

Favre J M, dos Santos L P, Reiners D; Eurographics Symposium on Parallel Graphics and Visualisation; Editors, May 2007.

Folini D, Walder R, LeVeque R J, and Favre J M; Supersonic turbulence as an agent of structure formation in space; Proceedings of ICIAM07 in Applied Mathematics and Mechanics, 27 November 2007.

Kunszt P; Grid Middleware Development in Large International Projects – Experience and Recommendations; Conference Proceedings of the IEEE Second International Conference on Software Engineering Advances, Aug.25-31 2007, Cap Esterel, France.

Montagnat J, Frohner A, Jouvenot D, Pera C, Kunszt P, Koblitz B, Santos N, Loomis C, Texier R, Lingrand D, Guio P, Brito Da Rocha D, Sobreira de Almeida A, and Farkas Z; A Secure Grid Medical Data Manager Interfaced to the gLite Middleware; Journal of Grid Computing, Springer Verlag, Jan. 2008.

Oganov A R, Yanming Ma, Colin W. Glass, Mario Valle, "Evolutionary crystal structure prediction: overview of the USPEX method and some of its applications", The k network, newsletter 84, December 2007.

Perrig A, Valle M, Farhat M, Parkinson E, Favre J M, and Avellan F; Onboard flow visualisation in a Pelton turbine bucket; in Proceedings of the 23rd IAHR Symposium on Hydraulic Machinery and Systems, (Yokohama, Japan), Oct. 17-21 2006.

Quandt A, Hernandez P, Kunszt P, Lisacek F, Maffioletti S, Pautasso C, and Heinz Stockinger; High-throughput Data Analysis of Proteomic Mass Spectra on the SwissBioGrid; to appear in the Handbook of Resesarch on Computational Grid Technologies for Life Sciences, Biomedicine and Healthcare, editor Mario Catannaro, Dec. 2007.

Sawley M, Biddiscombe J, Favre J, “Advanced Visualisation Of Large Datasets For Discrete Element Method Simulations” Discrete Element Methods (DEM) 07, Brisbane, Australia August 27-29, 2007.

Stringfellow N; ”Prioritization and Scheduling on a Cluster of XT3 Systems”; CUG 2007, Seattle, USA.

Ulmer D. & Stringfellow N. (2007): ALPS – the Swiss Grand Challenge Programme on the Cray XT3.- Proceedings of CUG07, Seattle, May 7.-10, 2007.

Valle M; Visualisation support to chemistry research, in Proceeding of IEEE Visualisation 2006, (Baltimore, USA), Oct. 29 - Nov. 3 2006. (Selected as one of the 5 Best Poster Candidates of IEEE Visualisation 2006).

Valle M; Representations that promote cognition: the case of chemistry visualisation tools; in Proceeding of SIGGRAPH 2006, (Boston, USA), July 30 - Aug. 3 2006. (poster).

Valle M: Representations that promote cognition: the case of chemistry visualisation tools; in Proceeding of the third symposium on Applied Perception in Graphics and Visualisation, (Boston, USA), July 28-30 2006. (poster).

Invited talks and seminars

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

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

Valle M; ”From Tradition to Insight Support - What we can demand from our Chemistry Visualisation Tools”, April 2007,University of Manchester, UK.

Members of Advisory Board

Anwar Osseyran, SARA Computing and Networking Services, NL, Chairman of the Board
Guy Brasseur, National Centre for Atmospheric Research (NCAR), USA
Mehdi Jazayeri, Università della Svizzera Italiana (USI), CH
Klaus Schulten, University of Illinois, Urbana-Campaign, USA
Hors Simon, Lawrence Berkeley National Laboratory, USA

Impressum

CSCS Swiss National Supercomputing Centre
Via Cantonale
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:
OK Haller Druck, Zürich

Print-run:
650

Meeting of Advisory Board (SB) in 2008
June 17th, Dresden, Germany

Annu

An

A

Ann

Annual R

Annual Rep

Annua

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

Annual Report

Annual Report