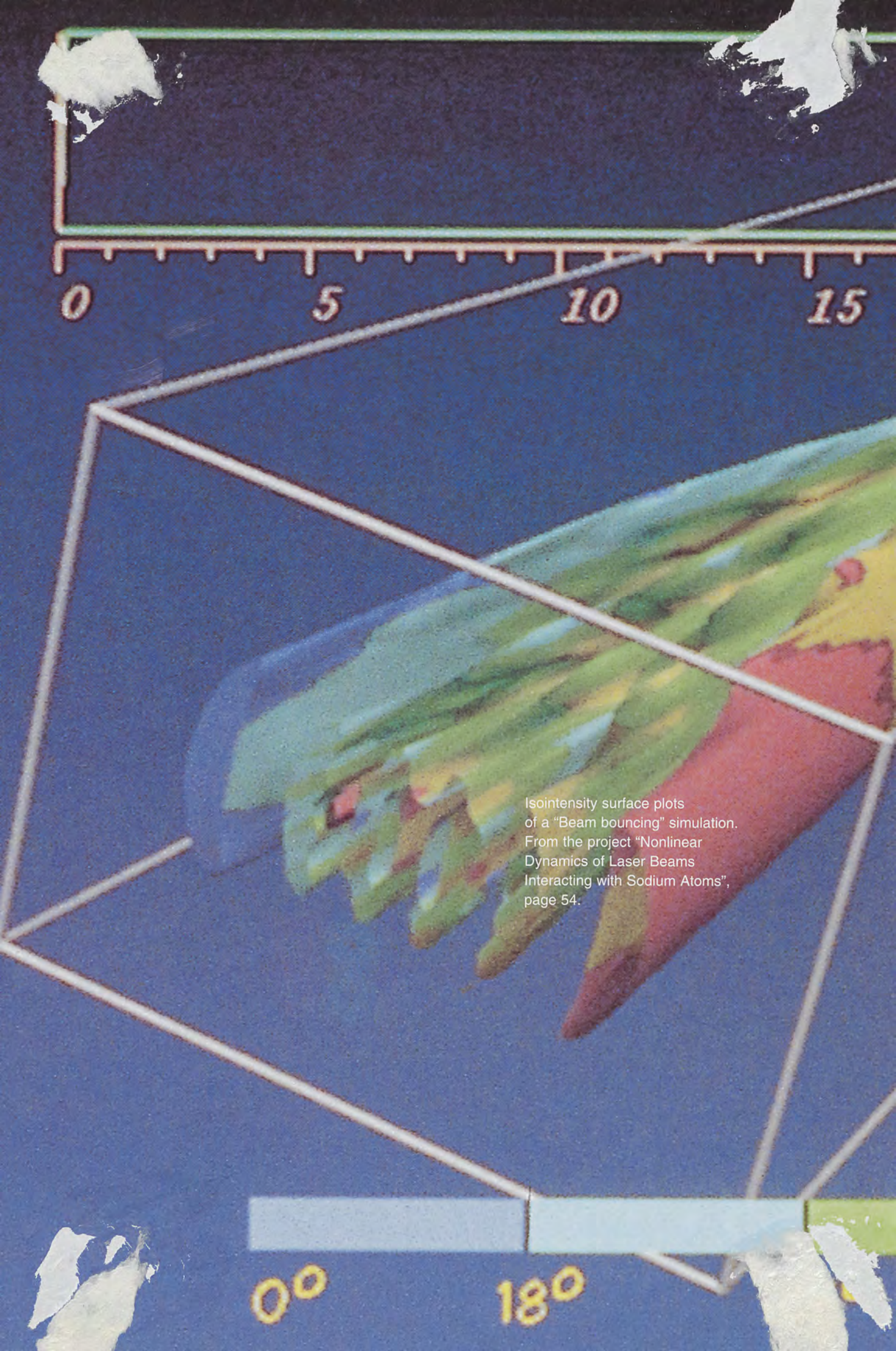
Centro Svizzero di
Calcolo Scientifico

Swiss Center for
Scientific Computing

ETH Eidgenössische Technische Hochschule Zürich
Ecole polytechnique fédérale de Zurich
Politecnico federale di Zurigo
Swiss Federal Institute of Technology Zurich

PROJECT DIRECTORY 1995



Isointensity surface plots of a “Beam bouncing” simulation. From the project “Nonlinear Dynamics of Laser Beams Interacting with Sodium Atoms”, page 54.

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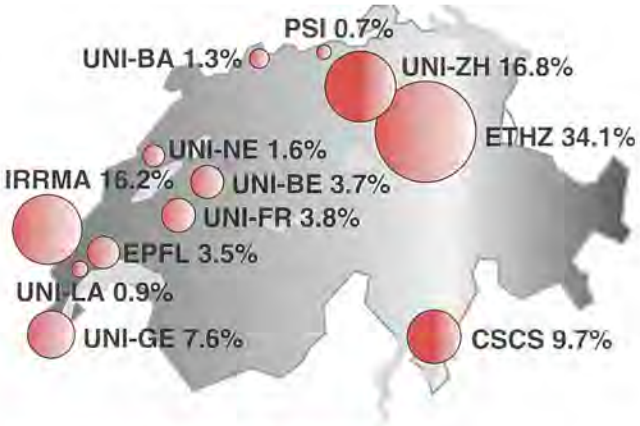
In 1995 an efficient problem and solution tracking system was enabled by the CSCS User Support group and help desk. It serves as the central point of contact for users, providing additional information and documentation as well as improved assistance in porting and optimizing codes for the computer facilities. The User Support group evaluates user and project needs against the center's available resources, targeting the platforms and applications which best suit the circumstance.

The continuous improvement of graphics hardware and software for workstations has brought increased quality to visualization of scientific data.

The user community furthermore profits from a recently installed assortment of standard application packages in computational chemistry and other project-specific software applications. Extended user support capability, in the form of the PRSS (Project-Related Student Stages) mobility program, was also carried out for the first time (see "CSCS's Educational activities in 1995", next page).

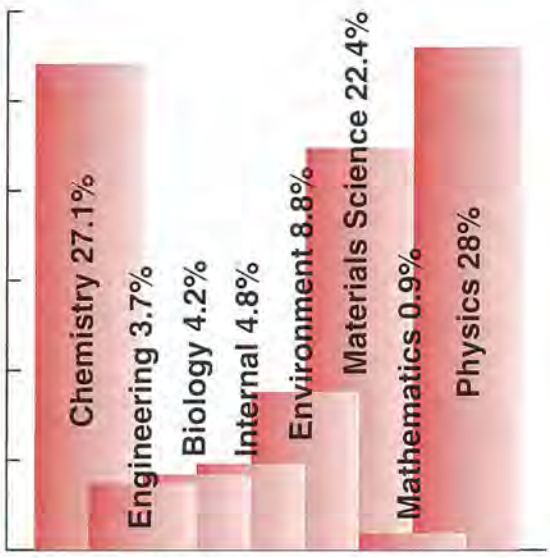
The CSCS Local Coordinators, a first line of user support present in universities and organizations where a large user community exists, met in Manno in the spring to familiarize themselves with the user support procedures, and to offer input on further improvements.

Various communication platforms, including WWW pages, the *CROSSCUTS* newsletter and electronic mailings, were employed to maintain information flow between the center and the user community.

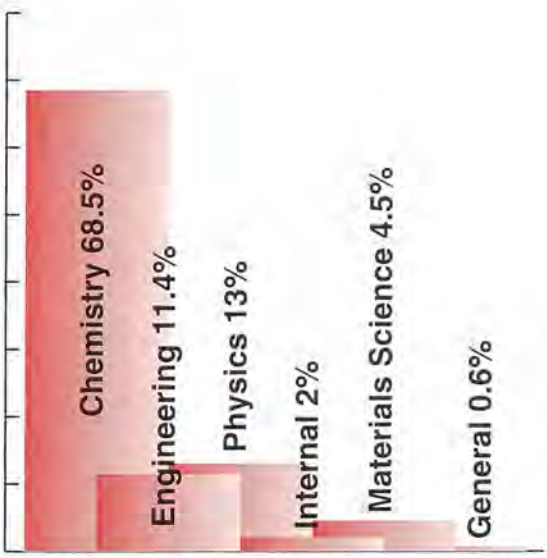


NEC SX-3, CPU usage by organization

As can be seen in the graphs, utilization of CSCS resources continues to follow a trend with regards to distribution of CPU time between universities and the two Federal Institutes of Technology (ETHZ and EPFL). The latter, as was the case in 1994, were responsible for 40% of the total CPU utilization for 1995. While the disciplines of physics, chemistry, material and environmental sciences constitute the core of computational work performed on the NEC SX-3, on the HP Cluster the dominant field was chemistry, accountable for 68.5% of the total utilization for that system.



NEC SX-3, 1995 CPU usage by application field



HP Workstation Cluster, 1995 CPU usage by field

CSCS's educational and local outreach activities in 1995 ranged from highly-specialised training to general computer education sessions. Teaching and training activities aim at CSCS staff, external users of the CSCS environment in Swiss academia, staff of industrial and commercial companies and school students.

With the PRSS (Project-Related Student Stages) mobility program, started in August 1995, CSCS set up an initiative which offered young researchers and students from Swiss Academia the opportunity to move to Manno and work/live close to the center for up to three months. It gave them a chance to experience a first-hand working environment at the center, profiting from direct access to specialists responsible for the center's file and archiving environment, the Convex Exemplar parallel and SX-3 vector programming environments and the visualisation laboratory, while carrying on their specific projects. In addition, special application field-related courses were offered that were based on the scientific profile of the different topics. As a result, participants returned to their home university with a programming, computing and visualisation environment customised at CSCS in order to best fit their particular needs.

CSCS did also benefit from this initiative, through the national exposure and by embedding itself in the country's scientific environment. In this respect, the PRSS program forms part of the active policy to improve the information flow and synergies between the center and the Swiss universities and technical institutes. The initiative was positively received, and several professors applied for the participation of one of their PhD students. Discussions between organisers, students and consultants brought helpful input in determining the schedule and tenor of the presentations and lectures held in the framework of the program. The topics of the participants' projects covered many different domains ranging from solid state physics to physical chemistry. The participants wrote a final report about their experience, published later in CSCS's newsletter *CROSSCUTS* 5(1).

Moments from PRSS '95 and SSIP '95

The "Summer Student Internship Program" (SSIP), CSCS's summer course for undergraduate and graduate students, carried out for the third time in 1995, focuses on Switzerland's integration in an international network of research and education. The internship program exposing university students to the field of parallel computing, came to a close in October. In a two-week introductory course the students were taught basic skills in programming distributed memory parallel processors. In the following eleven weeks, each student worked on and completed a small research project. The topics involved aspects of parallel computing and well known programming problems of distributed memory parallel processing, i.e., the development of programming tools, new algorithms and applications for such machines. Each participant gave an intermediate talk, held a final presentation on the last day of the course and provided a report documenting his/her project, along with the completed software itself.

SHPCS "Swiss High Performance Computing Seminars" have been organised and carried out at CSCS on a regular basis.

The initiatives undertaken in the framework of the Canton of Ticino "Progetto Scuola" are a result of common efforts with the Canton. Its goals are to develop material on applied computing for different school levels and offer hands-on experience on high performance computers. One of the programs, the Computing and Communications Camp C^3, extended nationally. C^3, which was organised in collaboration with the group "Ingenieure für die Schweiz von morgen", offered in 1995 for the first time camps/courses in applied computing and computer communication to talented scholars who already had basic knowledge of computers. The participants took a practical approach to computer applications and were able to carry out simulations, gaining at the same time access to the world of science and technology. Students from all over Switzerland participated in one camp for Canton Ticino and two camps for the German speaking part of Switzerland. The students handed in a project proposal in which they described what investigations they would like to do and their proposals were reviewed by a jury.

Furthermore, courses were held by CSCS staff members at Scuola Tecnica Superiore in Manno in vectorial and parallel programming. They covered various aspects like scientific applications, hardware architecture, introduction to Fortran, compilers and optimisation.

LARGE USER PROJECTS

CSCS's "Large User Projects" are projects requiring more than 10 CPU hours per month on one NEC SX-3/24R processor.

This section summarizes Large User Projects conducted at CSCS in 1995, covering a variety of scientific domains such as biology, chemistry, engineering, geography, materials science, physical chemistry and physics.

In addition to the twenty-eight projects presented (twenty-three abstracts and five reports), five prominent CSCS users share their views on High-performance Computing and on CSCS: Prof. Jacques Weber (University of Geneva), Prof. Themistocles Dracos (ETHZ), Dr. Anthony Cooper (EPFL), Stefan Dangel (University of Zurich) and Prof. Leonhard Kleiser (ETHZ).

Institutes can be cross-referenced to the address list found later in this document.

Structure and Dynamics of Proteins in Solution

RESPONSIBLE INSTITUTE:
Institut für Molekularbiologie und Biophysik, ETHZ

PROJECT LEADER:
Dr. M. Billeter–Institut für Molekularbiologie und Biophysik, ETHZ

Our project on the NEC SX-3 is focused on the study of the dynamic properties of macromolecules. For this purpose we have written the program OPAL for simulations of the evolution with time of large molecular systems; the results are then directly compared to experimental data obtained in our laboratory from NMR spectroscopy. OPAL features a user-friendly interface, high efficiency (over 1.5 GFLOPS on the NEC SX-3) and flexibility.

The most CPU-intensive project of 1995 was the simulation of the dynamic behavior of the solvated complex formed by the homeodomain from the *Antennapedia* protein with a target DNA. This protein-DNA-water system (with about 10'000 atoms) was followed for 2 nanoseconds (in time steps of 2.5 femtoseconds). The analysis of the resulting molecular dynamics (MD) trajectory shows fluctuations of the protein-DNA interactions in the range of about 100 picoseconds. The penetration of water molecules into the intermolecular interface occurs at somewhat slower rates. These data help to explain the mechanisms with which the protein recognizes the DNA in a specific manner and the pathways taken by water molecules to penetrate the protein-DNA complex [2].

OPAL was also used for MD simulations of the protein *hirudin*, a potent inhibitor of blood coagulation obtained from leeches, in order to characterize transient hydrogen bonds that were identified previously by two-dimensional 1H-NMR experiments and site-directed mutagenesis [4]. Opening and closing of hydrogen bonds was observed in the 100 ps time range. Further experiments and MD simulations are planned on a cyclic analogue of a loop in *hirudin* that shows a network of three time-shared hydrogen bonds.

MD calculations using time-averaged instead of instantaneous distance restraints were used to characterize a disordered helical region in the (Cys39->Ser, Trp56->Ser)-mutant *Antennapedia* homeodomain protein for which the NMR measurements cannot be explained by a static structure [1].

In addition to the studies of protein dynamics, the NEC SX-3 and OPAL were used in a routine fashion for refinements of protein structures calculated from NMR data with distance geometry techniques. These include the N-terminal region of the molecular chaperone *DnaJ* [5, 6], a killer toxin from yeast, the pheromone *Er-11* and the pathogenesis-related plant protein *P14A* [3].

References:

[1] Bartels, C., D. Resendez-Perez, P. Güntert, D. Braun, W. J. Gehring and K. Wüthrich. 1996. Nuclear magnetic resonance solution structure of the Antp(C39S,W56S) Homeodomain. *J. Mol. Biol.*, submitted.

[2] Billeter, M., P. Luginbühl, P. Güntert and K. Wüthrich. Homeodomain-type DNA recognition. Lecture, *21st. EMBO Symposium*, Heidelberg, Germany (1995).

[3] Fernández, C., T. Szyperski, T. Bruyère, E. Mösinger and K. Wüthrich. The NMR solution structure of the pathogenesis related protein P14A. Lecture, *21st EMBO Symposium*, Heidelberg, Germany (1995).

[4] Güntert, P., T. Szyperski and K. Wüthrich. Transient hydrogen bonds on the surface of hirudin. Presented at the *First European Symposium of the Protein Society*, Davos, Switzerland (1995).

[5] Pellecchia, M., T. Szyperski and K. Wüthrich. NMR solution structure of the N-terminal region (2-108) of the Escherichia coli molecular chaperone DnaJ. Presented at the *First European Symposium of the Protein Society*, Davos, Switzerland (1995).

[6] Szyperski, T., M. Pellecchia, D. Wall. C. Georgopoulos and K. Wüthrich. 1994. NMR structure determination of the Escherichia coli DnaJ molecular chaperone: Secondary structure and backbone fold of the N-terminal region (residues 2-108) containing the Highly Conserved J Domain. *Proc. Natl. Acad. Sci.* U. S. A., 91: 11343–11347.

Structure and Rearrangements of Organic Ion-Molecule Complexes

RESPONSIBLE INSTITUTE:
Institut de Chimie Physique, Université de Fribourg

PROJECT LEADER:
Prof. T. Bally–Institut de Chimie Physique, Université de Fribourg

When a charged molecule encounters a neutral molecule, attractive Coulombic (ion-induced dipole) and dispersive interactions develop between the two species. At large distances these (classically treatable) interactions dominate. However, as the two species move closer to form a so-called **ion-molecule complex (IMC)**, covalent interactions come into play which require a *quantum chemical description* of some kind.

The title project focusses on IMC's where these latter interactions are predominant, such as in π-complex cations between olefins or aromatic compounds and in σ-bonded complexes formed between molecules carrying lone pairs, where the frontier molecular orbitals of the two constituent species are close in energy and can develop sufficient spatial overlap.

In particular, model calculations on the reactions of ethylene (Et) and acetylene (Ac) with their corresponding radical cations ($Et^{+\bullet}$ and $Ac^{+\bullet}$, respectively) have revealed the importance of so called "long-bond" complexes which rearrange subsequently to more tightly bound species $Et_2^{+\bullet}$, $Ac_2^{+\bullet}$, or $Et\text{-}Ac^{+\bullet}$. Our calculations, which were partially carried out at the CSCS, have also provided an answer to the question why IMC's (and rearrangement products originating from those) can be observed upon ionization of neutral dimers of Et but *not* of Ac.

Our work relates to experiments carried out in crossed effusive beams of ions and neutral molecules or in supersonic beams containing pre-formed clusters as well as to condensed phase work on ion-molecule reacations which are important in several realms of science.

Computational Coordination Chemistry

RESPONSIBLE INSTITUTE:
Institut de Chimie inorganique et analytique, Université de Fribourg

PROJECT LEADER:
Dr. C. Daul–Institut de Chimie inorganique et analytique, Université de Fribourg

INVOLVED PERSONS:
Computational Chemistry Group–Institut de Chimie inorganique et analytique, Université de Fribourg

Basically chemistry is concerned with the structure, spectroscopy and reactivity of molecules and this project will consider the contributions that theoretical methods related to experimental studies can offer to our understanding of these aspects. Starting from first principles or from empirical models, we are able to determine the energy and electronic structure of metal complexes in different electronic states with good accuracy (typically: 120kJ). Hence we can predict their spectra, electric and magnetic properties, and reaction energies. At the same time the study of potential energy surfaces and nuclear motion provides information of dynamic nature of reactivity and reaction probabilities. The knowledge of the structure and reactivity of an isolated molecule is often only the first step in the development of a quantitative theory whose results can be compared to experimental data. Experimental chemistry, whether in gas phase, in solution or in solids, involves large numbers of molecules and we need to use the methods of statistical mechanics to relate the results of a quantum-mechanical treatment of a single molecule to experimental data. Comparison of these predictions with experimental results is essential for 2 reasons: (i) to improve and refine the theoretical models; (ii) it does provide information to design new experiments.

Calculation of Molecular Properties in Liquids and Bulk Properties of Liquids

RESPONSIBLE INSTITUTE:
Institut für Physikalische Chemie, Universität Basel

PROJECT LEADER:
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J. Solca–Institut für Physikalische Chemie, Universität Basel

Within this project, for the first time the structure of a liquid was calculated with experimental accuracy from pure theory (see Figure 1). Most simulations of liquids are performed in the framework of classical mechanics and the approximation of additivity of pair potentials. Besides errors due to the approximate pair potential, this leads to errors due to quantum effects and the neglect of many-body interactions. By calculating the radial distribution function from pure theory for liquid neon and argon with a quantum effective Wigner-Kirkwood potential and comparison with experiments, it was shown that quantum effects are sizable for liquid neon at lower temperatures, whereas many-body effects are negligible.

References:

[1] J. L. Yarnell, M. J. Katz, R. G. Wenzel and S. H. Koenig. 1973. *Phys. Rev.* A 7: 2130.
[2] D. E. Woon. 1993. *Chem. Phys. Letters* 204: 29.
[3] A. K. Soper. 1986. *Chem. Phys.* 107: 61.

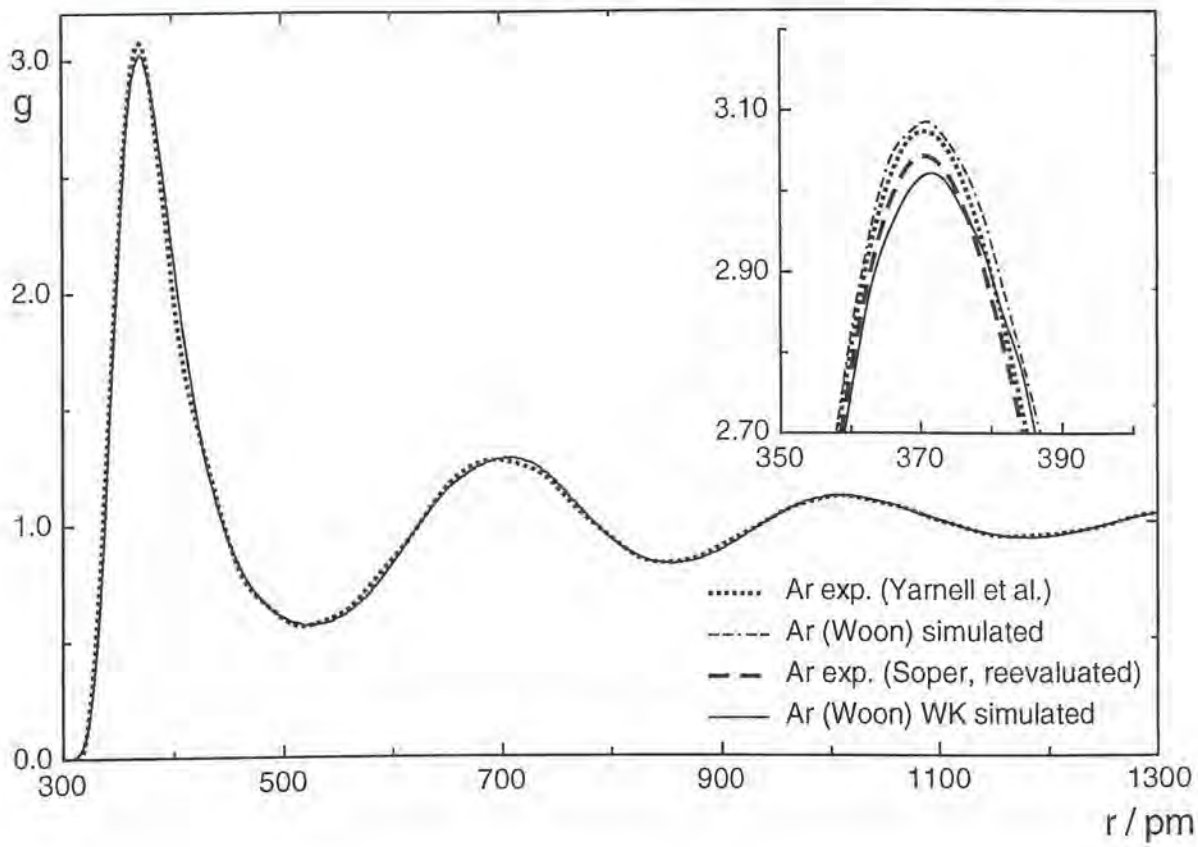

Figure 1: Radial distribution function of liquid argon at 85 K. The inset is a blow-up of the peak maximum. The experimental curve is from Yarnell et al. [1] and shows a nearly perfect agreement with the classical simulation with an *ab initio* potential by Woon [2], whereas the curve obtained with the Wigner-Kirkwood quantum effective potential shows a smaller amplitude, but is in excellent agreement with the reevaluated experiment by Soper [3]. The curves are cubic spline functions fitted through the experimental and calculated points, respectively.

An *Ab Initio* Derived Four-Dimensional Stretching/Torsional Potential Energy Surface for $(H_2O)_3$

RESPONSIBLE INSTITUTE:
Institut für anorganische, analytische und physikalische Chemie, Universität Bern

PROJECT LEADER:
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S. Graf–Institut für anorganische, analytische und physikalische Chemie, Universität Bern
Dr. W. Klopper–IPS-ETHZ

An intermolecular potential energy surface was derived for the cyclic homodromic hydrogen-bonded water trimer as a function of four intermolecular coordinates: these are the three torsional ω_1, ω_2, ω_3 coordinates [1-4], and the intermolecular symmetric stretching coordinate R(O•••O) [4] using equal O•••O distances, with fixed and equal intramolecular geometry of each H_2O molecule. The surface is partly based on previous MP2-R12 *ab initio* calculations [1, 2], which involve very large basis sets and the most extensive treatment of correlation energy for calculations of $(H_2O)_3$ so far.

In going beyond the 75 *ab initio* interaction energies previously computed as a function of the $\{\omega_1, \omega_2, \omega_3\}$ coordinates for a *fixed* O•••O distance of 2.80 Å [1, 2], we have now calculated 100 further points at the same $\{\omega_1, \omega_2, \omega_3\}$ coordinates, but over a range R(O•••O)= 2.65 - 2.95 Å. These 175 points, multiplied by six due to the S_6 symmetry of the surface, are now being fitted using a modified EPEN-2 [3] water - water intermolecular potential energy function (PES), denoted *modEPEN* [1, 2, 6].

Figure 1 shows four cuts through the PES as a function of the R(O•••O) coordinate, at four torsional stationary points. Figure 2 (following page) shows an isopotential rendering of the *modEPEN* potential at -530 cm^{-1}, as a function of two torsional $\{\omega_1, \omega_3\}$ coordinates and the *R* stretching coordinate. Note the two—out of a total of six—(*upd*) torsional transition structure "bottleneck" regions.

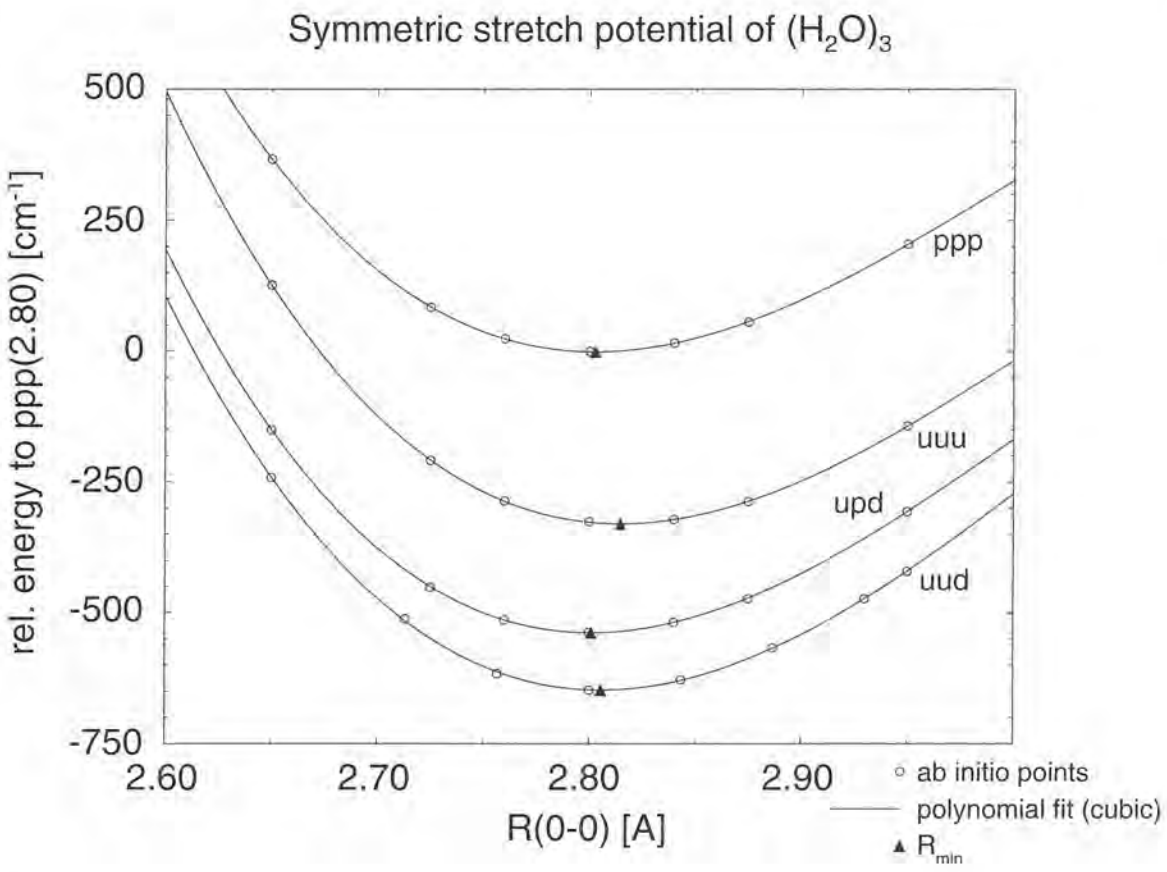


Figure 1.

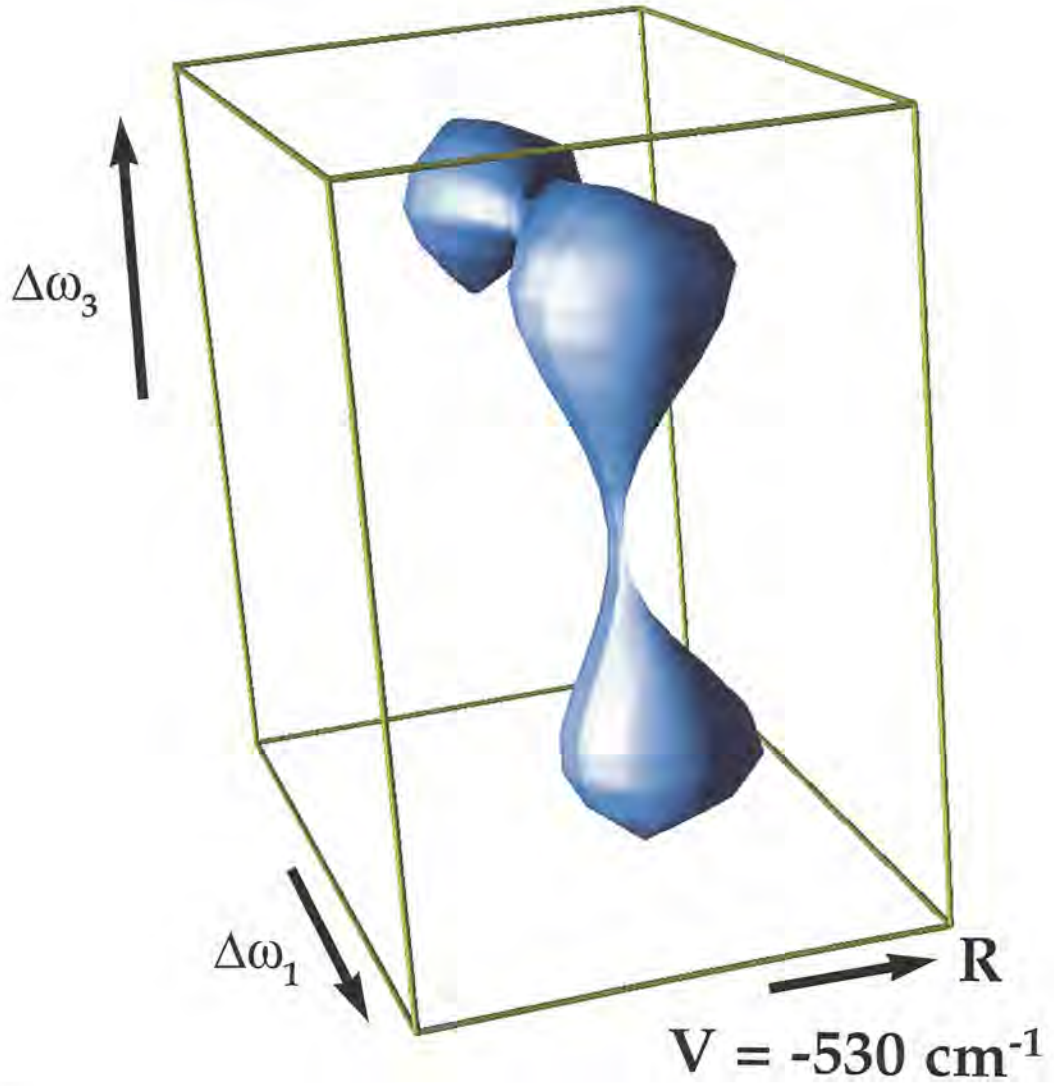


Figure 2.

The *modEPEN* potential provides a rapidly computable analytical expression for use in quantum mechanical calculations of intermolecular vibrational eigenfunctions, eigenvalues and other properties of $(H_2O)_3$ [4–6]. Torsional eigenfunctions were previously calculated in model calculations, using one-dimensional [4], and two-dimensional [5] subspaces of the ω_1, ω_2, ω_3 coordinates.
Very recently, we have performed a fully three-dimensional torsional calculation [6] using the *modEPEN* potential. The low-lying torsional wavefunctions are easily classifiable according to their nodal properties and the symmetries in S_6 [4, 6]. The eigenfrequencies and transition moments [4–6] are extremely useful for predicting and analyzing the far-infrared torsional vibrational spectrum of the water trimer [7].

References:

[1] Bürgi T., S. Graf, S. Leutwyler, and W. Klopper. 1995. *J. Chem. Phys.* 103: 1077.
[2] Klopper W., M. Schütz, H. P. Lüthi, and S. Leutwyler. 1995. *J. Chem. Phys.* 103: 1085.
[3] Owicki J. C., L. L. Shipman, and H. A. Scheraga. 1975. *J. Phys. Chem.* 79: 1794.
[4] Schütz M., T. Bürgi, S. Leutwyler, and H. B. Bürgi. 1993. *J. Chem. Phys.* 99: 5228.
[5] Klopper W. and M. Schütz. 1995. *Chem. Phys. Letters* 237: 536.
[6] Sabo D., Z. Bacic, T. Bürgi, and S. Leutwyler. 1995. *Chem. Phys. Letters* 244: 283.
[7] Pugliano N. and R. Saykally. 1992. Science 257: 1937; Liu K., J. Loeser, M. J. Elrod, J. A. Rzepiela, N. Pugliano and R. Saykally. 1994. *J. Am. Chem. Soc.* 116: 3507.

Spectroscopy and Dynamics of Molecules and Clusters

RESPONSIBLE INSTITUTE:
Laboratorium für Physikalische Chemie, ETHZ

PROJECT LEADER:
Prof. M. Quack–Laboratorium für Physikalische Chemie, ETHZ

INVOLVED PERSONS:
PD Dr. M. Suhm–Laboratorium für Physikalische Chemie, ETHZ

The motion of hydrogen atoms in molecules and even more so in hydrogen-bonded clusters is highly anharmonic, strongly coupled and significantly non-classical. Thus, its accurate description requires global quantum methods. While state of the art basis set methods are limited to tri- and tetratomic molecules, quantum Monte Carlo methods can be applied to selected excitations of much larger systems. Their algorithmic simplicity makes them appropriate for benchmark calculations and for high-speed vector computers. In combination with our spectroscopic studies and potential energy surfaces of HF clusters, we have calculated rovibrational excitations in $(HF)_2$ [1, 2] and $(HF)_{3\text{-}5}$ [3] as well as ground state properties up to $(HF)_8$ [4]. For $(HF)_3$, the anharmonic hydrogen bond vibrations are predicted near 150, 160, 375, 450, 560, and about 750 cm^{-1}. These predictions should facilitate future experimental gas phase assignment. We have also studied the fully anharmonic dynamics in 9 dimensions for the CH_4 molecule in view of fundamental questions [5, 6].

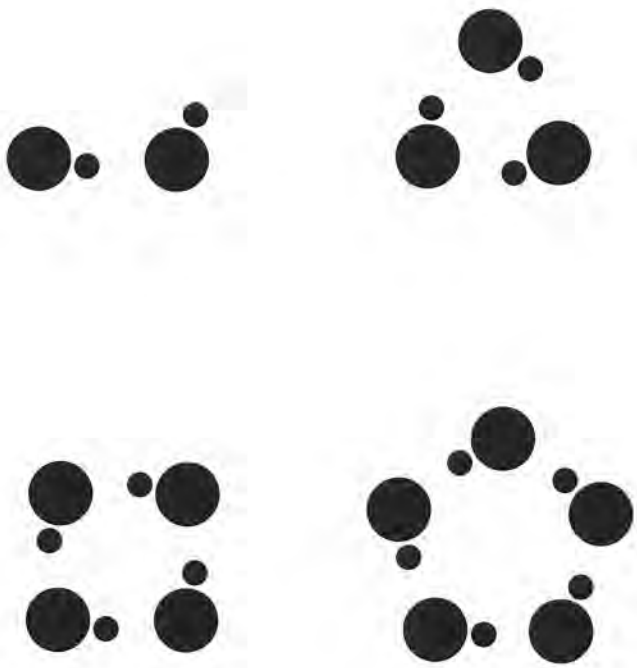


Figure 1: Illustration of $(HF)_n$ cluster structures. The large circles represent F atoms, the small ones H atoms.

References:

[1] Quack, M. and M. A. Suhm. 1995. *Chem. Phys. Lett.* 234: 71–76.
[2] Quack, M. and M. A. Suhm. 1996. *Theor. Chim. Acta* 93, 61–65.
[3] Luckhaus, D., M. Quack, U. Schmitt and M. A. Suhm. 1995. *Ber. Bunsenges. Phys. Chem.* 99: 457–468.
[4] Suhm, M. A. 1995. *Ber. Bunsenges. Phys. Chem.* 99: 1159–1167.
[5] Hollenstein, H., R. R. Marquardt, M. Quack and M. A. Suhm. 1994. *J. Chem. Phys.* 101: 3588–3602.
[6] Hollenstein, H., R. R. Marquardt, M. Quack and M. A. Suhm. 1995. *Ber. Bunsenges. Phys. Chem.* 99: 275–281.

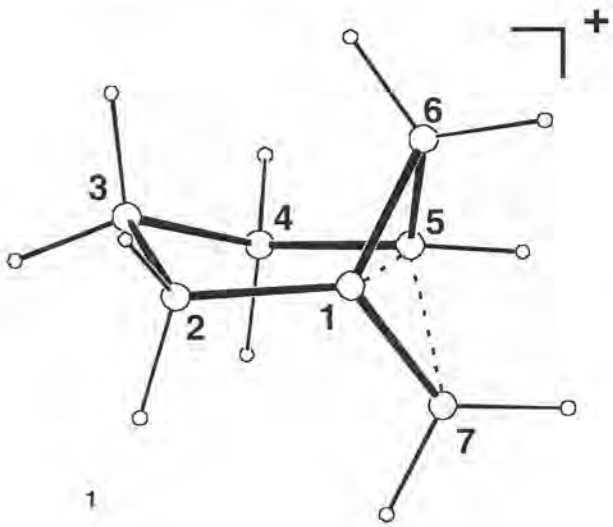
Quantum Chemical Studies of Reactive Intermediates and Mechanisms of Organic Reactions

RESPONSIBLE INSTITUTE:
Département de Chimie organique, Université de Genève

PROJECT LEADER:
Dr. J. Mareda–Département de Chimie organique, Université de Genève

The experimental observation of the short lived species such as carbocations or carbenes is difficult, and in most cases impossible. The theoretical calculations of accurate geometries and energies, especially for short-lived reaction intermediates and for transition states are therefore of particular interest.

The aim of the present research project is to investigate the properties and rearrangements of bridgehead carbocations, by means of high level quantum chemical methods. For example, we examined in particular the nature of the bicyclo[3.1.1]hexyl cation and its isomers [1], in order to provide a rational for the enhanced reactivity of corresponding halides. This enhanced reactivity is due to the fact that the pivotal intermediate on the $C_7H_{11}^+$ ion potential energy surface is a nonclassical carbocation **1**. The cyclopropylcarbinyl cation **2**, also located on this surface, has a substantial homoallyl character. Such unusual species represent a significant challenge to quantum chemistry methods. Several high level quantum chemical calculations were therefore used, and their accuracy for the carbocation **1** and its isomers were evaluated. The substituent and solvent effects on these ions, as well as their rearrangement mechanisms, are presently studied.



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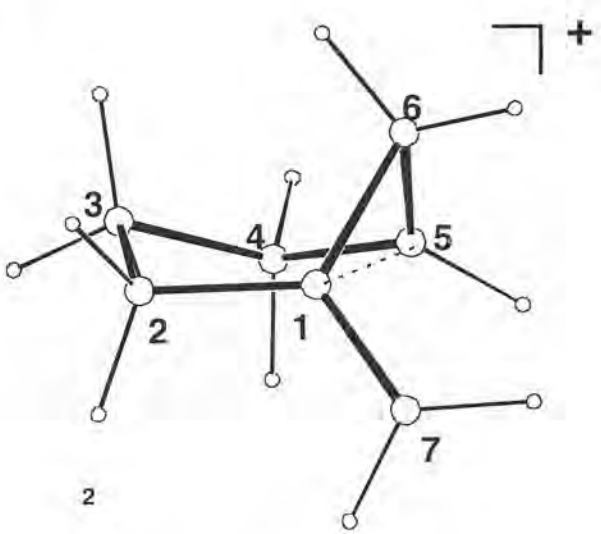

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In a continuous effort to investigate bridgehead reactivities [2], we study also the factors influencing the electronic structure, energy and conformations of a whole range of selected bridgehead carbocations.

In a separate project, the carbene cycloadditions are computationally examined. Singlet carbenes may undergo either 1,2- or 1,4-cycloadditions with conjugated dienes. Previously we investigated the mechanisms and selectivities of intramolecular carbene cycloadditions [3], using computational methods. Yet, the factors controlling selectivity are so far unexplained in the case of intermolecular cycloadditions. We are therefore studying the intermolecular dihalocarbene cycloadditions to dimethylenecycloalcans.

References:

[1] Mareda J. and C. Chiancone. Presentation at the *Current Trends in Computational Chemistry*, Jackson, Mississippi, U. S. A., November 1995, submitted for publication.

[2] Müller P. and J. Mareda. 1990. Cage Hydrocarbons. Edited by Olah, George Andrew. Wiley: New York, N. Y.: 189;
Mareda J. 1993. *J. Chem. Soc.*, Chem. Commun.: 1280;
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[3] Evanseck J. D., J. Mareda and K. N. Houk. 1990. *J. Am. Chem. Soc.*, 112: 73.

Quantum-Chemical Calculations of Potential Surfaces

RESPONSIBLE INSTITUTE:
Organisch-chemisches Institut, Universität Zürich

PROJECT LEADER:
Prof. W. Thiel–Organisch-chemisches Institut, Universität Zürich

INVOLVED PERSONS:
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V. Jonas–Organisch-chemisches Institut, Universität Zürich
D. Werner–Organisch-chemisches Institut, Universität Zürich

Ab initio calculations at the SCF, MP2, and CCSD(T) levels have been used to predict the equilibrium structures, the harmonic and anharmonic force fields, and the vibration-rotation spectra of several small reactive molecules including FCCCl [1], FCCBr, ClCCCl, HSF, XeF_4 [2], and BiH_3 [3]. The theoretical predictions facilitate the spectroscopic identification of such short-lived molecules and guide the analysis of the observed high-resolution spectra.

Density functional calculations with nonlocal gradient-corrected exchange-correlation functionals (e.g. BP86) provide surprisingly accurate geometries, vibrational frequencies, and bond dissociation energies for many transition metal carbonyls [4]. Analogous systematic calculations have been performed for transition metal complexes with other ligands (work in progress) which may play a role in catalytic processes. A detailed study of iron carbonyl olefine complexes has been motivated by empirical correlations between reactivity and NMR chemical shifts.

Semiempirical calculations on large icosahedral fullerenes (C_{180}, C_{240}, C_{540}, C_{960}) have established the facetted structures to be significantly more stable than their spherical counterparts [5]. For the smaller fullerenes (C_{180}, C_{240}) this has been confirmed by *ab initio* SCF and density functional computations.

References:

[1] Breidung J., H. Bürger, M. Senzlober and W. Thiel. 1995. *Ber. Bunsenges. Phys. Chem.* 99: 282.
[2] Bürger H., S. Ma, J. Breidung and W. Thiel. 1996. *J. Chem. Phys.* 104: 4945.
[3] Breidung J. and W. Thiel. 1995. *J. Mol. Spectrosc.* 169: 166.
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[5] Bakowies D., M. Bühl and W. Thiel. 1995. *J. Am. Chem. Soc. 117*: 10113.

Computation of Unsteady Three-Dimensional Flows in Complex Geometries

RESPONSIBLE INSTITUTE:
IET/LVV-ETHZ

PROJECT LEADER:
Prof. M. K. Eberle–IET/LVV-ETHZ

INVOLVED PERSONS:
Dr. K. Boulouchos–IET/LVV-ETHZ
L. Kaiktsis–IET/LVV-ETHZ

Our HLR-Project "Computation of Unsteady Three-dimensional Flows in Complex Geometries" has focused on problems in channels with sudden expansion, where we have studied transition and early turbulence. A major part of this work has focused on the canonical flow over a backward-facing step.

A study of the stability and transition of the two- and three-dimensional flow over a backward-facing step with a nominal expansion ratio of two has been performed up to Reynolds number $Re = 2{,}000$, using direct numerical simulation (DNS). In two dimensions, a high-order spectral element method is employed for the simulations, whereas three-dimensional simulations are based on a spectral element/Fourier method. The interpretation of results is based on concepts of modern instability theory.

During the course of our investigation of the flow in a backward-facing step we found that the flow is convectively unstable in a large portion of the flow domain for Reynolds numbers in the range $700 \leq Re \leq 2{,}000$: upstream generated disturbances propagate downstream at amplified amplitude with a space-dependent speed, but all flow states up to $Re = 2{,}000$ are time-independent in the absence of any external excitation. For small excitation disturbances, the amplitude of the resulting waveform is proportional to the disturbance amplitude. However, selective sustained external excitation even at small amplitudes can alter the behaviour of the system and lead to time-dependent flow at large times. The effect of two different types of excitation imposed at the inflow was studied: (1) monochromatic wave with frequency chosen to be either close to or far from the shear layer frequency; and (2) random noise. It was

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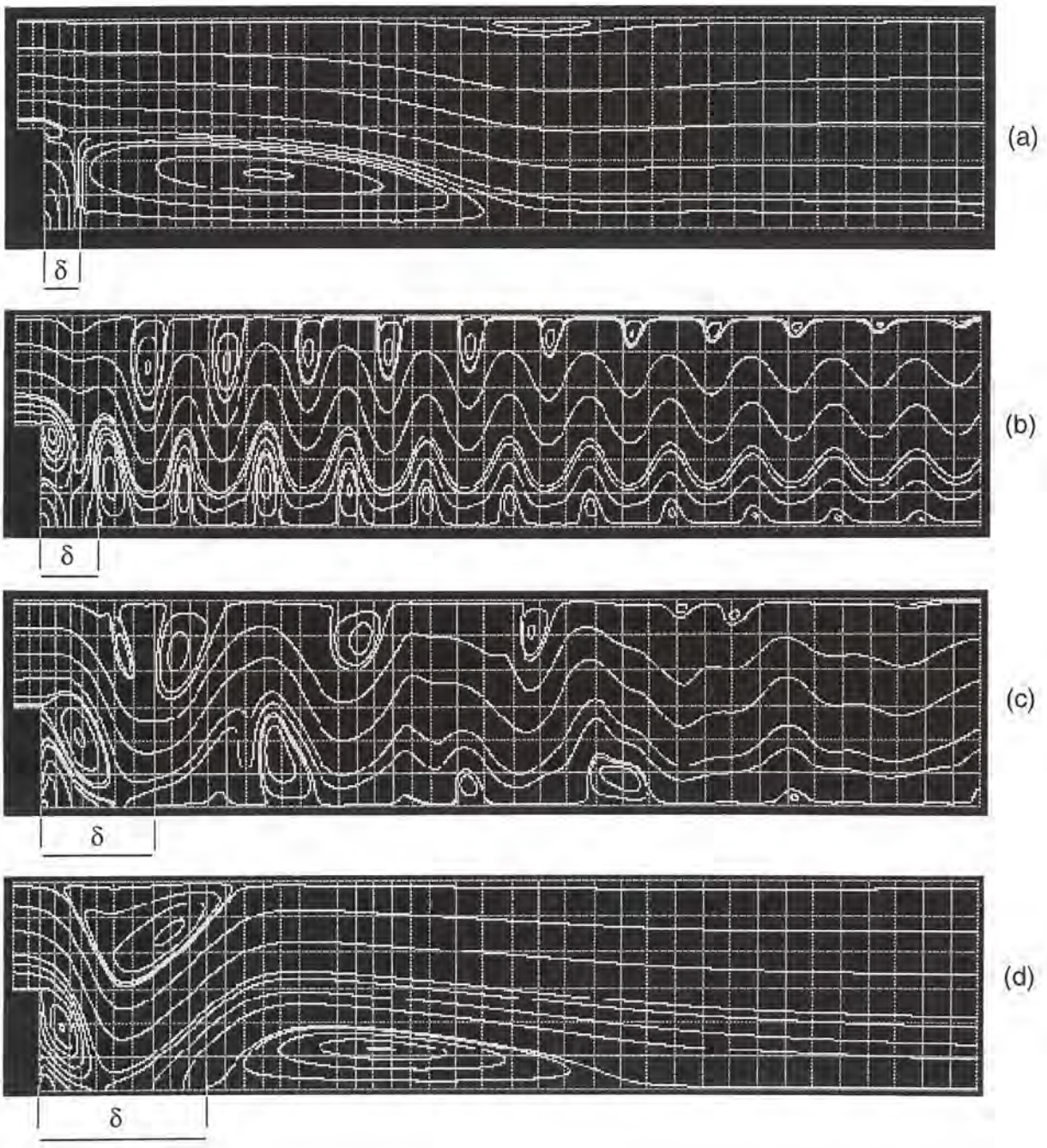


Figure 1: Flow over a backward-facing step: instantaneous streamlines for suction at the step wall and blowing at the low wall (the x scale is compressed by a factor of 4): (a) δ=1.25, (b) δ=2.0, (c) δ=4.0, (d) δ=6.0.

found that for small amplitude monochromatic excitation the flow acquires a time-periodic behaviour if perturbed close to the shear layer frequency, whereas the flow remains unaffected for high values of the excitation frequency. On the other hand, for the random noise case, an unsteady behaviour is obtained with a fundamental frequency close to the shear layer frequency. A detailed presentation of this work can be found in [1].

Generating global unsteadiness in the backward-facing step flow is of interest for practical applications; one important application is the performance enhancement of combustors by efficient flame stabilization. Using direct numerical simulation of the two-dimensional flow, we showed that in the low Reynolds number regime an oscillatory flow can result from simultaneous suction at the step wall and blowing at the low wall. For a nominal expansion ratio of two, Reynolds number $Re = 1{,}000$, and fixed suction and blowing mass flow-rates, a steady or time dependent flow is obtained, depending on the extent of the region where blowing is applied (see figure). Results are discussed in [2].

For the same geometry and problem definition as in the two-dimensional flow, it was found that the three-dimensional flow is stable to three-dimensional temporal perturbations for Reynolds numbers $Re \leq 1{,}000$. At $Re = 2{,}000$, a shear layer instability develops, leading to unsteady three-dimensional flow. Results are presented in [3].

References:

[1] Kaiktsis, L., G. E. Karniadakis & S. A. Orszag. 1995. Unsteadiness and convective instabilities in two-dimensional flow over a backward-facing step. *Journal of Fluid Mechanics*, to appear.

[2] Kaiktsis, L. and P. A. Monkewitz. 1995. Generating global unsteadiness in flow over a backward-facing step. In preparation.

[3] Kaiktsis, L. 1995. Instability classification and transition in flow over a backward-facing step. *PhD thesis*, Institut für Energietechnik, ETH-Zürich.

Ocean and Climate, Modelling the Biogeochemical Cycle of Carbon

RESPONSIBLE INSTITUTE:
Physikalisches Institut, Universität Bern

PROJECT LEADER:
Prof. T. Stocker–Physikalisches Institut, Universität Bern

Climate variability is strongly influenced by the global ocean circulation. Abrupt climatic changes reconstructed by the analysis of various ocean and ice sheet paleoclimate archives suggest that these changes have been triggered by fresh water input in the high latitudes. A sequence of disturbances of the ocean circulation was initiated at different geographical locations with different intensities in a 3-dimensional ocean general circulation model. The response of the ocean shows a teleconnection of southern disturbances with northern response and vice versa. That is, local variations can induce global climatic changes.

Understanding the climate of the past goes hand in hand with understanding present climatic change. One of the most prominent and best documented concerns the atmospheric emission of CO_2. Exploring the part of the carbon cycle with a 3-dimensional ocean tracer transport model allows us to determine the marine uptake of anthropogenic CO_2 of the last decades. Such a study combines numerical simulations of the global ocean circulation with the simulation of the biochemical reactions in the ocean. To validate such a carbon cycle model we use data sets based on observations. On the other hand, calculation of transport processes allows for further interpretation of these off-shore measurements from a mechanistic point of view.

Large-scale ocean models involve many parametrizations. One of them handles the transport of waters into the deep ocean. Such deep convection takes only some days and occurs on length scales of kilometers. It is the feeding process of the ocean's deep waters which preserves the climatic fingerprint of today for the next 1000 years. To obtain better parametrizations of this important small-scale process a high resolution model is used. This model resolves most of the processes down to a length scale of some meters and allows the systematic study of the sub-grid physics of low resolution global models.

Climate Simulation

RESPONSIBLE INSTITUTE:
Geographisches Institut, ETHZ

PROJECT LEADER:
Dr. M. Beniston–Geographisches Institut, ETHZ

The Climate Simulation project has the main objective of simulating at high spatial and temporal resolution current climate to improve our understanding of the fundamental mechanisms of the climate system, and future climate in order to assess the magnitude of changes to be expected in the next century under conditions of anthropogenically-induced "greenhouse gas" forcing. The numerical parts of the project have been partitioned into a number of steps, which converge towards the final objective of providing an operational modeling system for use to the climate research community investigating climate change and its potential impacts on a number of natural and socio-economic systems. The steps are as follows:

1. Simulation of current climate with the high-resolution General Circulation Model (GCM) and exhaustive analysis of the model performance using available observational datasets,
2. Simulation of current climate (January and July daily climatologies) with the high-resolution Limited Area Model (LAM) and exhaustive analysis of the model performance, in particular of boundary-layer physics and precipitation,
3. Simulation of future climate (climate change scenario based on a doubling of equivalent CO_2 concentrations in the atmosphere compared to 1990 values) with the GCM. Analyses of the changes in dynamic and thermodynamic field with respect to current climate,
4. Simulation of future climate with the LAM. Analyses of changes in the behavior of temperature and precipitation in the Alps.

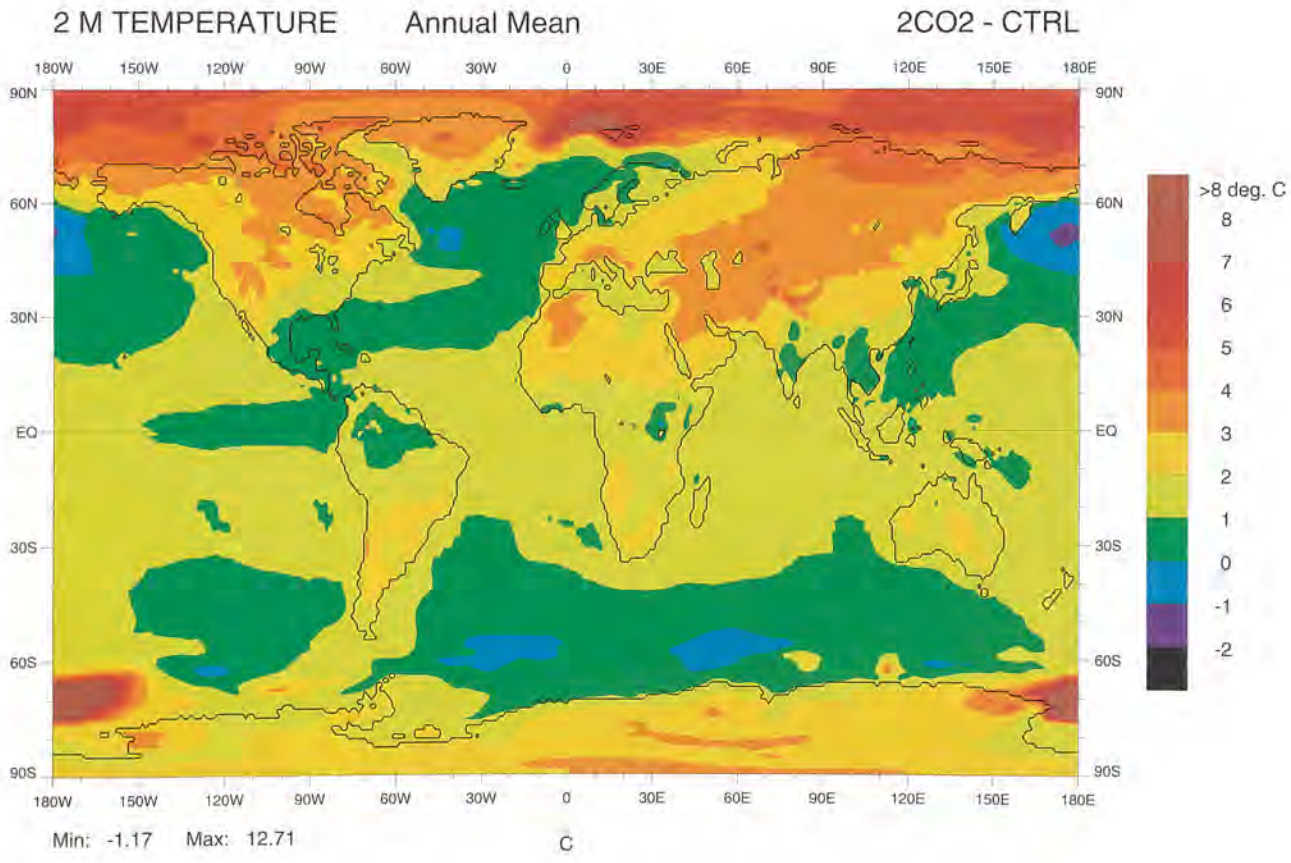


Figure 1: Global distribution of annual mean surface air temperature changes as simulated by the ECHAM3 climate model in a doubling CO_2 time slice experiment.

Ab Initio Molecular Dynamics Study of First-Order Phase Transitions

RESPONSIBLE INSTITUTE:
IRRMA-EPFL

PROJECT LEADER:
Prof. R. Car–IRRMA-EPFL/ Département de Physique de la matière condensée, Université de Genève

INVOLVED PERSONS:
Dr. O. Sugino–IRRMA-EPFL/ Fundamental Research Laboratories, NEC Corporation

Prediction of phase transformations of real materials from first-principles microscopic quantum theory is a long standing goal of condensed matter physics. A major difficulty is that, in order to predict phase stability at finite temperature, the free-energies of different phases of a given substance must be calculated. This is particularly difficult for a liquid phase for which a simple quasi-harmonic approximation is not valid. In this work accurate techniques of thermodynamics integration, previously used only in the context of classical molecular dynamics simulations based on empirical interatomic interactions, have been extended to first-principles simulations. These allow to compute the free-energy difference along a reversible thermodynamic path connecting two different systems. This approach has been used to study the melting transition in silicon and to predict a number of thermodynamic properties of this material at the melting point, showing overall a rather good agreement between theory and experiment [1]. This approach has been subsequently used to study the thermodynamics of amorphisation of silicon. Presently, we are applying the same approach to elucidate some aspects of the phase diagram of carbon at high temperature that are not fully understood experimentally.

References:

[1] Sugino, O. and R. Car. 1995. *Phys. Rev. Lett.* 74: 1823.

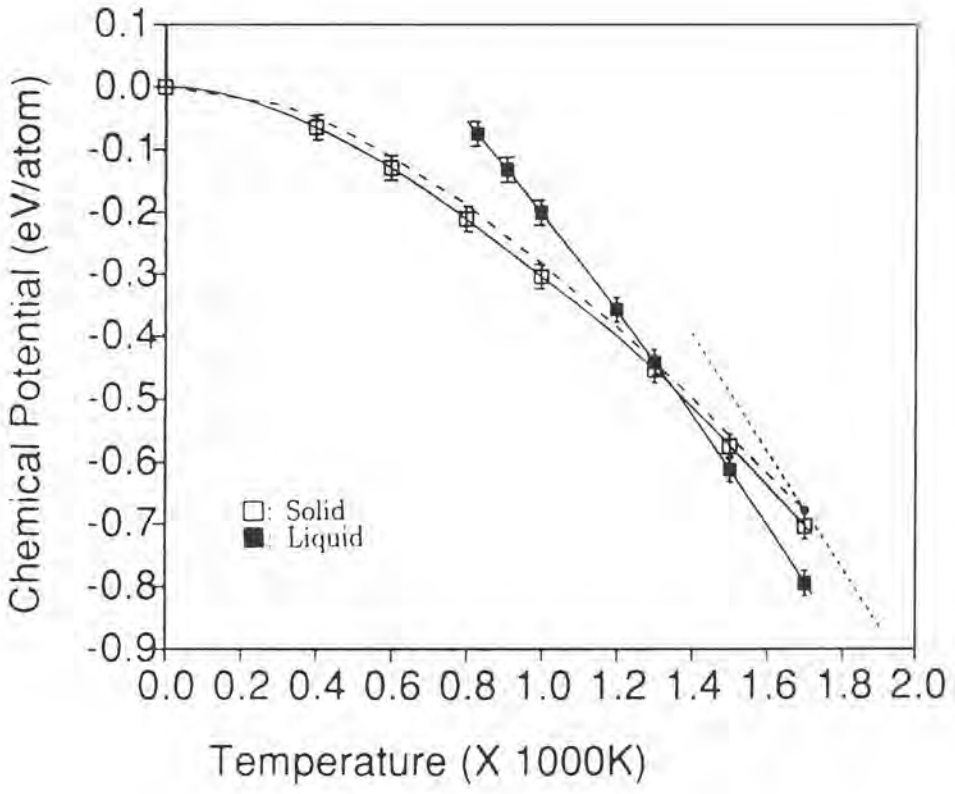


Figure 1: Chemical potential for solid silicon (open squares) and liquid silicon (filled squares). Full lines correspond to theory and broken lines to experiment.

Investigation of the Properties of SiO_2 and of its Interface with Si(001)

RESPONSIBLE INSTITUTE:
IRRMA-EPFL

PROJECT LEADER:
Prof. R. Car–IRRMA-EPFL/ Département de Physique de la matière condensée, Université de Genève

INVOLVED PERSONS:
Dr. M. S. Hybertsen–AT&T Bell Laboratories (U. S. A.)
Dr. A. Pasquarello–IRRMA-EPFL
Dr. J. Sarnthein–IRRMA-EPFL/ Technische Universität Wien (Austria)

The current degree of device miniaturization in silicon-based technology calls for an understanding of the structural properties of the Si(001)-SiO_2 interface at the microscopic level. However, despite the use of a large variety of experimental techniques, the detailed bond pattern at this interface remains essentially unknown. In order to increase our insight in the structural properties of the amorphous SiO_2 component, we performed a molecular dynamics study in which liquid SiO_2 was quenched to low temperatures [1]. This study yielded a chemically ordered amorphous network, whose structure factor was in excellent agreement with experiment. In addition, detailed structural information, such as bond lengths and bond angles, became available. Approaching the problem along different lines, we set up model interface structures by attaching tridymite, a crystalline form of SiO_2 , to Si(001), and then allowing for full relaxation. The bond-density mismatch was adjusted as shown in the figure. The structural properties of the oxide compared well with our model of the amorphous [1]. By calculating Si 2p core-level shifts and comparing with photoemission experiments, we supported the interpretation of the spectra which assigned the suboxide peaks to differently oxygen-coordinated silicon atoms [2].

References:

[1] Sarnthein J., A. Pasquarello, and R. Car. 1995. *Phys. Rev. Lett.* 74: 4682; *Phys. Rev.* B 52, November 1995.
[2] Pasquarello A., M. S. Hybertsen, and R. Car. 1995. *Phys. Rev. Lett.* 74: 1024.

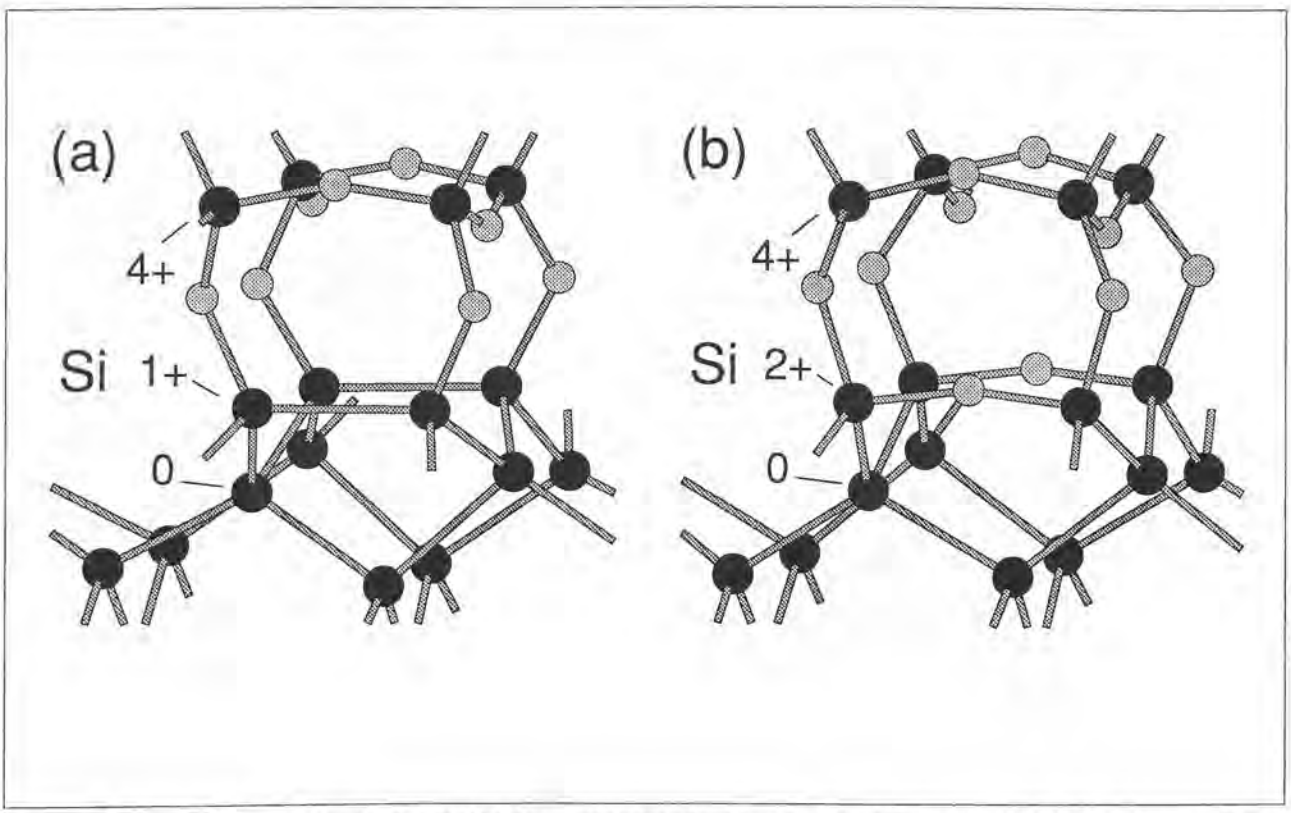


Figure 1: Ball and stick models of the Si(001)-SiO_2 interface, as found upon full relaxation in Ref. [2]. The bond-density mismatch is fixed (a) allowing for dimerization or (b) introducing oxygen bridges. The Si partial oxidation states are indicated.

Si Control Layers at GaAs/Al(100) Schottky Junctions

RESPONSIBLE INSTITUTE:
IRRMA-EPFL

PROJECT LEADER:
Prof. A. Baldereschi–IRRMA-EPFL

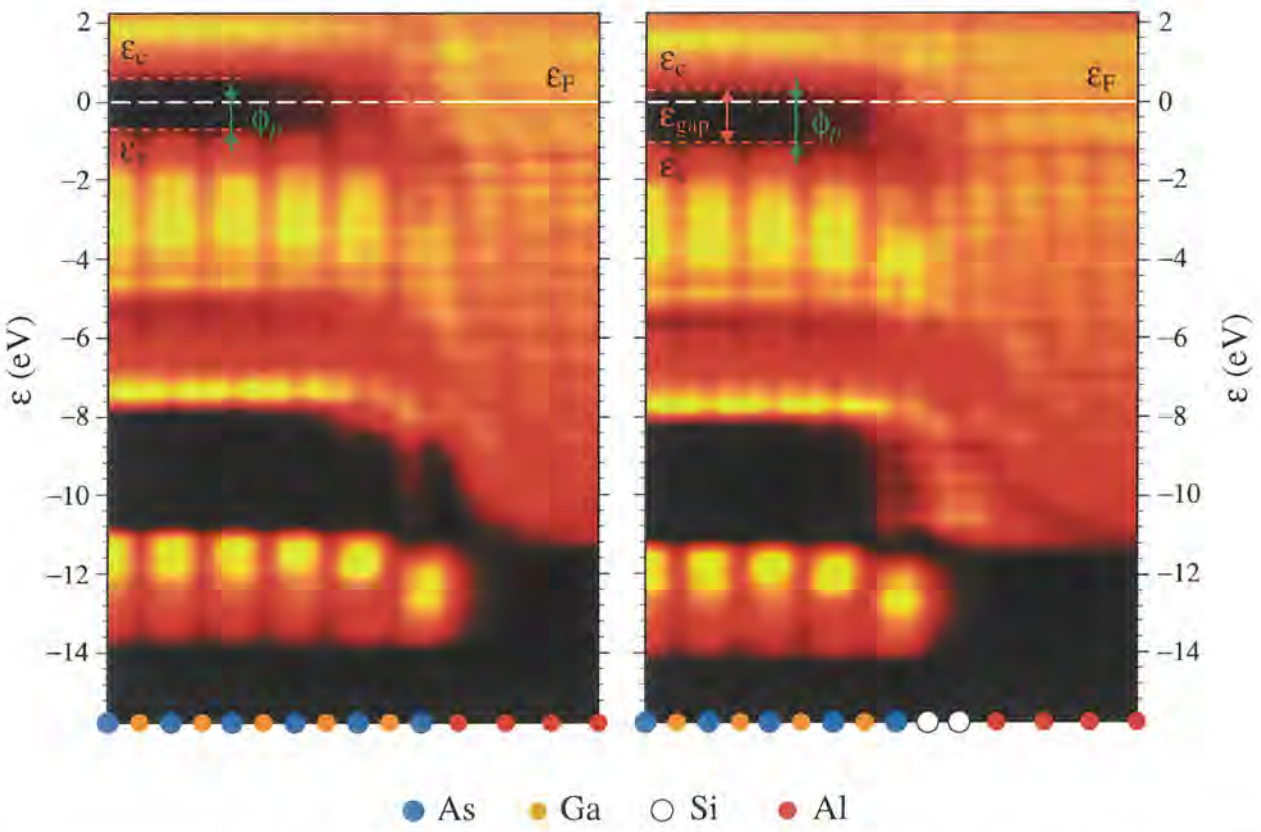
INVOLVED PERSONS:
C. Berthod–IRRMA-EPFL
Dr. N. Binggeli–IRRMA-EPFL

Metal-semiconductor interfaces are widely used in semiconductor device technology either as rectifying or as ohmic contacts. The Schottky barrier height is the fundamental parameter which controls the transport properties of the contacts. The purpose of our work is to identify by first-principles computational studies the structural and electronic parameters which influence Schottky barrier heights, and to explore the mechanisms which can be used to control the barrier heights. We studied, in particular, the tuning of the GaAs/Al(100) Schottky barrier by means of ultrathin Si layers which are deposited at the interface.

The barrier modification results from the heterovalent nature of the interlayers, and the calculated barrier values quantitatively explain the experimental data for Si coverages in the submonolayer to 2 monolayers range [1]. We analyzed this effect on the atomic scale by probing the screening of interfacial perturbations by the metal wave-functions, and by examining the Si induced changes in the local density of states. Based on this microscopic analysis, we have developed a model for predicting the barrier modifications in terms of screened local interface dipoles [2].

References:

[1] Cantile, M., L. Sorba, S. Yildirim, P. Faraci, G. Biasiol, A. Franciosi, T. J. Miller and M. I. Nathan. 1994. *Appl. Phys. Lett.* 64: 988.
[2] Berthod, C., N. Binggeli and A. Baldereschi. *EUROPHYS. LETT.* (in press).



Si Control Layers at GaAs/Al(100) Schottky Junctions. Figure 1: Energy-band profile as given by the computed local electronic density of states map at GaAs/Si/Al(100) junctions for zero (left) and 2 monolayers (right) Si coverages. The density of states increases from black (zero) to yellow (highest density). The Fermi level ε_F of the metal, the semiconductor valence band edge ε_v, and the Schottky barrier height, ϕ_p, are also indicated.

First-Principles Studies of Surfaces, Interfaces and Amorphous Materials

RESPONSIBLE INSTITUTE:
Département de Physique de la matière condensée, Université de Genève

PROJECT LEADER:
Dr. T. Jarlborg–Département de Physique de la matière condensée, Université de Genève

INVOLVED PERSONS:
E. Moroni–Universität Wien (Austria)

The Vienna *ab-initio* Molecular Dynamic program (VAMP) using Vanderbilt ultrasoft pseudopotentials has been tested, and successfully applied for studies of structural and magnetic properties of Fe, Ni and Co in bcc, hcp and fcc structures. Both the VAMP approach and all electron linear-muffin-tin-orbital (LMTO) method are used for studies of different iron-silicides. The influence of random Fe defects on the structural and electronic properties is also investigated for several FeSi cubic phases.

The study of the magnetic and structural properties of Fe_3Si is mainly motivated by the fact that such systems are used as components of magnetic multilayers together with bcc Fe. Our study shows that the local moments of the different sites of Fe depend strongly on the local coordination. Addition of silicon to iron causes some important changes in the magnetic and mechanic properties of bcc Fe, pushing the stability of the bcc structure to higher temperature.

FeSi stabilises in the cubic *B*20 structure having eight atoms per unit cell. At low temperature, the peculiar feature is a small gap (50 meV). At larger temperature, spin-fluctuations become important and influence strongly the magnetic properties with a maximum of the susceptibility at 500 K. The *FeSi* compound in the *B*20 structure is found to be only a fraction of a mRy more stable than the metallic B2 FeSi.

The continuation of this work will be the study of metal-semiconductor interfaces (e.g. $Si/FeSi_2$) and magnetic multilayer (e.g. $Fe/FeSi$ and $Fe_3Si/FeSi$).

Program Environment for User Support in Computational Chemistry and Materials Science

RESPONSIBLE INSTITUTE:
CSCS

PROJECT LEADER:
Dr. D. Maric–CSCS

At CSCS more than 60% of the CPU time is allocated to the user projects performing microscopic simulations (very large scale electronic structure calculations and molecular dynamics simulations). These methods are employed by research groups studying problems in chemistry, biochemistry, pharmacology, solid state physics and materials science.

Most of the computational methods used for microscopic simulations at CSCS have been developed by Swiss research groups. CSCS has actively supported these authors in porting and optimising their programs on the CSCS high performance computing facilities, as well as has partly interfaced these programs to the CSCS visualisation tools.

Besides the construction and maintenance of this integrated simulation environment which should allow the simultaneous usage of different software packages on the heterogeneous hardware in a connected way, the showcase applications of these tools to the challenging problems from biochemical and materials science applications are carried out.

Numerical Simulation of Cluster Deposition on Surfaces

RESPONSIBLE INSTITUTE:
IPE-EPFL

PROJECT LEADER:
Dr. C. Massobrio–IPE-EPFL

The main goal of the project, carried out within the IPE-EPFL, is the study of electronic, structural and dynamical properties of clusters. Both isolated and supported systems have been investigated by using first principles molecular dynamics in the first case [1] and effective n-body interatomic potentials in the second [2]. Among the results obtained in 1995 we recall:

a) the analysis of atomic diffusion underlying the formation of a surface alloy in the Pd/Ag case, in conjunction with photoemission experiments and
b) the study of finite temperature effects in Cu_7^-.

In the first case we obtained diffusion barriers in excellent agreement with experiments, together with a microscopic description of the mechanism leading to the formation of the alloy [3]. In the second we were able, for the particular cluster size N=7, to achieve a more refined interpretation of the photoelectrum spectra and obtain thermally averaged distributions of excitation energies. The project on Cu clusters has been carried out in collaboration with Dr. Alfredo Pasquarello and Prof. Roberto Car of IRRMA.

References:

[1] Massobrio C., A. Pasquarello and R. Car. 1995. *Phys. Rev. Lett.* 75: 2104 and to be published.
[2] Blandin P., C. Massobrio and P. Ballone. 1994. *Phys. Rev. Lett.* 72: 3072
[3] Patthey F., C. Massobrio and W. D. Schneider, to be published.

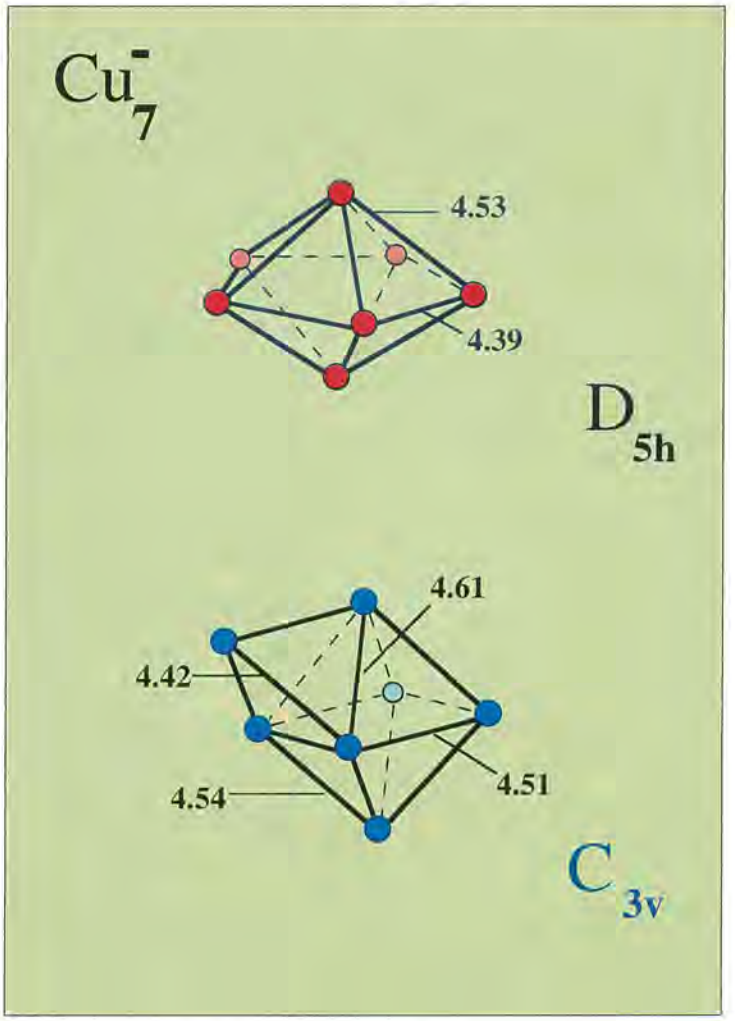


Figure 1.

Simulation of Solid Polymers

RESPONSIBLE INSTITUTE:
Institut für Polymere, ETHZ

PROJECT LEADER:
Prof. Dr. U. W. Suter–Institut für Polymere, ETHZ

INVOLVED PERSONS:
Group of Macromolecular Chemistry–Institut für Polymere, ETHZ

The computational activities in the group of Macromolecular Chemistry constitute a theoretical and numerical counterpart to traditional polymer synthetic work. The general goal of these activities is the investigation of the relationship between molecular structure and properties in polymeric systems, mostly in the glassy state or in the melt. In most calculations, a fully atomistic representation is used.

The NEC SX-3 in Manno has been applied mainly on the following three areas:

- Development of **new Monte Carlo methods** for the sampling of polymer configuration space: the efficient generation of truly independent and representative polymer configurations is one of the toughest problems polymer simulators are confronted with. A suite of MC algorithms including Metropolis MC, Simple Reptation and Configurational Bias was applied to short- and long-chain alkanes as model compounds for linear polymers of the polyethylene type. An improved force field was developed that allows accurate prediction of PvT properties over a wide range of temperatures and pressures.
- Computation of the **effects of small molecules in amorphous polymeric matrices**: the presence of small molecules in a polymeric structure can have a strong influence on the behaviour of polymers. The softening effect of water on the mechanical properties of Nylon has been investigated by atomistic simulation. The figure (next page) represents water molecules in an amorphous Nylon structure (water concentration: 10 wt%, temperature: 300 K, cell edge 20 Å; water shown as CPK model, polymer represented as a wire model). Additionally, the solubility of water in Nylon is being investigated using Widom's standard insertion technique for the calculation of the chemical potential.
- Mesoscopic simulation of **composite materials**: amorphous polymers are frequently used as the continuous phase in a wide range of industrially relevant composite materials. The understanding of their properties and very especially, of their anisotropy or direction dependence, is a key step in their use as structural materials. Given the characteristic length scales of the reinforcing particles, the description of both polymer and filler cannot be performed at the atomistic level. We are currently investigating the use of continuum-mechanical (Finite Element) techniques to the prediction of direction-dependent macroscopic mechanical properties of composite materials with a polymeric basis.

Towards the Accurate Computation of Properties of Transition Metal Compounds: The Binding Energy of Ferrocene

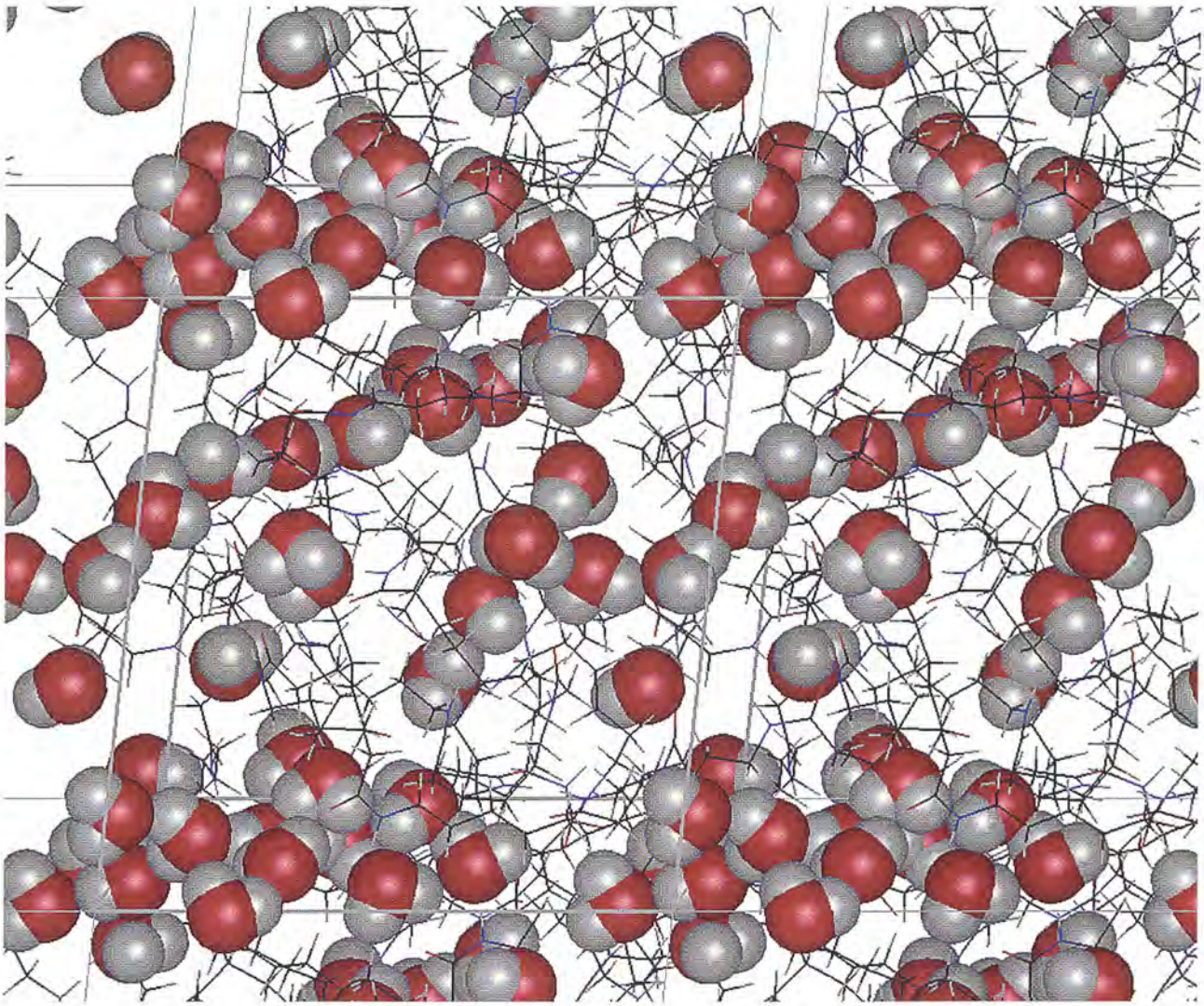
RESPONSIBLE INSTITUTE:
IPS-ETHZ

PROJECT LEADER:
Dr. H. P. Lüthi–IPS-ETHZ

INVOLVED PERSONS:
Dr. W. Klopper–IPS-ETHZ

A number of recent studies show that due to the progress made in quantum chemical method development, structural and thermodynamic properties of transition metal complexes can now be computed with (near-) experimental accuracy. It therefore becomes important to analyze the remaining sources of error in a *quantitative* way in order to provide error bars for the data computed. Errors introduced by basis set truncation and basis set superposition, by lack of size consistency and/or size extensivity, or by neglect of relativistic effects are among the items to be investigated.

This investigation aimed at an error analysis for the computed binding energy of ferrocene as published by B. O. Roos and by T. Helgaker and coworkers. Using data from MP2-R12, coupled cluster and DFT studies generated by us, we were able to critically review the theoretical *and* the experimental data for that particular observable. The computations performed on CSCS' NEC SX-3 were MP2-R12 calculations (program SORE) addressing the basis set truncation error. From our study it appears that—for the very first time—quantum chemical investigations were to challenge experimental data for ferrocene, one of the most systematically explored molecules. A manuscript describing this work has been accepted for publication in *Chemical Physics Letters*.



Simulation of Solid Polymers. Figure 1: Atomistic microstructure of amorphous Nylon-6 with 10% by weight of water. (The water is drawn as space-filling molecules, the polymer chain is represented by light bonds.

Cosmological Structure Formation with Topological Defects

RESPONSIBLE INSTITUTE:
Département de Physique Théorique, Université de Genève

PROJECT LEADER:
Prof. R. Durrer–Département de Physique Théorique, Université de Genève

Within standard big bang cosmology, the formation of structure in the universe (i.e., inhomogeneities in the matter distribution like galaxies, clusters, superclusters, voids and walls and anisotropies in the cosmic microwave background) is still an essentially unsolved problem. We investigate models where fluctuations in matter and radiation are seeded by global topological defects which may form during a phase transition in the early universe. These models, like scenarios where perturbations are induced during an inflationary epoch, lead to a scale invariant spectrum of fluctuations as it has been observed by the DMR experiment aboard the COBE satellite [1]. It is an attractive feature of our models, that the only free parameter is the phase transition temperature, i.e., the results are independent of the precise shape of the scalar field potential.

We numerically evolve the order parameter (scalar field, Higgs field) inducing the phase transition. This amounts in solving a coupled system of hyperbolic nonlinear partial differential equations. We then determine the gravitational action of the scalar field on matter and radiation in first order perturbation theory. We calculate the cosmic microwave anisotropies (the figure, next page, shows a false color image of these anisotropies from one realization) and the dark matter fluctuations to compare our models with observations. Results of our simulations can be found in the references below.

References:

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[3] Durrer, R. and Z.-H. Zhou. 1995. *Phys. Rev. Lett.* 74: 1701.
[4] Durrer, R. and Z.-H. Zhou. 1995. In *Seventeenth Texas Symposium on Relativistic Astrophysics and Cosmology*, edited by. H. Böhringer, G. E. Morfill and J. Trümper: 688.
[5] Durrer, R. and Z.-H. Zhou. 1996. *Phys. Rev.* D 53: 5394.
[6] Durrer, R., A. Gangui and M. Sakellariadou. *Phys. Rev. Lett.* (in print). (astro-ph/9507035).

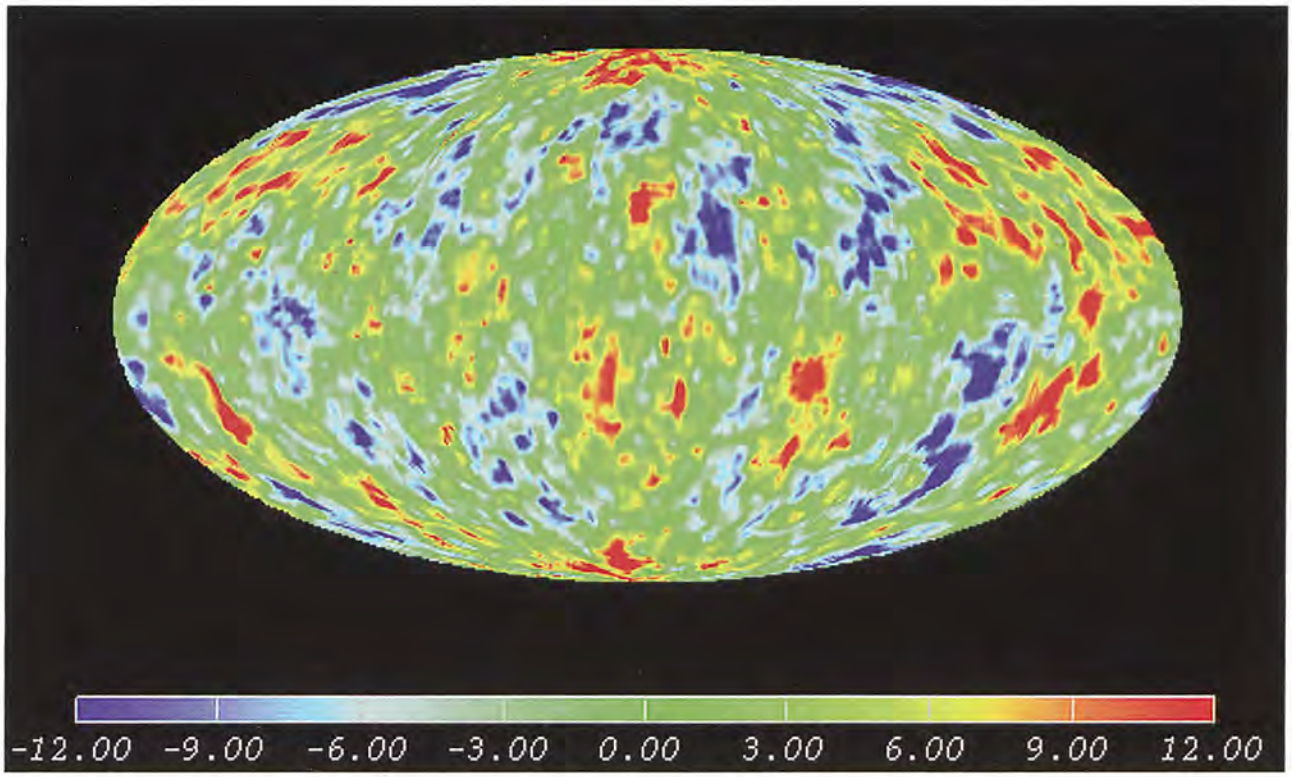
Calculation of the Electronic Structure of Impurities in Solids

RESPONSIBLE INSTITUTE:
Physik-Institut, Universität Zürich

PROJECT LEADER:
Prof. P. F. Meier–Physik-Institut, Universität Zürich

During the past year we investigated the microscopic structure of hydrogen-like impurities in semiconductors. Different approaches to solve the many-electron problem have been employed, such as the density functional method (DFM) using localized basis sets as provided by the packages DeFT, a derivate of the DeMon program and Gaussian/DFT. Our own DFM code uses plane waves as basis sets and state of art methods like the conjugate gradient technique and decoupled norm conserving pseudopotentials. This provides us with a fast, well optimized code running on different types of computers. For instance, on the NEC SX-3/24R, the program runs consistently at 1.7GFlops with a vectorization rate of 99.5%.

We performed extensive calculations using these methods. In particular, we investigated the electric field gradients induced by hydrogen at impurity nuclei and we studied the equilibrium structures of crystal silicon containing a boron-hydrogen or a phosphorous-hydrogen impurity pair along with the vibrational frequencies. Furthermore, hyperfine properties in spin polarized systems were calculated and we found that they are very sensitive to gradient corrections to the local spin density approximation.



Cosmological Structure Formation with Topological Defects. Figure 1.

Adaptive P^{3}M Gravitation Code

RESPONSIBLE INSTITUTE:
IPS-ETHZ

PROJECT LEADER:
Dr. W. P. Petersen–IPS-ETHZ

A vector/parallel adaptive P^{3}M (particle-particle, particle-mesh) N-body simulation code has been developed. Much progress has been made in algorithmic development: the short-range P-P portion of the code has been vectorized and shared memory parallelized, and a robust and flexible FFT (Fast Fourier Transform) package has been written and installed. The interesting physics, however, remains to be done. We are continuing with this cosmic structure formation project. Gravity is phase space separating, hence the problems are more difficult than in plasma simulations or chemical kinetics, although the parallel methods are applicable to these phase space saturating problems. In particular, this code has attracted some interest from the Physical Chemistry Department. Currently, the code is well vectorized (Cray machines and NEC SX-3) and micro-tasked (Cray machines). On four processors the load is well balanced, but currently doesn't seem to scale well for more CPUs. An interesting analysis by Klaus Gärtner seems to show this effect is an inherent memory band-width limitation. Our objectives for the coming year will be (1) to do more physics, and (2) study and optimize the load balancing using microtasking on the SX-4, our target machine.

Numerical Investigation of the Simulation of Strongly Correlated Fermions

RESPONSIBLE INSTITUTE:
Institut für Theoretische Physik, ETHZ

PROJECT LEADERS:
Prof. T. M. Rice–Institut für Theoretische Physik, ETHZ
PD Dr. D. Würtz–IPS-ETHZ

INVOLVED PERSONS:
B. Ammon–IPS-ETHZ
B. Frischmuth–IPS-ETHZ
Dr. M. Troyer–IPS-ETHZ
Dr. H. Tsunetsugu–IPS-ETHZ

High temperature superconductors are a big challenge to theoretical solid state physics, as they are a typical example of strongly correlated electron systems. In these systems, owing to the strong interactions, various analytical approximations often lead to results controversial to each other. Exact numerical investigations are therefore very important to obtain rigorous results free from the approximations.

The numerical methods themselves are also a big task because of the huge number of states involved. In the past three years we have improved a variety of numerical methods to study the t-J model to get as much information as possible within the capacity and speed of current super-computers. Our central interest is the t-J model, which is believed to be the simplest model correctly describing the high temperature superconductors. The one-dimensional t-J chains are well understood, and a nearly complete phase diagram is now available.

To understand the superconducting and related phases expected for the two-dimensional t-J model, we have tried to describe important correlations starting from some one-dimensional systems, based on the idea of dimensional crossover. In particular, the underdoped region of the YBCO compounds is characterized by the presence of spin gap (or pseudo-gap), which is expected to relate with the mechanism of superconductivity. We have proposed that this phase may be described by a new type of the charge density wave stabilized by quantum spin fluctuations. We have semi-quantitatively determined the phase transition from this phase to the superconducting phase, by using the numerical simulations on one-dimensional systems combined with a mean-field treatment for the couplings in the other direction.

An important point is that as far as the spin gap phase in two dimensions is concerned t-J ladders consisting of two coupled chains would be more appropriate as the starting onedimensional system than single chains. The dimensional crossover would then be smooth since the ladder shares the spin gap nature. On the other hand, the t-J chains have no spin gap near half filling, implying the presence of a phase transition as the interchain couplings increase.

The single t-J ladder has been numerically investigated in detail as the starting point, with emphasis on its excitation spectrum and dynamical correlations. An important result is that the excitations change their nature depending on the energy scale. Most notably the lowest excitations are a collective charge mode, responsible for superconducting fluctuations with a modified d-wave internal symmetry. There are quasiparticle excitations with a finite spin gap, in addition to the collective spin mode in a higher energy sector. At low hole dopings these quasiparticles form a dilute Fermi gas with a strong attraction. However, the

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Fermi wave number is proportional to the electron density rather than the hole doping, corresponding to a large Fermi surface observed in the planar compounds by photoemission experiment.

The undoped ladders are by themselves intriguing since they are also realized in some quasione-dimensional materials. We have studied their thermodynamics in detail and have calculated the temperature dependence of a variety of quantities, e.g., the magnetic susceptibility, spin correlation length and the nuclear spin lattice relaxation rate $1/T$. We found good agreement with experimental measurements. An interesting phenomena is that ladders consisting of an even number of coupled chains exhibit a finite gap in the spin excitation spectrum, while odd-width ladders are similar to a single chain and have gapless spin excitations.

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Prof. Jacques Weber–
Département de chimie physique, Université de Genève (Computational Quantum Chemistry Applied to Inorganic and Organometallic Systems, page 34).

PhD in physics in 1969, full professor at the physical chemistry department of the University of Geneva since 1989 and chairman of the section of chemistry since 1995, professor Weber's background includes collaborations with the University of Florida as an invited professor, with IBM research laboratory, San José (California) as invited researcher, and with the University of Paris 7. His research domains are computational chemistry, molecular modelling and infographics, quantum chemistry applied to organometallic and inorganic compounds, and molecular dynamics.

Q: What impact does high-performance computing currently have on your research activities?

A: High-performance computing has undoubtedly an important impact on our research activities, as it enables us to tackle large systems which are totally out of the range of conventional workstations. This is mainly due to the limited amount of core memory and disk space on the latter systems, but the very long CPU times required are also a factor which has to be taken into account. For example, is it reasonable to run jobs which may take weeks of CPU on a typical workstation? I would say that this might be a possible solution in exceptional cases, but generally speaking you can not run routinely production jobs of that size on single processor workstations. You then have to turn to supercomputers, would they be of vector type or of massively parallel architecture. A question which is frequently asked to us, specially by managers of computer facilities, is why do we always turn to larger and larger systems to calculate using computational chemistry techniques? In other words, why do we almost immediately saturate their machines after costly upgrading, which, we have to admit this, must be somewhat frustrating for them? The answer is fairly easy. As most scientific disciplines, computational quantum chemistry is a rapidly expanding field where all kinds of modellizations have already been performed for small gaseous molecules. The progress in quantum chemistry methodologies and computer hardware is such that it is possible to perform calculations for these small systems with a higher accuracy than that of best experimental techniques. However, as most of these theoretical methods scale at least as N^3, where N is the number of atoms of the system, the computational effort increases very rapidly as a function of the complexity of the system. As most of the important chemical processes take place in solution, on surfaces or in solid materials, realistic modellizations in chemistry involve several tens, or hundreds, of atoms and they are therefore very costly. This is unfortunately the case for practically all challenging problems in today's chemistry: the search for novel heterogeneous or homogeneous catalysts, more efficient new materials, polymers, etc. To summarize abruptly, the fact that computational chemists saturate high-performance computer centers is an indication that they are tackling "real" chemical problems with a good chance to lead to significant progresses in this discipline.

Q: Do you have a vision regarding how your research area and high-performance computing will evolve in the future? If so, please describe your vision:

A: As mentioned above, computational chemistry and, in particular, its arsenal of tools based on quantum theory are going to evolve towards more and more realistic modelling, i.e., taking account of solvent, temperature, time evolution, etc., of complex processes such as those involved in rational drug design, selection and synthesis of new materials, design of new catalysts, and modelling of environment (climate change, stratospheric ozone depletion, etc.). However, for computational chemistry to be even more successfully involved in such research issues, new methodological developments and synergistic

combinations of different theoretical methods have to be introduced. This will allow an extension of theoretical investigations to realistic modelling of many-particle phases in which chemistry takes place, such as solute/solvent, liquids, solid materials and biological macromolecules. To summarize, computational chemistry will probably be able to treat non-ideal heterogeneous systems with a large number of particles and components. Clearly, the evolution of high-performance computing is difficult to assess, as it depends on many technical and economical aspects. Most probably, massively parallel architectures are going to dominate with peak performance of the order of teraflops. The role of networking and graphics is going to be increasingly important for the benefit of end users in scientific computing. However, one may predict that it will be more and more difficult to adapt the existing program packages so as to fully exploit the tremendous compute power of these new machines. This is actually a major point of concern for scientists without high-level specialization in computer science: how are they going to be able to make an efficient use of these very powerful computers without investing too much in code development and optimization? It seems to me that the only possible answer is to do more and more team work, with specialists in computer science playing an important role in developing adequate computing tools.

Q: Does CSCS meet your expectations of a high-performance computing center?

A: I think CSCS is playing an important role in providing CPU time on high-performance computers for Swiss scientists, specially for those affiliated with Universities where such equipments are generally not available. We have been undoubtedly able to perform large-scale calculations at CSCS which would have been impossible to carry out on our own workstations, specially in the field of first-principles (Car-Parrinello) molecular dynamics simulations of materials.

Q: What do you find of particular value at CSCS?

A: The availability of several powerful computers (HP cluster, Convex, etc.) in addition to the NEC SX-4 is certainly an asset. I would also mention the large range of programs available on the SX-4, and on these other machines as well, in the field of computational chemistry.

Q: What do you think should be improved at CSCS?

A: The documentation available on these program packages is not always sufficient. There should be some on-line documentation accessible by the users.

Q: Please comment on the relationship between your research team and CSCS staff.

A: To the best of my judgement, these relations are generally good and my coworkers have no apparent reason to complain.

Computational Quantum Chemistry Applied to Inorganic and Organometallic Systems

RESPONSIBLE INSTITUTE:
Département de chimie physique, Université de Genève

PROJECT LEADER:
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Dr. A. Selloni–Département de chimie physique, Université de Genève
Dr. T. Wesolowski–Département de chimie physique, Université de Genève

It is clear today that computational chemistry plays an increasing role in the modelling of complex systems, with applications such as *rational drug design, selection and synthesis of new materials, design of new catalysts, and modelling of the environment*. In this context, quantum chemistry is the method of choice when information related to electronic structure is required or, more generally, when parameters of classical methods are not available. However, in computational quantum chemistry, it is undoubtedly much easier to perform realistic modellizations for organic than for inorganic compounds [1]. It is indeed by no means an easy task to carry out state of the art *ab initio* quantum chemical calculations on transition metal complexes, mainly for the following reasons : (i) a significant amount of electron correlation must be introduced; (ii) multiplet structure effects can in general not be ignored; (iii) large one-electron basis sets must be used, which significantly increases the computational effort [2]. This explains why, in spite of the spectacular development of computer hardware, high-level *ab initio* investigations of realistic transition metal systems are still rather scarce. It is therefore not surprising that alternatives to the *ab initio* techniques are widely used for transition metal complexes. These are essentially of two types.

First, *semi-empirical methods*, such as the extended-Hückel (EH) model [3], have been extensively used for calculations of electronic structures and, provided an additional account is made of interatomic repulsions [4, 5], of molecular geometries. In addition, the EH wavefunctions and energies are useful to carry out more detailed investigations of the chemical bonding and reactivity of the species using the following techniques : *fragment analysis* [6], *second-order perturbation theory* [7] or *reaction potentials* [8]. Other semi-empirical schemes are also available for transition metal complexes, such as ZINDO [9], or PRDDO [10].

The second alternative concerns methods based on *density functional theory* (DFT) which have made a remarkable breakthrough in computational quantum chemistry during the last few years [11, 12]. With the introduction of so-called non-local gradient corrections to the (local) exchange and correlation functionals used previously, they are able to lead to an accuracy comparable to that obtained in *ab initio* calculations performed at the Hartree-Fock plus second-order Møller-Plesset (MP2) perturbation level [13], though requiring a significantly reduced computational effort. Actually, DFT methods have become *de facto* the standard techniques for routine modelling of coordination compounds, organometallic and inorganic systems such as clusters, catalysts, new materials, etc.

Important developments have been also performed in the field of *the first-principles molecular dynamics* (MD) method proposed by Car and Parrinello [14], which basically allows the user to carry out quantum (DFT) MD simulations at temperatures above 0 K. Indeed, this model has recently been successfully applied to systems of great interest in chemistry, namely : the properties of water dimer [15], with possible extension to condensed water, the structure and vibrational frequencies of ferrocene [16], and the physisorption of water on MgO surfaces [17]. In spite of the significant computational effort which is still necessary to perform such MD simulations, there is no doubt that this technique may be considered as a very powerful and promising tool to model the structure and properties of "real" systems.

We incline to think that all the conditions are met today, after long years of intense methodological developments, to carry out reliable and chemically meaningful modellizations of organometallic and inorganic systems. This is the major research topic of our Geneva group and we would like to illustrate it by presenting two applications devoted to large scale calculations performed on CSCS' equipment, and also a methodological development leading to an easier treatment of large systems.

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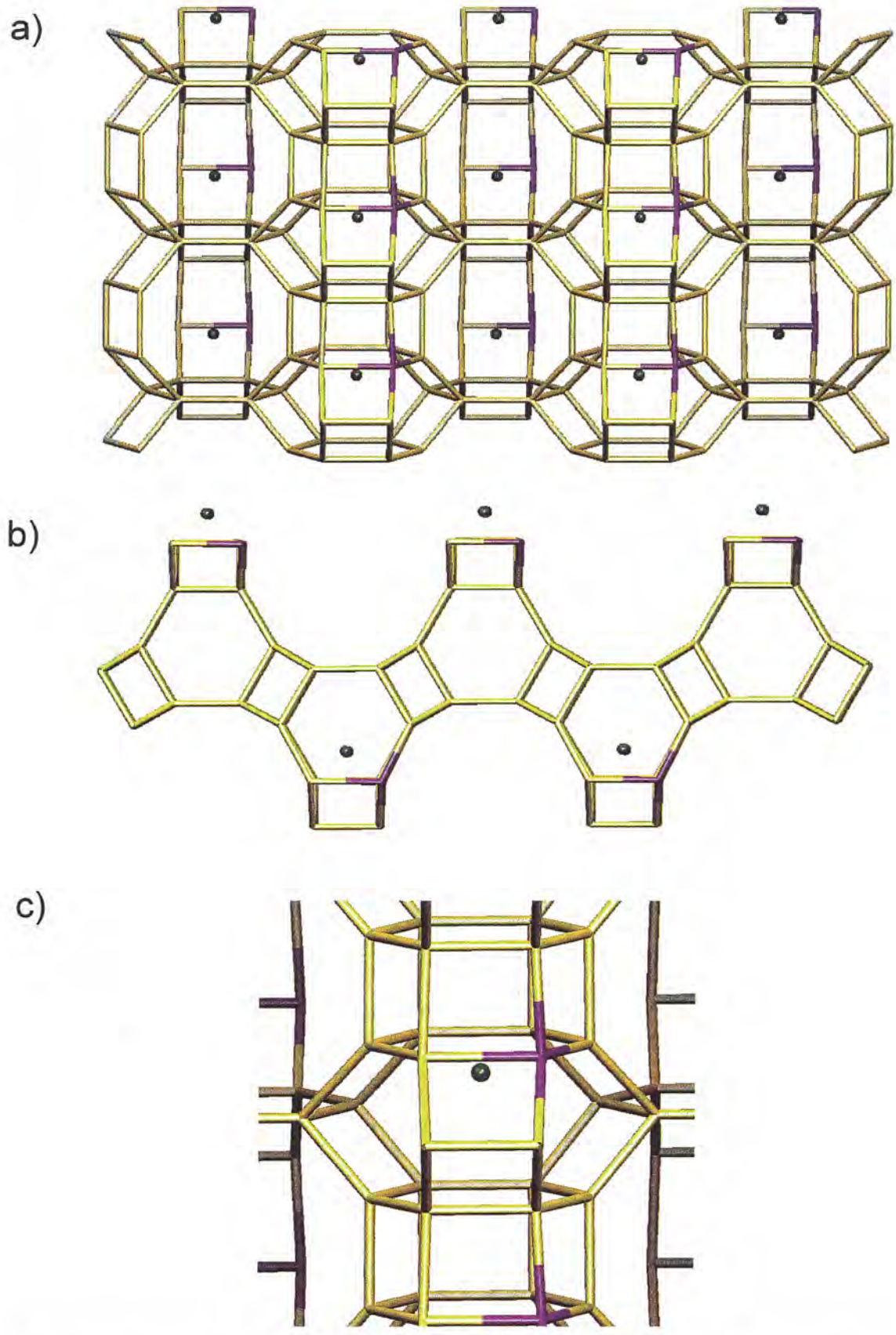

Figure 1: Structure of the most stable H^+ binding site inside the cancrinite cage of offretite. Only silicon (yellow) and Al (purple) atoms of the framework are shown, the oxygen atoms being located approximately halfway between the tetrahedral vertices. Protons are represented by the green spheres. a) Side view. b) Top view. Both a) and b) show several unit cells of offretite. c) Enlarged view of a single cancrinite cage.

First-principles Molecular Dynamics Calculations Performed on Zeolites

Zeolites are microporous aluminosilicate materials which are widely used for hydrocarbon conversion, size and shape selective catalysis, gas separation, ion exchange, sorbing processes, etc. [18]. Zeolites are composed of three dimensional networks of corner sharing TO_4 tetrahedra, where T can be either Si or Al. These tetrahedra give rise to *channels* and *cages*, where positive inorganic or organic ions, counter-balancing the negative charges associated with each AlO_4 unit, are located.

Knowledge of the cation distribution in zeolites is extremely important for understanding their activity. The most widely used charge-balancing counterions are protons, which are known to be firmly bonded to the lone pairs of the bridging oxygen species. These acidic hydroxyl groups play a crucial role in the catalytic activity of zeolites. We have used local density functional theory, within the framework of the Car-Parrinello approach [14], to study the dependence of the acidic properties of a particular zeolite, offretite, on the local atomic structure around the Al centres. Unlike most previous quantum chemical studies on zeolites, which were typically based on cluster models of rather limited size, the full periodicity of the lattice is taken into account in our study. Moreover, all atomic positions are fully relaxed, without constraining some atoms at their experimental geometry, as it is often the case in cluster calculations.

An important result of our work is that there is a strict correlation between the $Si^{4+}/(Al^{3+},H^{+})$ substitution energy and the proton affinity at a given site, the most stable sites being those with the largest proton affinity (lowest acidity). Figure 1 presents several views displaying the most stable H^{+} binding site in such a substituted zeolite. In addition, the most acidic sites appear to be characterized by AlOSi and AlOH bond angles which are larger and smaller than average, respectively. A large AlOSi bond angle is indeed related to a stronger admixture of the O 2*s* orbital into the AlO and SiO bonds, thus implying a weaker (i.e. exhibiting less *s*-character) bond of the bridging oxygen to the proton [19].

As an alternative to proton counterions, monovalent (e.g. Na^{+}, K^{+}), divalent (e.g. Ca^{2+}), or trivalent (e.g. La^{3+}) cations can be incorporated into extra-framework sites of the zeolite, in order to neutralize the negative charge resulting from substitution(s) of Si^{4+} by Al^{3+} ions. These cations are generally found in well-defined locations within the framework. We have investigated the structure and energetics of different $Si^{4+}/(Al^{3+},M^{+})$ substitutions in offretite in the case M^{+}=Na^{+},K^{+}. Our results show that the nature of the counterion has an important influence in determining the relative stability of different binding sites.

For potassium counterions, we find that the preferred site lies inside the so-called cancrinite cage, and corresponds to Al in T_1, which is one of the two inquivalent tetrahedral sites of offretite, and belongs to the hexagonal prism [20]. This result is in complete agreement with crystallographic data and with sorption experiments for offretites with low Al content. Moreover, in the case of K^{+} we find that site selectivity is quite pronounced, as the large size of this cation gives rise to important steric effects in the offretite framework. For Na^{+} counterions, instead, the spread in the relative substitution energies of different binding sites is very small, e.g. there are as much as four low-lying sites within a range of 2.5 kcal/mol. In addition, substitution energies are smaller than in the case of K^{+} counterions. These results are consistent with the experimental fact that offretite cannot be synthesized with Na^{+} cations, the presence of a majority of K^{+} cations being necessary in order to achieve crystallization.

Applications of the PRDDO/M Method to Organometallic Compounds

As stated above, modelling applications of systems containing transition metal centers are the major research topic of our laboratory. To this end, it is important to have at hand a quantum chemical method less demanding in computer time than DFT for geometry optimizations of large systems. Indeed, organometallic compounds present some characteristic features which make them attractive from a chemical point of view, but their large size leads generally to a tremendous computational effort when accurate modelling is needed. This problem may be solved by resorting to semi-empirical quantum chemical methods such as PRDDO/M [10], which may be considered as an approximate *ab initio* Hartree-Fock technique without introducing empirical parameters.

We present here preliminary results obtained for organometallic systems using the PRDDO/M program recently installed on the NEC SX-3 at CSCS. In a first step we have performed some calculations on standard systems in order to test the reliability of the method for the type of compounds we are interested in. Molecules such as ferrocene [$Fe(Cp)_2$], bis(benzene)chromium [$Cr(C_6H_6)_2$] and (η^6-benzene)tricarbonylchromium [$(C_6H_6)Cr(CO)_3$] have been chosen. The results obtained for the geometries are quite reasonable when compared with experimental values, i.e. the error bars on bond distances lie in a range of 0.02-0.08 Å, the corresponding values for bond angles being 2-5°.

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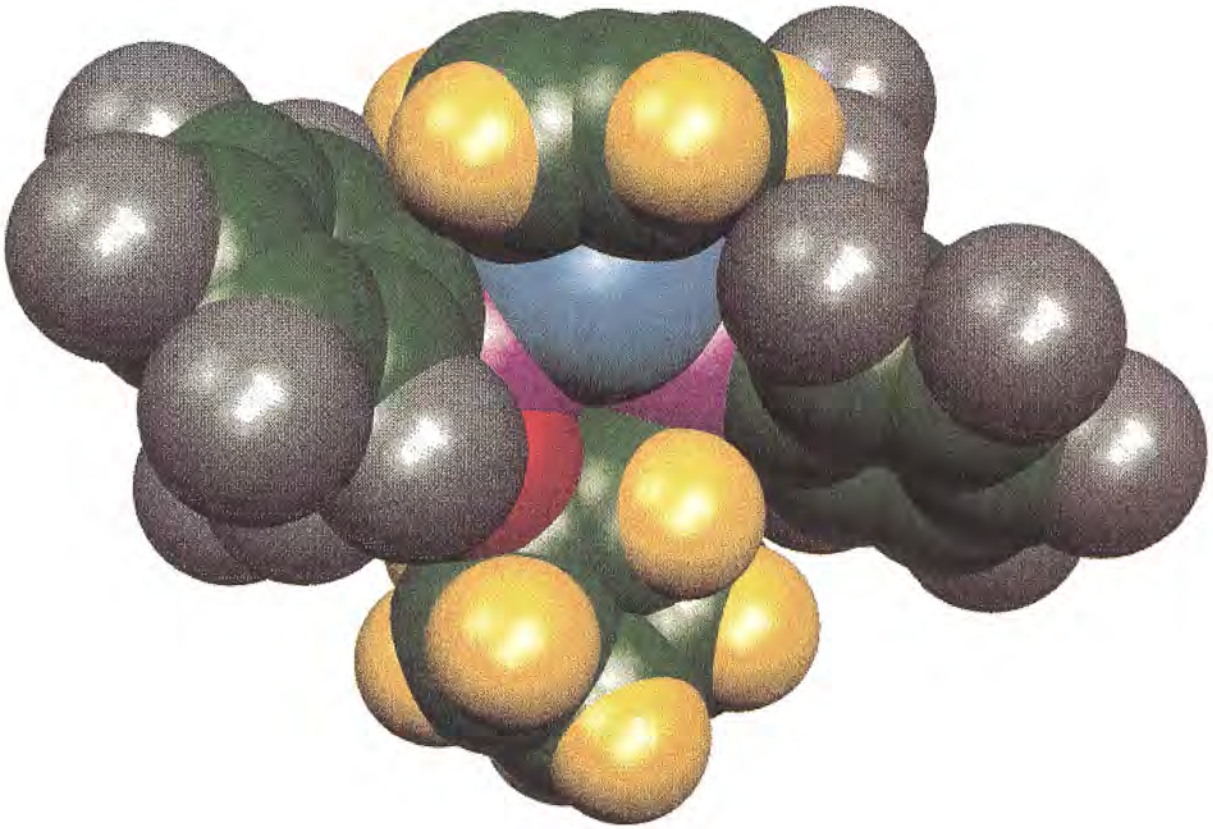

Figure 2: Space-filling model of the chiral Lewis acid $[Cp(C_5H_8(OP(C_6F_5)_2)_2)Fe]^+$ Color coding of the atoms: blue Fe; purple P; grey F; red O; green C; yellow H.

These encouraging results prompted us to turn to larger systems for which modelling studies are required, namely Fe(II)-based Lewis acids synthesized in the laboratory of Prof. E.P. Kündig at the University of Geneva. Indeed, these compounds have been shown to play a crucial role in the catalysis of enantioselective Diels-Alder reactions between dienes and dienophiles [21]. The purpose of the modelling studies is to rationalize the enantioselective catalytic reaction mechanism by predicting the geometry of the transition state in these reactions, which could lead to the design of better catalysts for this important chemical process. Figure 2 presents a molecular model of the chiral Lewis acid $[Cp(C_5H_8(OP(C_6F_5)_2)_2)Fe]^+$ which depicts clearly the cavity with the vacant complexation site able to host the prospective reactants. The first results obtained using PRDDO/M method for these systems indicate that this technique is able to lead to realistic results.

Applications of the Kohn-Sham Equations with Constrained Electron Density

We are also working on a new formalism for obtaining the ground-state energy and electron density of large systems, such as macromolecules or compounds in solution. These methodological developments are based on density functional theory and consist of partitioning the electron density ρ of a system in two parts, ρ_1 and ρ_2 such as $\rho = \rho_1 + \rho_2$, one of them (ρ_2) being temporarily frozen while the other one (ρ_1) is calculated in a self consistent procedure (SCF) [22]. The equations used for obtaining the non-frozen electron density are indeed solved in a self consistent way similar to that used in the standard Kohn-Sham DFT procedure. This approach is computationally advantageous when compared to a quantum mechanical treatment of the whole complex. Recently, we developed a computational procedure that allows the frozen electron density to relax in a series of iterations [23] (Figure 3). The initial stage of the implementation of this ➔

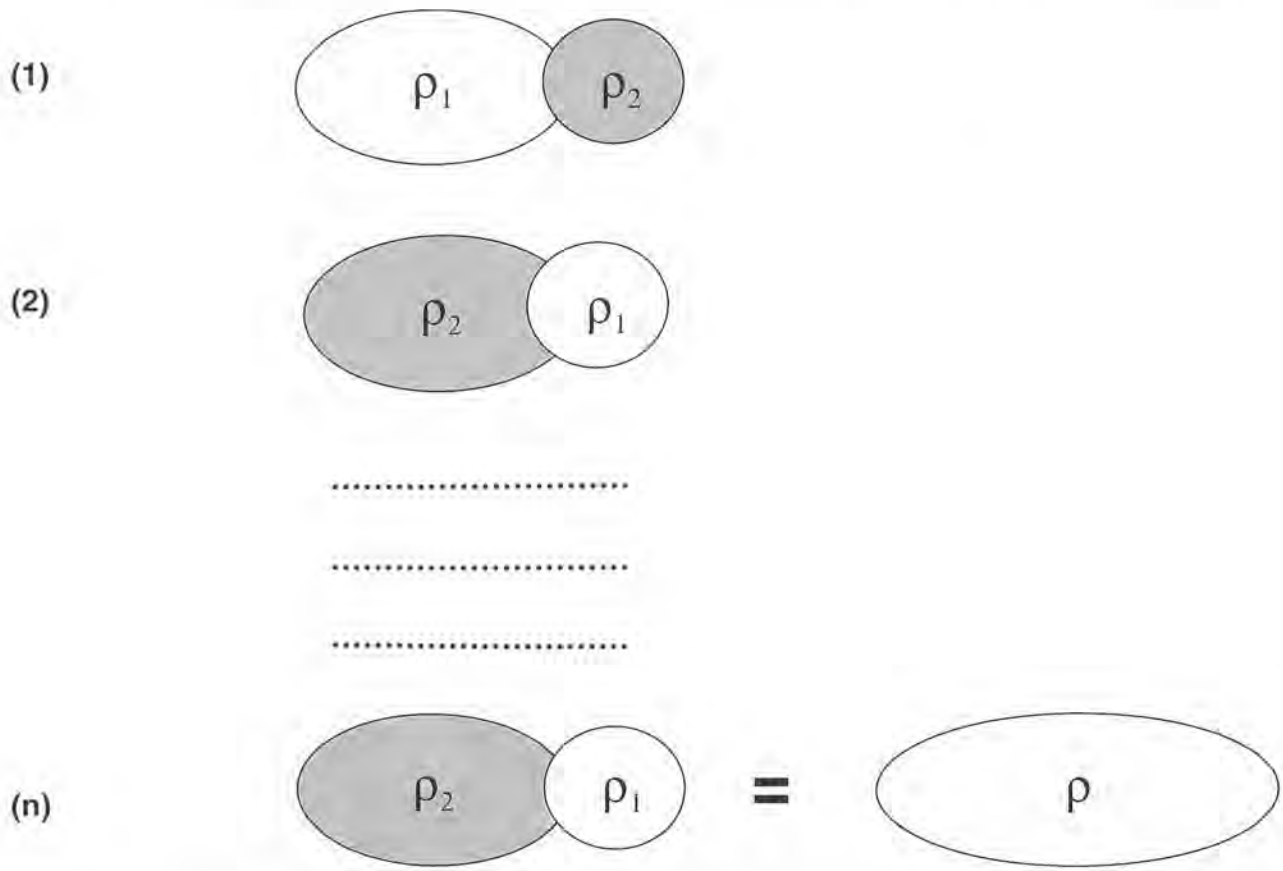

Figure 3: Iterative evaluation of the electron density $\rho = \rho_1 + \rho_2$ of a large system obtained by the constrained electron density approach. At each step, ρ_1 (white) is calculated using the SCF Kohn-Sham procedure while ρ_2 (grey) is kept frozen. Consecutive iteration steps allow to interchange ρ_1 and ρ_2. At the end of the procedure, the results are equivalent to those obtained by SCF treatment of ρ itself (supermolecule approach).

formalism into the standard DFT based program *deMon* has been completed. The fundamental issue of this approach concerning the approximate kinetic energy functional together with its functional derivative has been addressed [24]. The studies of model weak complexes (H_2..NCH, HF..NCH, and N_2..CO) lead to a very good agreement between the ground state electron densities obtained using the standard DFT based approach for the whole system and the present approach used iteratively for individual molecules forming a complex. Larger molecular complexes are currently being studied in our laboratory.

As a conclusion, there is little doubt that the progresses recently achieved in advanced computational chemistry techniques will lead to a more realistic modelling of systems with a large number of particles and components, such as inorganic and organometallic compounds, chemisorbed species on surfaces, solid materials, and biological macromolecules.

Acknowledgements

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Prof. Themistocles Dracos– Institut für Hydromechanik und Wasserwitschaft, ETHZ. (Direct Numerical Simulation of a Turbulent Open Channel Flow, page 42).

With a background in civil engineering, Professor Dracos was appointed ordinary professor at ETHZ in 1979. He worked as Head of the department for civil engineering, head of the "Institut für Hydromechanik und Wasserwirtschaft" and as member of the following committees: Aufnahmeprüfungskommission, Forschungskommission, and Dozentenkommission (president).

Q: What impact does high-performance computing currently have on your research activities?

A: The flow of viscous fluids at sufficiently high Reynolds numbers is turbulent. It can be described by a set of non-linear equations called the Navier-Stokes equations. The analytical solutions of these equations cannot be found for such kind of flows whose characteristic is the unpredictability. The high-performance computers made it however possible to numerically solve these equations for moderate Reynolds numbers and simple geometries. This enabled the study of turbulent flows by performing numerical experiments with a large number of realisations of the flow field. High-performance computing in many cases replaces the physical experiments and becomes an indispensable tool complementing the physical experiments in turbulence research.

Q: Do you have a vision regarding how your research area and high-performance computing will evolve in the future? If so, please describe your vision:

A: Turbulent flows have a large spectrum of scales which becomes broader with increasing Reynolds number. With the existing computing capabilities, the spectrum one can resolve extends a little bit more than two decades. This is not yet sufficient for a complete statistical analysis of the flow. The hope is that the rapidly increasing performance of computers will allow to extend this range to at least three decades. The increase of the computing performance will also hopefully allow to perform computing for more complicated geometries. This may open the way for the application of direct numerical simulations of turbulent flows to solve real-life problems.

Q: Does CSCS meet your expectations of a high-performance computing center?

A: The high-performance of the center made it possible to compute a turbulent channel flow with high temporal and spatial resolution for a Reynolds number which is still moderate but high enough to ensure that turbulence is well developed. However this project already reaches the computing limits of the center. This is typical of this kind of problems and most probably will be the case also for the next generation of computers, as the need for memory space and for increased computational speed increases nearly with the third power of the Reynolds number.

Q: What do you find of particular value at CSCS?

A: During the period of our cooperation with CSCS, which extends to about one and a half years we could follow how the services of the

centre have been continuously improved. We especially appreciate the help of the group helping to optimising the codes, which is of great value when PhD students are involved.

Q: What do you think should be improved at CSCS?

A: Although the electronic mail makes communication and cooperation over long distance easy, we sometimes miss the possibility of personal contact with CSCS staff. This is mainly due to the remote location of the center which has no connection to the main public transportation lines.

Q: Please comment on the relationship between your research team and CSCS staff.

A: We want to thank CSCS staff for their help and the good cooperation which runs with a minimum of bureaucratic work.

Direct Numerical Simulation of a Turbulent Open Channel Flow

RESPONSIBLE INSTITUTE:
Institut für Hydromechanik und Wasserwirtschaft, ETHZ

PROJECT LEADER:
Prof. T. Dracos–Institut für Hydromechanik und Wasserwirtschaft, ETHZ

INVOLVED PERSONS:
H. Merava–Civil Engineering Faculty, Slovak Technical University Bratislava (Slovakia)

Introduction

Numerical modelling is one of the possible approaches for investigating turbulence. The basic governing equations for turbulent flow modelling are the continuity equation and the Navier-Stokes equations. To solve this nonlinear system of partial differential equations analytically is, except for very simple cases, impossible. Recently, the direct numerical simulation became a promising approach for turbulent flow calculation. This method incorporates the solution of time-dependent three-dimensional Navier-Stokes equations directly without usage of any turbulence models, and all essential flow field scales are resolved on the computational grid. To be able to resolve the smallest turbulence scales, the computational grid resolution has to be high enough, and appropriate numerical methods have to be employed. For their high convergence rate and accuracy, spectral methods are frequently used for this kind of calculations. The solution is represented in space in terms of orthogonal function series, mostly Fourier series and Chebychev polynomials. To optimise the performance of the algorithm, some of the operations are carried out in physical space. This methods, called pseudospectral, involve therefore numerous transformations from Fourier to physical space and backwards and are still quite time consuming. The time advancement of the solution is usually carried out by a finite difference method. To ensure numerical stability of difference methods, the integration time step has to be kept small, so the computation has to be continued for a large number of time steps. That is why the direct numerical simulation became feasible only with the advent of high-speed and large-memory computers. Even the capability of supercomputers is sufficient only to simulate turbulent flows at moderate Reynolds numbers.

Problem Definition

The aim of the present project was to perform a simulation of a three-dimensional turbulent open channel flow in order to generate a turbulence database. The flow's Reynolds number based on the channel depth and the average velocity is Re=8500. The corresponding Reynolds number based on the channel depth and the wall shear velocity is Re_τ=423. The basic governing equations were solved numerically using a no-slip boundary condition for the bottom of the channel, and the free-slip boundary condition for the surface. Because the flow is assumed to be homogeneous in the streamwise and spanwise directions, periodic boundary conditions were used in these directions. To speed up the first stage of the calculation, the initial condition was a turbulent velocity field obtained from the University of California, Santa Barbara computed for the Reynolds number Re_τ=171.

Numerical Solution

The problem at hand was solved numerically using the Fourier-Chebychev pseudospectral method described. Fourier series were employed in space in the streamwise and spanwise directions, and Chebychev polynomial expansions in the normal direction. The advantage of using Chebychev polynomials in the normal direction is that such a representation gives very good resolution in regions close to the boundaries. For the problem considered the resolution close to the wall is important not only because of the large gradients of the solutions occurring there, but also to be able to investigate the near-wall flow structure. The time advancement was carried out by the Crank-Nicholson scheme for the diffusion terms and by the Adams-Bashforth scheme for the nonlinear terms of the Navier-Stokes equations.

The computational domain size was $4\pi h$ and $2\pi h$ in the streamwise and spanwise directions respectively, and h in the normal direction (h is the depth of the channel). To resolve the smallest turbulence scale, which is the Kolmogorov scale, the necessary spatial grid resolution for our Reynolds number is 256x256x129 modes in the streamwise, spanwise and normal directions respectively. The computational memory requirements for such a grid are 1.2 GB. This requirements could be met by the NEC SX-3, running the code in the dedicated mode. The direct numerical simulation of fully developed turbulent flow has to be →

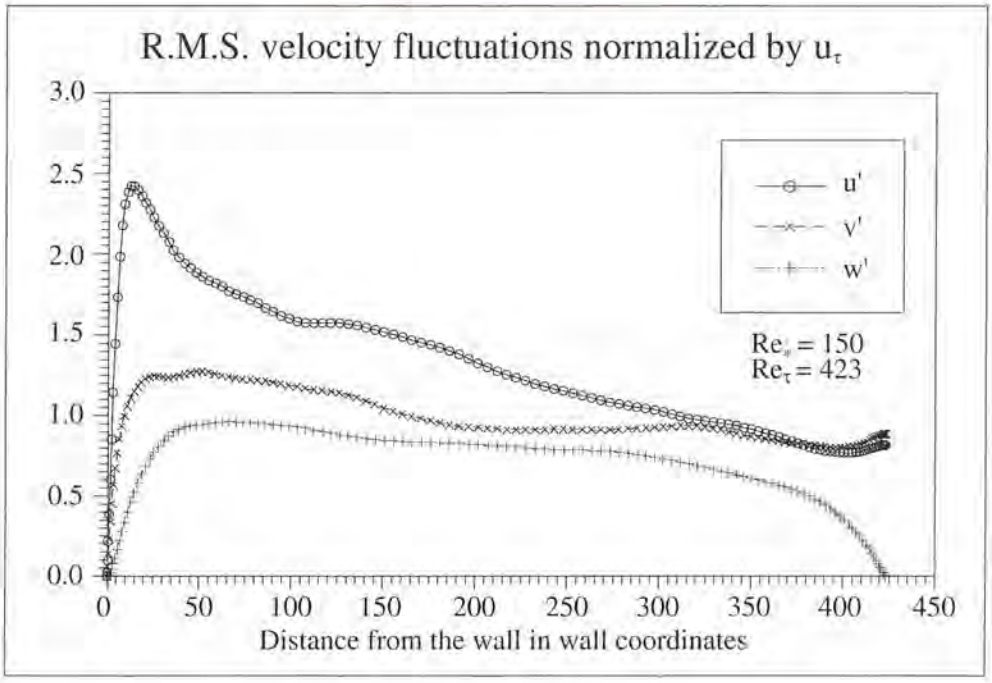

Figure 1: Distribution of turbulence intensities normalized by u_τ.

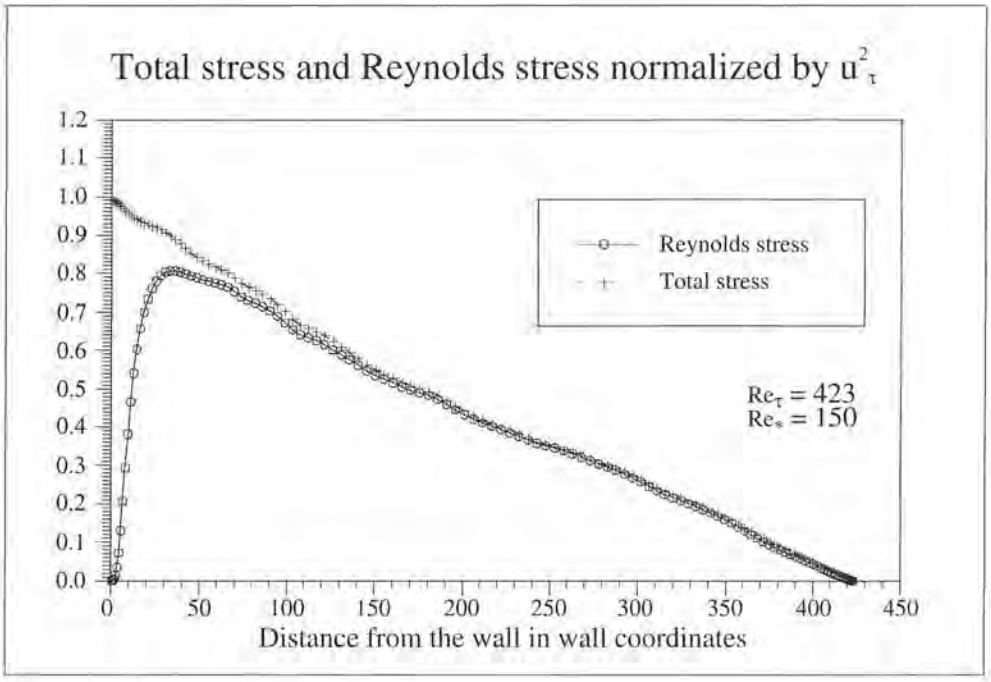

Figure 2: Shear stress profiles.

performed in two basic steps. First the statistically steady state has to be reached, then the computation is continued for additional time steps to store the results in the database. The statistical stability is indicated by a stable distribution of the turbulence intensities, and a linear shear stress profile. This profiles are shown in Figures 1 and 2. Because of using pseudospectral method, most of the computational time is spent by Fourier transforms. To speed up the computations, the original code was optimised at CSCS, and the NEC SX-3 scientific library Fast Fourier Transform routines were utilised. The speed of execution of the code increased this way by about a factor of 10, and the achieved final performance was about 1.1 GFLOPS.

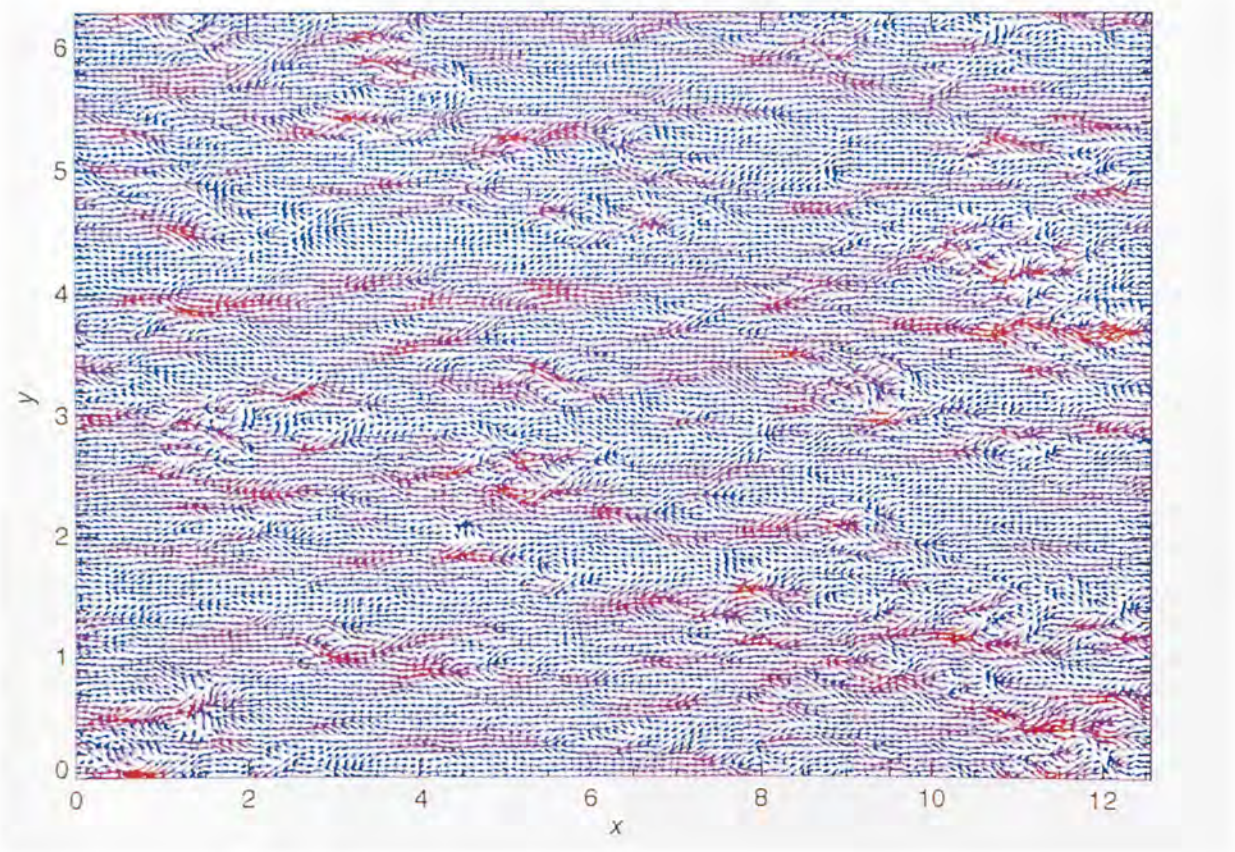

Figure 3: Shear stress distribution on the wall.

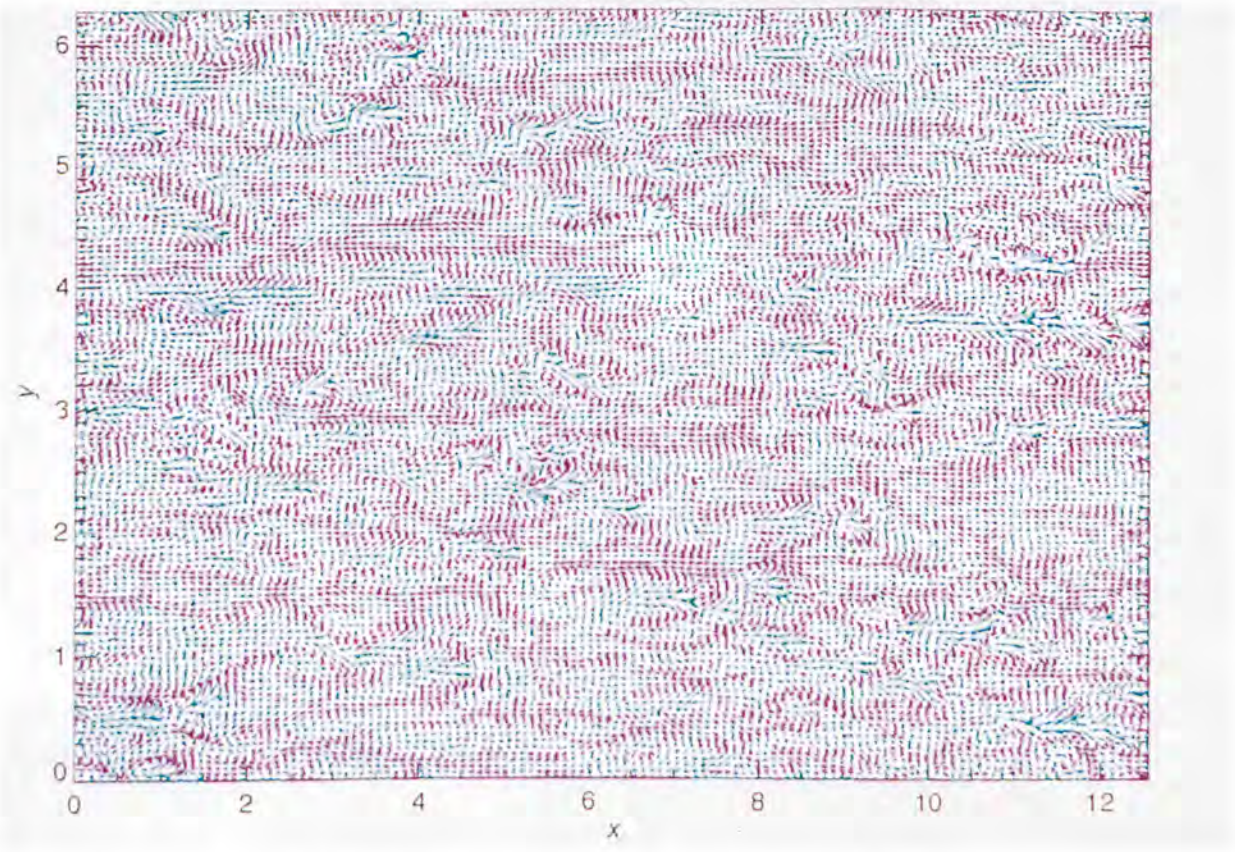

Figure 4: Distribution of velocity fluctuations on the plane at the distance of 5 wall units.

Results

We present the results obtained from the direct numerical simulation stored in a database in context with the investigation of incipient motion of sediments at the bottom of the channel. The instantaneous wall shear stress distribution is computed and compared to velocity and vorticity distributions on levels at a distance of 5 and 15 wall units from the bottom.

In Figure 3 we show the shear stress distribution on the wall, in Figure 4 the distribution of the velocity fluctuations on the plane at the distance of 5 wall units. Events observed in the bottom shear stress distribution show good agreement with the events in the velocity distribution. Similar correlation is gained also for vorticity. Good agreement between the events in the wall shear stress distribution and the velocity and vorticity distribution at a distance of 15 wall units from the wall can be shown, too. This analysis gives us better insight into the processes near the boundary of the open channel and can improve understanding the near-wall turbulence phenomena.

Outlook

Databases can contribute to increase understanding turbulence, and they have proved to be an effective research tool. They provide instantaneous velocity and pressure fields in three-dimensional space. Their advantage in comparison to experimental results, where the resolution is often low, is that the flow can be analysed without any extrapolations from incomplete data. There are different possibilities to use the data provided by a turbulence database, e.g.:

- investigation of the geometry of the flow,
- examination of turbulence structures,
- particle tracking,
- flow visualisation,
- calibration of experimental measurements.

The database will be put to disposal of the ERCOFTAC SWISS "EULER CENTER" and it can serve as a basis for future turbulence research for Swiss and foreign scientists as well.

Acknowledgements

We would like to thank Professor Paul Rys from the Laboratory of Technical Chemistry, Swiss Federal Institute of Technology, and to the staff of the Swiss Scientific Computing Center in Manno for their support. The project was supported by the Swiss National Science Foundation.

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Dr. Anthony Cooper–
CRPP-EPFL
(Computation of Stellarator Coils, Equilibrium and Stability, page 48).

Dr. Anthony Cooper was born in Valparaiso, Chile in 1950. He received a PhD degree in Nuclear Science from the University of Michigan, Ann Arbor (U. S. A.) in 1979 and was employed at the Oak Ridge National Laboratory from 1980 to 1986. Since 1986 he has been at the Centre de Recherches en Physique des Plasmas (CRPP) of the EPFL in Lausanne. He has concentrated his work on the investigation of the magnetohydrodynamic (MHD) equilibrium and stability of three dimensional (3D) magnetic fusion plasma confinement configurations. He was a partner in the team that developed the 3D ideal MHD stability code TERPSICHORE that won Cray Gigaflop Performance Awards in 1989 and 1990.
His present interests focus on the identification and the development of 3D vacuum magnetic confinement configurations that could offer optimal properties with respect to ideal MHD stability.

Q: What impact does high-performance computing currently have on your research activities?

A: High-performance computing plays a vital and indispensable part of our efforts in Fusion Energy Research. Without it, the level of knowledge and understanding we have achieved would be unattainable.

Q: Do you have a vision regarding how your research area and high-performance computing will evolve in the future? If so, please describe your vision:

A: In the future, high-performance computing as it evolves should allow us to examine more diverse magnetic fusion confinement configurations and to apply more rigourous and sophisticated physical models with the increased resolution that such models require.

Q: Does CSCS meet your expectations of a high-performance computing center?

A: CSCS has provided us with the means to achieve in our computational efforts so far the targets we have set ourselves in our research activities. With this, we believe that we lead the world in the domains we concentrate on despite much more limited manpower resources.

Q: What do you find of particular value at CSCS?

A: It has been our experience that the CSCS system management has been to date very attentive to listen to our suggestions and to accommodate our requests. We have appreciated the availability of CSCS staff to assist us when we have encountered problems and difficulties. We hope that this continues in the future.

Q: What do you think should be improved at CSCS?

A: In our past work on other supercomputer systems, we have generally been able to store massive amounts of data that have resulted from our calculations. The limited amount of storage capacity at CSCS caused at first difficulties in our modus operandi. But we have come to realize that because we consult back to only a small fraction of the data we have generated, it is acceptable to store just the much more compact essential input data and rerun cases that need to be re-evaluated. This may in fact be more cost effective in the long run. Our calculations tend to use a lot of memory and generate a lot of data with modest CPU consumption.

Q: Please comment on the relationship between your research team and CSCS staff.

A: We have maintained a very close working collaboration with CSCS staff. Our successes so far are in many ways attributable to the advice and help we have received specifically from Mauro Ballabio through his efforts to port and optimize the programmes we run on CSCS computers.

Computation of Stellarator Coils, Equilibrium and Stability

RESPONSIBLE INSTITUTE:
CRPP-EPFL, Association Euratom-Confédération Suisse

PROJECT LEADER:
Dr. W. A. Cooper–CRPP-EPFL, Association Euratom-Confédération Suisse

INVOLVED PERSONS:
M. Ballabio–CSCS
Dr. R. Gruber–CSCS
P. Merkel–MPIPP-Euratom Association (Germany)

1. Scientific Part

The stellarator concept is one important branch of achieving toroidal magnetic confinement for nuclear fusion. Stellarator design has undergone a deep change recently. The geometry of coils generating a stellarator confinement region is no longer considered to be the basic starting point for investigating physics properties. Rather, stellarator optimization which is indispensable for the viability of stellarators as reactors is more adequately performed with the geometry of the plasma boundary determining the properties of the confinement region. This approach requires—after having obtained an optimal confinement region—the computation of coils generating this confinement region. This task is performed with the NESCOIL code which—in particular—computes a modular coil set. Finding optimal coils constitutes a second intricate optimization task with NESCOIL as its basic tool and has to take into account a large variety of physical and technical constraints.

The stellarator Wendelstein 7-X proposed by IPP as a European stellarator project was designed as described above. As an experimental project it needs a meaningful flexibility of its magnetic configuration. For this purpose not only a single modular coil set was designed but a second modular system with a smaller number of coils and smaller currents in them will be superimposed to achieve this flexibility. With respect to these two coils systems it is desirable to answer a number of detailed questions to corroborate the options considered so far and to investigate possibilities for worthwhile improvements.

The free-boundary NEMEC (= VMEC + NESTOR) code is to be employed to determine three-dimensional (3D) magnetohydrodynamic (MHD) equilibria with nested magnetic flux surfaces of the configurations that result from the optimisation procedure of the NESCOIL code. The linear ideal MHD stability to local and global external modes of the equilibria obtained with VMEC are computed with the TERPSICHORE code.

Convergence difficulties of the equilibrium code for some classes of configurations motivate the development of a new 3D finite element code. In collaboration with CSCS, the code CLIO-3D is under construction.

2. Numerical Part

NESCOIL code (developed at IPP): Coil optimization by minimizing a functional with nonlinear constraints in combination with the solution of a Neumann boundary value problem. It is a highly efficient vectorized code with extremely long vectors and employs a NAG optimization routine.

NEMEC: VMEC code developed at the Oak Ridge National Laboratory, NESTOR code developed at IPP. NEMEC is well tested and highly vectorised.

TERPSICHORE code developed at EPFL. It is vectorised and parallelised very efficiently. Was a Cray Gigaflop Performance Award winner in 1989 and 1990.

All these codes are written in FORTRAN.

A new 3D finite element equilibrium code is to be developed.

3. Technical Part

1) **Computers to be Used:** NEC SX-3 because of the structure of the NESCOIL code and because TERPSICHORE requires large memory.
2) **CPU Time Required:** In 1994 the NESCOIL code was installed on the NEC SX-3 and achieved 1.5 GFLOPS. Thus, a typical production run takes of the order of one hour. About 30 production runs per month appear to be adequate, so 30 hours per month are needed.
   For each configuration identified with NESCOIL, we would calculate on average 4 equilibria with NEMEC at 6 minutes per run. This corresponds to 12 hours per month.
   In the Wendelstein 7-X configuration, there are 2 independent families of modes that can become unsta- →

ble. Thus 2 computations would be performed with TERPSICHORE at 3 minutes per run for each equilibrium calculation. This amounts to 12 hours per month. TERPSICHORE achieves typically 1.5-1.6 GFLOPS on one processor of the SX-3.
We estimate an additional 4 hours per month for the development of the new 3D equilibrium code. Therefore, the total request is 60 hours per month for 10 months out of a year (≡ 2 months are allotted to holidays and conference participations).

3) **Memory Requirements**: Small central memory (32 Mbytes) and no disk space needed for NESCOIL and VMEC. TERPSICHORE production runs require at least 256 Mbytes. Selected runs may require up to 800 Mbytes.
4) **I/O Charge, Graphics:** Very little I/O load. Visualization of coils for example with BASPL.

4. Abstract

4.1 Objectives of Wendelstein VII-X

Wendelstein VII-X is a research project of the Max-Planck-Institut für Plasmaphysik in Garching, Germany, for the realization of toroidal magnetic fusion. The project is in the final phase of European and national approval and is to be built in Greifswald at the Baltic sea. The overall goal of Wendelstein VII-X is progress in the understanding of physics and engineering relevant to stellarator fusion plasmas. Generally, stellarators are considered the leading alternative to tokamaks when recalling obvious inherent potential physics advantages: stationarity since the equilibrium does not rely on a net toroidal plasma current, no danger of disruptions for the same reason, less free energy because of the external generation of the entire confining field. The configuration selected for Wendelstein VII-X will be of the Helias type (HELIcal Advanced Stellarator) which is a toroidal plasma equilibrium with appropriately optimized properties. Added to the general advantages are potential engineering advantages resulting from the possibility for only one single coil system for generating the entire confining magnetic field. Furthermore, experimentation with Wendelstein VII-X and comparison of the results with those of tokamaks will allow investigations on the influence on transport of net toroidal plasma currents and of the different behaviour of trapped particle orbits so that Wendelstein VII-X may foster deeper understanding of toroidal magnetic confinement in general.

4.2 Selection of the Wendelstein VII-X Magnetic Configuration

The optimization of stellarator configurations was carried out with respect to the following set of criteria:

- high quality of vacuum-field magnetic surfaces (regular boundary, avoidance of low-order rational values of twist (or rotational transform) ι ('resonances'), adjustment of the shear, sufficiently small thickness of islands)
- good finite-β equilibrium properties (small shift of the magnetic axis [Shafranov shift], small change of ι with β at fixed external currents)
- good MHD stability properties (stability with respect to local resistive interchanges and ideal ballooning at $\langle\beta\rangle \approx 0.05$)
- small neoclassical transport in the $1/\nu$-regime (equivalent ripple $\delta_{\iota} \leq 0.02$)
- small bootstrap current in the lmfp-regime (ratio of bootstrap current in a stellarator to the bootstrap current in a tokamak with same aspect ratio and rotational transform, $I_{BS,stel} \leq 0.1\, I_{BS,tok}$)
- good collisionless α-particle containment at operational values of β (fractional prompt loss < 0.1)
- good modular coil feasibility (sufficiently large distance between coils and plasma, and a sufficiently small coil curvature)

The small axis shift and the small change of rotational transform and shear with increasing plasma pressure are a consequence of the achieved small parallel current density,

$$\left\langle j_{\parallel}^2 / j_{\perp}^2 \right\rangle \leq \frac{1}{2} .$$

More generally, compatibility and simultaneous achievement of all of the above criteria has been proven; in particular, the goals concerning the neoclassical behaviour have been surpassed. The nature of the optimization result can be characterized as follows:

The simultaneous achievement of the above set of criteria essentially determines the structure of the magnetic field strength distribution of the configuration, and its geometrical shape is then a consequence of this structure.

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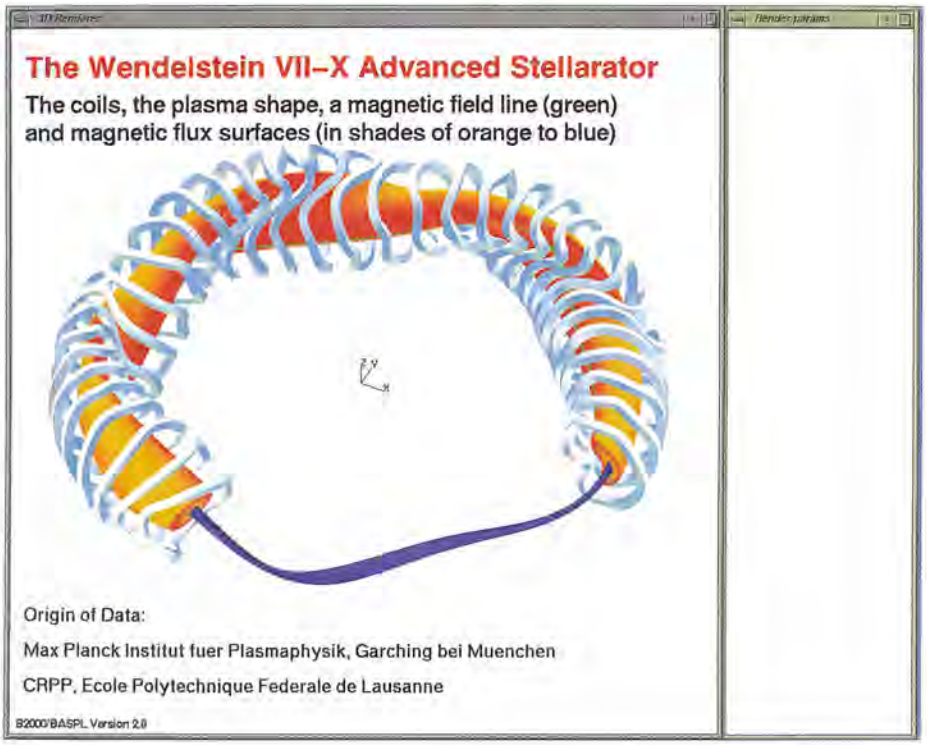

Figure 1: Sketch of Wendelstein VII-X basic configuration. Shown are three and a half periods of the plasma boundary (in orange), the kidney-shaped cross-section at the position of strongest plasma-column curvature, the triangular cross-section at the position of smallest plasma-column curvature, one and a half periods of the helix-like magnetic axis (in blue), a field line on the plasma boundary (in green), 36 of the 50 modular coils (in grey).

While the optimization only takes into consideration classical physics goals it also results in very interesting and desirable perspectives as far as anomalous transport is concerned: many conjectured mechanisms for exciting anomalous transport (stochasticity in vacuum and finite-β fields, trapped orbits, instabilities such as ballooning, tearing and trapped-particle drift modes) are reduced substantially. In addition, the observed potential of stably operating a stellarator at unusually high densities, with the confinement time found to increase with density, is another route to increase confinement.

As the result of the optimization Wendelstein VII-X will realize a 5-period Helias configuration. A sketch of the configuration is displayed in Figure 1.

4.3 Theory of Coils for Wendelstein VII-X

Finding the coils for a given plasma boundary constitutes a mathematically ill-posed problem in the sense that—as an elliptic Neumann problem at the plasma boundary—it cannot be solved as an initial value problem. While the relevant technique was developed relatively early for tokamaks the appropriate procedure for stellarators came relatively late. It of course depends on the type of configuration considered whether a *modular* realization—i.e., with coils closed along the short way around the torus—is appropriate. The geometry of optimized stellarators—viz. their not very tight aspect ratio per period and their indentation being not extended over the full length of a period—is well suited to modular realization.

With the solution of the Neumann problem as a basic step, an optimization procedure for the coils has been devised. In optimizations of the W7—X coil system till now the following six constraints have been considered: i) distances plasma to coils, ii) local coil curvature limit, iii) plasma-divertor distances, iv) coil-to-coil distances, v) average coil curvature limit, vi) circumferences of the coils. The last of these constraints is directly related to the magnetic energy of the coil system and, therefore, to the cost.

As a result of these optimizations the confining magnetic field of Wendelstein VII-X will consist of 50 non-planar coils, 10 per field period. There are only five geometrically different coil types. A system of 20 superimposed planar coils, four per field period, allows—for example—variation of the rotational transform by ± 0.2. Separate current feeds (five in total) to the groups of ten equivalent coils allow modification of the mirror field along the magnetic axis by up to 0.1.

→

As far as the technical realization is concerned the magnet will consist of *superconducting* coils and constitutes the major technical component of the overall device.

5. Realization of a MHD Programs Environment

The intensive collaboration between CSCS-ETHZ, CRPP-EPFL and MPIPP-Garching during the last two years, gave the possibility to collect a large number of MHD codes and let them run on the same platform. All codes have been ported on the NEC SX-3/24R and some of them also highly optimized. A very important effort has been given on the interaction between different (in terms of implementation) codes but with the same functionality. The MEMCOM system has been chosen to have the possibility to share, manage and visualise data in a simple and efficient way. Figure 2 shows the whole codes collection, integrated in MEMCOM.

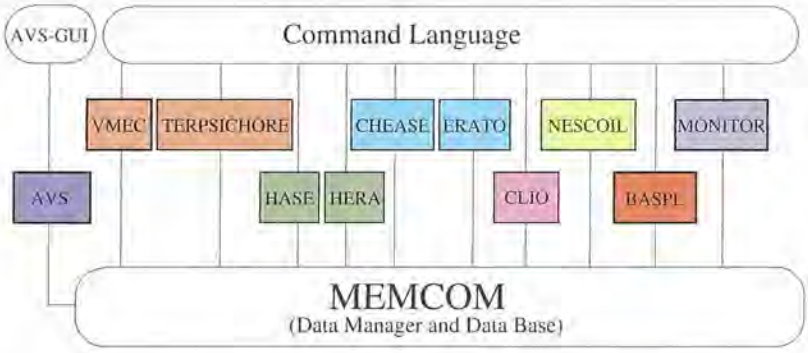

Figure 2: The MHD Programs Environment.

The existing MHD-codes can be essentially divided in 3 major domains:

- *plasma equilibrium* (CLIO, CHEASE, HASE, VMEC)
- *plasma stability* (ERATO, HERA, TERPSICHORE)
- *coil generation* (NESCOIL).

Typically equilibrium and stability codes are coupled together to build a solid and consistent stand-alone unit, as previously shown in Figure 2. The MHD Programs Environment offers now a good and efficient way to overcome the stand-alone problem of these codes and also could be used for the validation of part of them. For instance it is possible to compare results coming from the "standard" VMEC/TERPSICHORE package with those coming from VMEC/HERA. Or it is also possible to subdivide a module into different modules and substitute some of them with own generated modules.

Table 1 shows type, name and authors of the codes integrated in the environment.

All these codes can actually be executed on the SX-3. Some of them have been highly optimized to achieve the highest possible performance. We could achieve a top performance of 1.4 GFLOPS for a test case with NESCOIL and up to 1.6 GFLOPS for a test case with VMEC-TERPSICHORE. The maximum effort has been put on these 3 codes, because they are the most time (and memory) consuming. The remaining codes need only few minutes of CPU time and can reach up to 600 MFLOPS.

Graphical results can be directly produced by using a MEMCOM-integrated graphical system (BASPL) or by an AVS graphical user interface, that includes a special written module to read MEMCOM databases. Since some codes required special plotting libraries, which are not present on the SX-3, a SX-3 graphical library based on PHIGS has been realized to overcome this problem. The main advantage by using this library is that the computational part, usually done in batch mode via NQS, is fully separated from the graphical/interactive part.

It's probably the first time that so many MHD codes are present on a same platform. This could be a very good starting point for the development of new codes, which can be validated also by using some of the existing codes.

Type	Name	Author(s)
Helical equilibrium	HASE	P. Merkel, J. Nührenberg
Helical stability	HERA	D. Berger, R. Gruber, F. Troyon
3D ideal MHD equilibrium	VMEC	S. Hirshman, W.A. Cooper, R. Gruber, U. Schwenn, D.V. Anderson
3D ideal MHD stability	TERPSICHORE	S. Hirshman, W.A. Cooper, R. Gruber, U. Schwenn, D.V. Anderson
Coils optimisation	NESCOIL	P. Merkel
Asymmetric Tokamak equilibrium with X-points	CLIO	S. Semenzato
Cubic Hermite Element Axisymmetric Equilibrium	CHEASE	H. Lutjens
2D ideal MHD stability	ERATO	R. Gruber, F. Troyon, S. Gelato, A.Roy

Table 1: Integrated codes in the MHDPE.

Stefan Dangel–Physik-Institut, Universität Zürich.
(Nonlinear Dynamics of Laser Beams Interacting with Sodium Atoms, page 54).

Grown up in Pfaffhausen, Stefan Dangel studied Physics at the University of Zurich, conducting his Diploma work with Dr. R. Holzner under Prof. E. Brun in the Laser Laboratory.
He is currently working on his PhD with Dr. R. Holzner under Prof. J. Osterwalder at the University of Zurich.
In his free time, he studies bassoon with André Eichenberger and Manfred Sax, and plays the harp, giving about 30 concerts per year.

Q: What impact does high-performance computing currently have on your research activities?

A: For our research it is important to compare experiment and theory. This way we learn how our system works, we can use results from the experiment to modify the theory, and vice versa. Of course, as we learn more, the theoretical models become more complicated and solving them requires ever larger machines. On the computers we have at our institute, a typical calculation would take about a year to complete—more than we could afford to wait! After all, the best theoretical model is not very useful if you cannot calculate a solution.

Q: Do you have a vision regarding how your research area and high-performance computing will evolve in the future? If so, please describe your vision:

A: Well, as usual: more memory, more speed. Probably custom designed hardware (for one specific task only) and very carefully hand-coded software will play an increasing role, as the hardware reaches physical limits. For example, a dedicated FFT chip could be many times faster than the software used today. However, I would like to quote my grandmother who recently died at age 91 and had always been very interested in science: When confronted with the enormous number of operations per second the SX-3 can handle, she responded with "does mankind really need this?" Probably every researcher should think about this from time to time.

Q: Does CSCS meet your expectations of a high-performance computing center?

A: Oh, yes. The machines are taken care of, and when I need help I get help. What more could one expect ?

Q: What do you find of particular value at CSCS?

A: The Visualization Lab. Since we have three-dimensional and time dependent data, a movie is probably the best way to make it visible.

Q: What do you think should be improved at CSCS?

A: Developing software on the SX-3 is still a nightmare because of the slow turnaround times of the queuing system. I suggest a special queue open for developers only (versus “canned” software users).

Q: Please comment on the relationship between your research team and CSCS staff.

A: The contact with the staff is almost always uncomplicated and efficient. Also, the food at “La Stazione”, often enjoyed together, is excellent!

Nonlinear Dynamics of Laser Beams Interacting with Sodium Atoms

RESPONSIBLE INSTITUTE:
Physik-Institut, Universität Zürich

PROJECT LEADERS:
S. Dangel–Physik-Institut, Universität Zürich
Dr. R. Holzner–Physik-Institut, Universität Zürich

Introduction

The propagation of light through an atomic gas is probably one of the most fundamental interactions of light with matter. If such interactions take place, the optical properties of matter may change which in turn influences the behaviour of the light beam. One such interesting nonlinear matter-light interaction is optical pumping. Hereby circularly polarized light can trap formerly absorbing atoms into a nonabsorbing state. This may enhance the transmittency of the medium for the light beam up to complete transparency. Optical pumping of alkali atoms by polarized laser light causes a variety of other astonishing nonlinear effects, such as the formation of slow moving steep longitudinal intensity gradients ("pumping light fronts"), deflection of copropagating beams ("beam bouncing") [2], highly structured polarization and intensity patterns [5], asymmetry of absorption profiles [6], ring structure formation [7], "beam splitting" [8], "beam switching" [1] and "wire bouncing" [3].

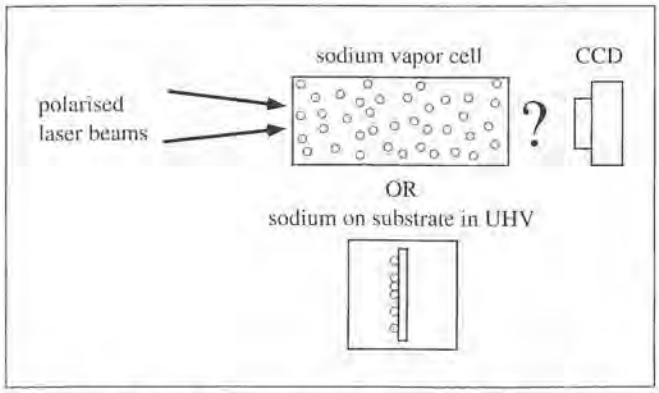

Figure 1: Simplified experimental setup. The laser beams, tuned near the atomic sodium D1-transition, pass through a glass cell filled with sodium vapor and Ar buffergas. The transmitted light is then detected by a CCD camera. For the 2-d experiments, the cell is replaced by a UHV apparatus containing a substrate onto which sodium atoms can be trapped.

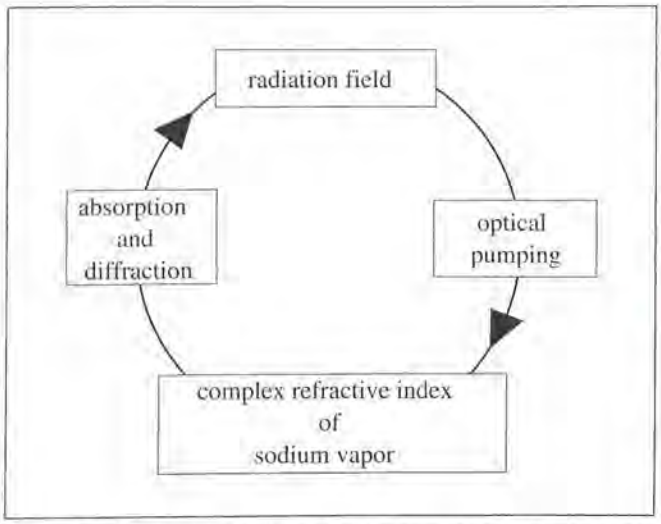

Figure 2: Basic mechanism of the interaction between laser light and sodium atoms.

These effects have been studied experimentally in our laser laboratory at the University of Zurich, using a setup shown in Figure 1. The theoretical description had long been restricted to the steady state (no time dependence). Even though the $J = 1/2$ to $J = 1/2$ approximation of the sodium D1-line had been used (neglecting the hyperfine structure), this old model described the measurements of steady state experiments well. However, when we developed the first time dependent model, we realized that the $J = 1/2$ to $J = 1/2$ approximation is no longer valid and all hyperfine levels must be considered to describe the dynamics of optical pumping correctly. To our knowledge, this current model is the first complete theoretical description of the temporal as well as the full 3-d spatial pattern formation dynamics of laser beams in an alkali vapor.

In late 1994 our group joined the newly formed surface physics group of Prof. J. Osterwalder. Using our combined knowledge, a UHV apparatus was added to our lab, permitting the study of a 2-d gas of sodium atoms on a surface by optical means. The dynamical model has been adapted for this case. Possible applications include a supersmall (on-chip) atomic clock, which would have a considerable impact on e.g. high-speed telecommunication technology or satellite navigation systems.

Theory

The basic mechanism of interaction between light and sodium atoms is shown in Figure 2: the laser light optically pumps the sodium atoms, therefore changing the index of refraction of the medium, which in turn leads to absorption and diffraction of the light. To describe the atoms, the density matrix formalism is used:

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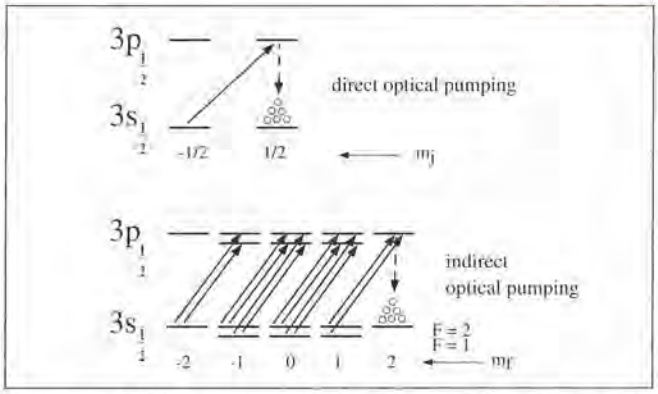

Figure 3: Optical pumping of the atomic D1-transition with circularly polarized light in a simplified (hypothetical) sodium atom without hyperfine structure (top) and in a real sodium atom (bottom). The "direct" pumping is about one order of magnitude too fast, whereas the "indirect" pumping is in good agreement with the measurements. Solid arrows denote the excitation by the circularly polarized light, whereas the dashed arrows indicate relaxation processes, most of which are not shown.

$$\frac{\partial \rho}{\partial t} = -\frac{i}{\hbar}[H, \rho] \qquad (1)$$

where ρ is the density operator. The Hamiltonian H is

$$H = H_0 + H_{laser} + H_{magnet} + \text{Relaxations.} \qquad (2)$$

Because the optical pumping process in a hypothetical sodium atom without hyperfine states is about one order of magnitude too fast as shown in Figure 3, all 16 states of the D1-line must be considered for an adequate description of the optical pumping mechanism. Equation (1) then leads to a system of 256 coupled ordinary differential equations. To exploit the symmetries of the system, it has been useful to develop the matrix ρ into the irreducible components [4]. For this task and to derive the equations finally used in the FORTRAN code, the computer algebra program "Mathematica" (which is installed at CSCS) has been used.
135 of the equations are relevant to calculate the atomic polarization $\vec{P}$ by which the atoms are coupled to the classical radiation field described by the 3-d wave equation (with slowly varying envelope approximation)

$$\frac{\partial^2 \vec{E}}{\partial x^2} + \frac{\partial^2 \vec{E}}{\partial y^2} + 2i\omega \frac{\partial \vec{E}}{\partial z} + 2i\omega \frac{\partial \vec{E}}{\partial t} = -\frac{\omega^2}{\varepsilon_0} \cdot \vec{P} \qquad (3)$$

for the laser light with frequency ω and electric field envelope $\vec{E}(\vec{r}, t)$. Equation (3) can be considered a 1-d wave equation combined with a 2-d diffusion equation.

Numerics

The 135 coupled ODE's of equation (1) are solved in parallel for each location in the sodium cell or on the surface (on a 3-d or 2-d grid, respectively). The PDE's are solved by transforming the wave equation part of equ. (3) into the integral equation

$$E(z,t) = \int_0^t dt' \, f\big(z-(t-t'),t'\big) + E(z-t,0) \qquad (4)$$

(where f is the inhomogeneous part) and using a 2-d FFT algorithm (scilib) to solve the "diffusion" part. For small resolutions (test calculations only) an algorithm which uses CSCS's M x M routine is faster. Special care has to be taken because the system of equations is stiff: the radiation field varies much faster than the atomic response due to optical pumping. The vectorisation is almost 100% and typical performances including in- and output on one SX-3 CPU are 2.1 GF for the FFT method and 4.5 GF for the M x M method. The bottleneck is the FFT routine! Typical resolutions for serious calculations are about 70 by 60 by 40, resulting in output files of between 1 and 2 Gb in size. The data from the simulations can be directly compared to the digitized signal of the CCD camera in the experiment. Also, thanks to Angelo Mangili and the CSCS graphics lab, time dependent 3-d solutions can be displayed as spectacular video animations. A sample picture from such a video showing the "beam bouncing" effect is shown in Figure 4.

In the case of a 2-d gas of sodium atoms on a surface and neglecting diffraction, Equation (4) reduces to

$$\vec{E}_{back}(t) = \vec{E}_{front}(t) + \frac{\rho i \omega}{2\varepsilon_0} \vec{P}(t) \qquad (5)$$

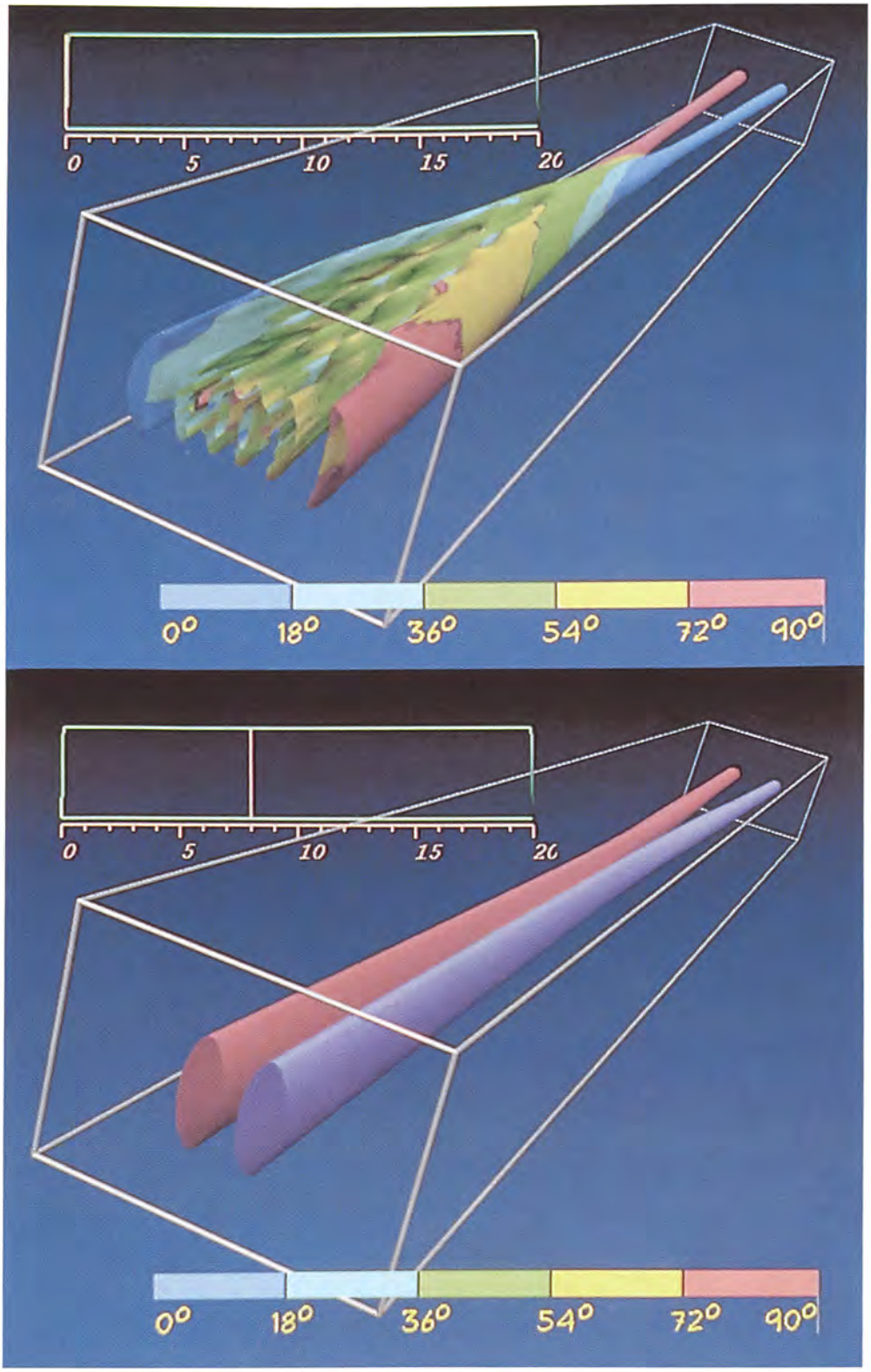

Figure 4: Isointensity surface plots of a "Beam bouncing" simulation. The beams have been turned on at t=0 and enter the sodium cell from the far side at a small angle. In the early stage (top, at less than 1μs) they still cross, as they would in vacuum or air, but some interaction is already visible. In the final state (bottom), they bounce off each other due to the optical pumping effect in sodium vapor. The polarisation of the light is indicated by the color.

where ρ is the surface density of sodium. The atomic polarization $\vec{P}(t)$ is again obtained by solving the coupled system (1). Figure 5 shows the calculated light intensity behind 0.001 monolayers of sodium after a laser beam has been turned on at t=0. Even though the stationary state shows almost no absorption, the dynamics of the signal could be used to derive the sodium density, relaxation rates and other important information in the forthcoming experiments. However, if the atoms are very close to the surface or close to each other, the hamiltonian H from equation (1) will have to be modified, resulting in a more sophisticated model.

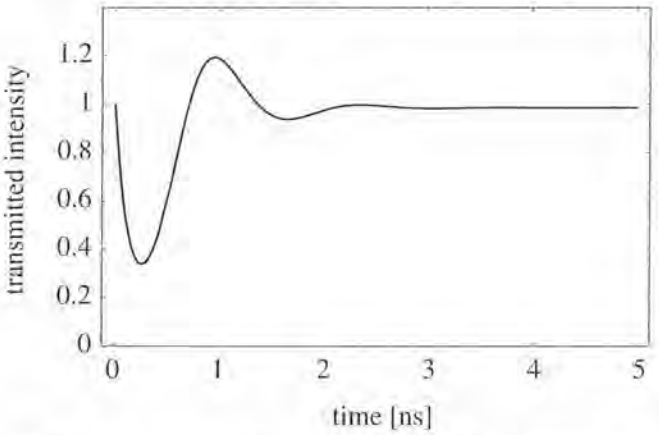

Figure 5: Calculated relative intensity behind a 0.001 monolayer of a 2-d gas of sodium atoms as a function of time after a laser beam of relative intensity 1 has been turned on at t=0.

Outlook

In 1995 several simulations of key experiments like "beam bouncing", "beam splitting", "beam switching" and "wire bouncing" have been calculated, many still in the J=1/2 to J=1/2 approximation. First calculations with the new model including hyperfine structure look promising and in 1996 we hope to:

- Optimize the performance of the new algorithm with hyperfine structure.
- Port the program to the SX-4 and parallelize the code. Previous tests show that almost 100% parallelization should be possible.
- Further develop the model for the 2-d case according to new experimental results.

Acknowledgments

We would like to thank the CSCS crew for their support, especially Angelo Mangili for the visualization and video production, James Brunson for SX-3 support and Claudia Moor for her help with all the other small and big problems we have had. Also we like to thank the "Schweizerischer Nationalfonds" and the "Ernst Hadorn Stiftung" for financial support.

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Prof. Leonhard Kleiser–Institut für Fluiddynamik, ETHZ (Numerical Simulation of Transitional and Turbulent Fluid Flows, page 60).

Full professor at ETHZ since September 1994 (Strömungslehre), his background includes studies in Mathematics and Physics, six years as a scientific collaborator at the "Kernforschungszentrum", Karlsruhe (Germany) and a PhD (Dr. -Ing.) obtained in 1982.
Before his call to the ETHZ, he worked at the Deutsche Forschungsanstalt für Luft- und Raumfahrt (DLR) in Göttingen, Germany.

Q: What impact does high-performance computing currently have on your research activities?

A: Our research is concerned with the investigation of turbulent fluid flows and the transition from the laminar to the turbulent state. Limited knowledge of these basic physical fluid phenomena and their appropriate modelling are major obstacles to the reliable flow computation in numerous problems of research and industry, ranging from the aerodynamics of turbomachinery to process engineering and numerical weather prediction, to name but a few. On this background, we are currently studying transitional and turbulent flows with the aim of obtaining an improved understanding of the physical processes and a better basis for the development of improved models. In particular, we are performing large-scale "direct" numerical simulations in which all relevant length and time scales of a flow must be resolved numerically in three-dimensional space and time. As the flows of interest show a large range of scales, very large computational resources are needed for such simulations: typically several million grid points in space and many thousands of timesteps (an overview of our current activities has been given in *CROSSCUTS* 4.2, April 1995). Therefore, our research crucially depends on the access to the most powerful supercomputers, appropriate periphery and software, and an adequate user support. Without this our research would be impossible. I am glad to say that at ETH Zurich and CSCS the conditions are very good.

Q: Do you have a vision regarding how your research area and high-performance computing will evolve in the future? If so, please describe your vision:

A: Demand for Computational Fluid Dynamics will continue to increase as it has done in the past, driven by the need for faster, more accurate and economical flow predictions. Likewise, more demanding fundamental problems of transition and turbulence will be studied, such as flows in more complex geometries, high-speed flows, shock-turbulence interaction and particle-laden flows. This will pose still greater demands on computing resources, which can be met by increased parallel computing. The migration from the SX-3 to the SX-4 in 1996 will be a first step in this direction. We expect that massively parallel computers will become more important in the future. At the same time, postprocessing needs to be developed further, notably the visualization and animation of three-dimensional, unsteady flows.

Q: Does CSCS meet your expectations of a high-performance computing center?

A: It very much does.

Q: What do you find of particular value at CSCS?

A: Computational facilities such as the NEC SX-3 are world-class. Our simulation codes run at up to 60% of the theoretically possible maximum computing speed, i.e., up to 4 GFLOPS on a single processor of the SX-3. This is about the maximum that can be achieved in practice, and enables us to use this expensive research tool very efficiently.

Q: What do you think should be improved at CSCS?

A.: Improvements have been made continuously when difficulties did arise. Based on initial experiences, the job scheduling has been optimised. Disk and mass storage space are being expanded in order to accommodate the huge databases produced by the simulations. Problems have appeared mainly with the postprocessing, which is done on the Convex. In this context it is important to realize that most of our postprocessing, i.e., the actual analysis of the data and production of scientific results, can be done only after the simulation runs have been completed. This work may extend over a period of several years, whereas the production runs take a few weeks or months of calender time. It is therefore necessary to find an optimal compromise between remote postprocessing in Manno and local postprocessing on the workstation on the desk of the scientist at ETH Zurich. This will be investigated in the near future.

Q: Please comment on the relationship between your research team and CSCS staff.

A: We are in continuous contact with staff members and management of CSCS and our relations are very good. We are getting good support, and a solution to any problem is usually found rather quickly.

Numerical Simulation of Transitional and Turbulent Fluid Flows

RESPONSIBLE INSTITUTE:
Institut für Fluiddynamik, ETHZ

PROJECT LEADER:
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INVOLVED PERSONS:
Dr. Y. Guo–Institut für Fluiddynamik, ETHZ
T. Mäder–Institut für Fluiddynamik, ETHZ
C. Mielke–Institut für Fluiddynamik, ETHZ
T. Wintergerste–Institut für Fluiddynamik, ETHZ

1. Introduction

The transition of a laminar flow to the turbulent state, beginning with disturbances of small amplitude, proceeds via a sequence of regular, increasingly complex intermediate stages, which are usually connected with flow instabilities. On modern supercomputers it became feasible to investigate laminar-turbulent transition processes up to the fully developed turbulence by direct numerical simulations (DNS). In direct numerical simulations the three-dimensional time-dependent Navier-Stokes equations are solved without any further model assumptions. All relevant scales of motion occurring in the flow have to be resolved. Numerical methods of high order are used for this purpose (see Kleiser and Zang [2]).

2. Simulations

The appropriate simulation codes have been developed and optimized on vector supercomputers during the past years. The work has been started on the NEC SX-3 at DLR Göttingen, Germany. In 1995 several large scale simulations have been performed to investigate fluid flows in three different physical cases. Each of these time-dependent simulations needs computing times on the order of 100 hours on the NEC SX-3.

- The first case was the simulation of the transition process in an incompressible three-dimensional boundary layer over a swept flat plate. The transition process in this boundary layer is initiated by the so-called crossflow instability. This instability arises in the boundary layer downstream of the leading edge of a swept aeroplane wing. The simulation was adapted to the transition experiment by Bippes et al. [1]. The influence of different amplitudes of the initially excited stationary crossflow vortex and travelling disturbances has been investigated. The computational domain was discretized by approximately 7.5 million grid points. The results show that a new vortical structure is generated during the late stages of transition. This new structure moves downstream with a velocity of approximately 70% of the free-stream velocity. The breakdown of the crossflow vortex and the onset of turbulence begins with the appearance of this new structure. The details of the breakdown process will be investigated next year.
- A second direct numerical simulation was performed of the subharmonic route from the laminar flow to the fully developed turbulence in a boundary-layer flow over a flat plate at Mach number $M_\infty = 4.5$. The Reynolds number based on the displacement thickness δ_1 was $Re_{\delta_1} = 10000$. The maximum resolution was $N_x \cdot N_y \cdot N_z = 128 \cdot 128 \cdot 240$ points in the streamwise, spanwise and wall-normal direction during the strongly nonlinear phase of the transition process.
  In the early stages of nonlinear breakdown a staggered pattern of finite amplitude lambda-vortices initiate the buildup of high-shear layers. A strong decrease of the shape factor, a strong increase of the skin friction coefficient (see Figure 1 next page) and the loss of spanwise symmetry due to formation and decay of new vortices indicate the final stages of breakdown to turbulence. The vortices as well as the shear layers become unstable and decay into new smaller vortices and shear layers. For engineering applications the effects of compressibility on turbulent kinetic energy are of interest. The results show that the dilatational dissipation—a measure of the influence of compressibility—is about three orders of magnitude smaller than the solenoidal and the pressure dissipation.
  These investigations will be extended to compressible three-dimensional boundary layers over swept configurations.
- Thirdly, a direct numerical simulation of a turbulent compressible boundary layer over a flat plate at Mach number $M_\infty = 3$ was performed. The code used computes the turbulent quantities locally with a temporal DNS approach, while the mean flow quantities are obtained by solving the Reynolds-averaged Navier-Stokes equations globally. The computational domain has 6.5 million grid points in the spatial directions. Four stations were simulated with a total of about 36000 time steps. The first results indicate a slow but continuous growth of the momentum thickness (i.e., decrease of the shape factor), as

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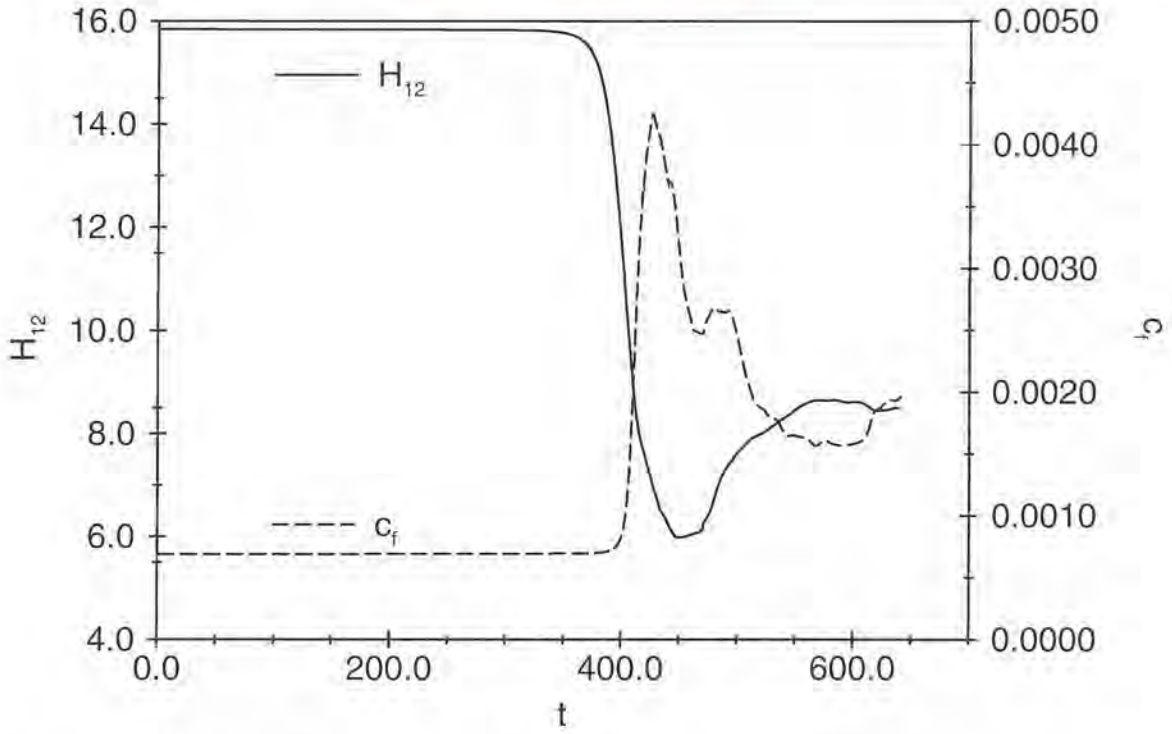

Figure 1: Evolution of shape factor and skin friction coefficient during the transition in a compressible boundary layer at Mach number $M_\infty = 4.5$.

well as two-point correlations of flow quantities that remain rather high near the center of the domain especially in the spanwise direction. This could be caused by the smallness of the computational domain, which does not allow to capture the largest structures of the flow.
It would be desirable to increase the size of the computational domain while keeping the same spatial resolution. However, this appears very difficult as the memory limits of the NEC SX-3 machine have almost been reached.

3. Visualization

After a simulation has been performed, an intense postprocessing is necessary to analyse the results of the simulations. The time-development of integral quantities like the shape factor or skin-friction coefficient is of interest. Another important aspect of the physical processes during transition is the development of vortical structures. Other important phenomena are the development, the instability, the roll up and finally the decay of shear layers. These processes are developing during transition and dominate the transfer of kinetic energy from the large scale structures to the small scales where the kinetic energy is dissipated. Shear layers are visualized by contour plots of the components of the velocity gradient tensor. The visualization of vortical structures in compressible and incompressible, transitional and turbulent flows by different criteria is part of our investigations.

Our data sets reach a size of several hundred MBytes. The ability to do postprocessing efficiently at CSCS is very important for our work. Visualization of three-dimensional instantaneous flow fields plays an important role during the postprocessing. We are using mainly the AVS package for this purpose. The flow visualizations were conducted partly on the CONVEX 3820 at CSCS due to the large memory requirements of our flow data.

4. Future Work

The current investigations will be continued and extended in the next year. New simulations with different initial conditions will be done. Furthermore the flow data computed during the last year have to be evaluated. A new topic to be started is the simulation of shock/boundary layer interaction of turbulent compressible fluid flows.

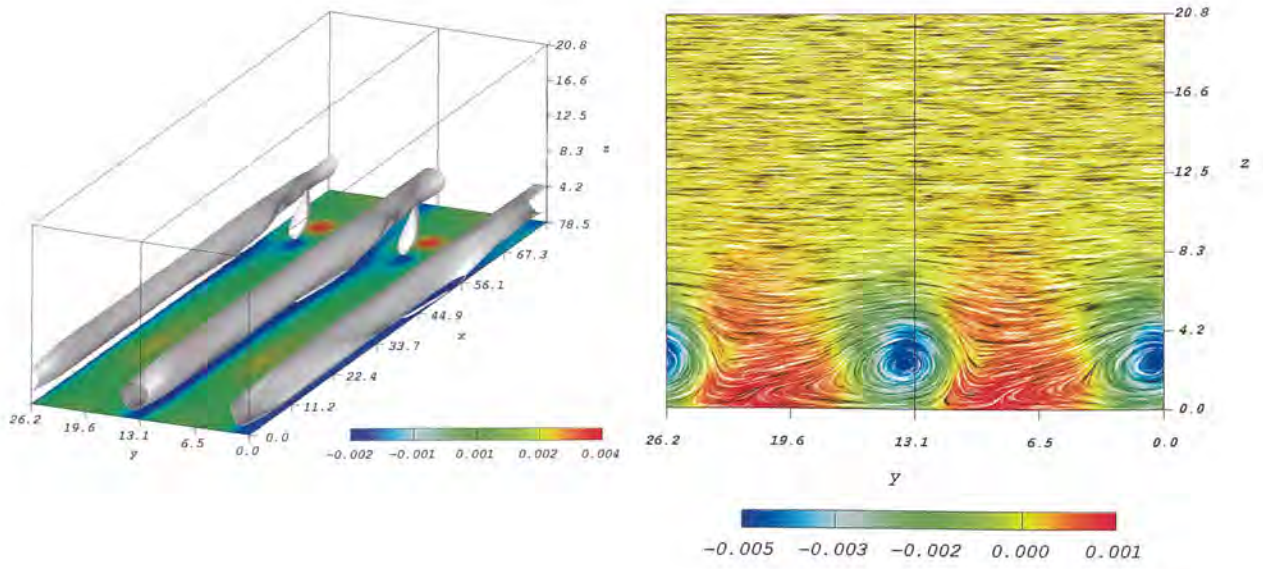

Figure 2: Visualization of crossflow vortices in an incompressible three-dimensional boundary layer by isosurfaces of low static pressure (left). The wall pressure distribution is shown by colour coding. Sectional streamlines and pressure distribution in cross-section x = 13.91 (right).

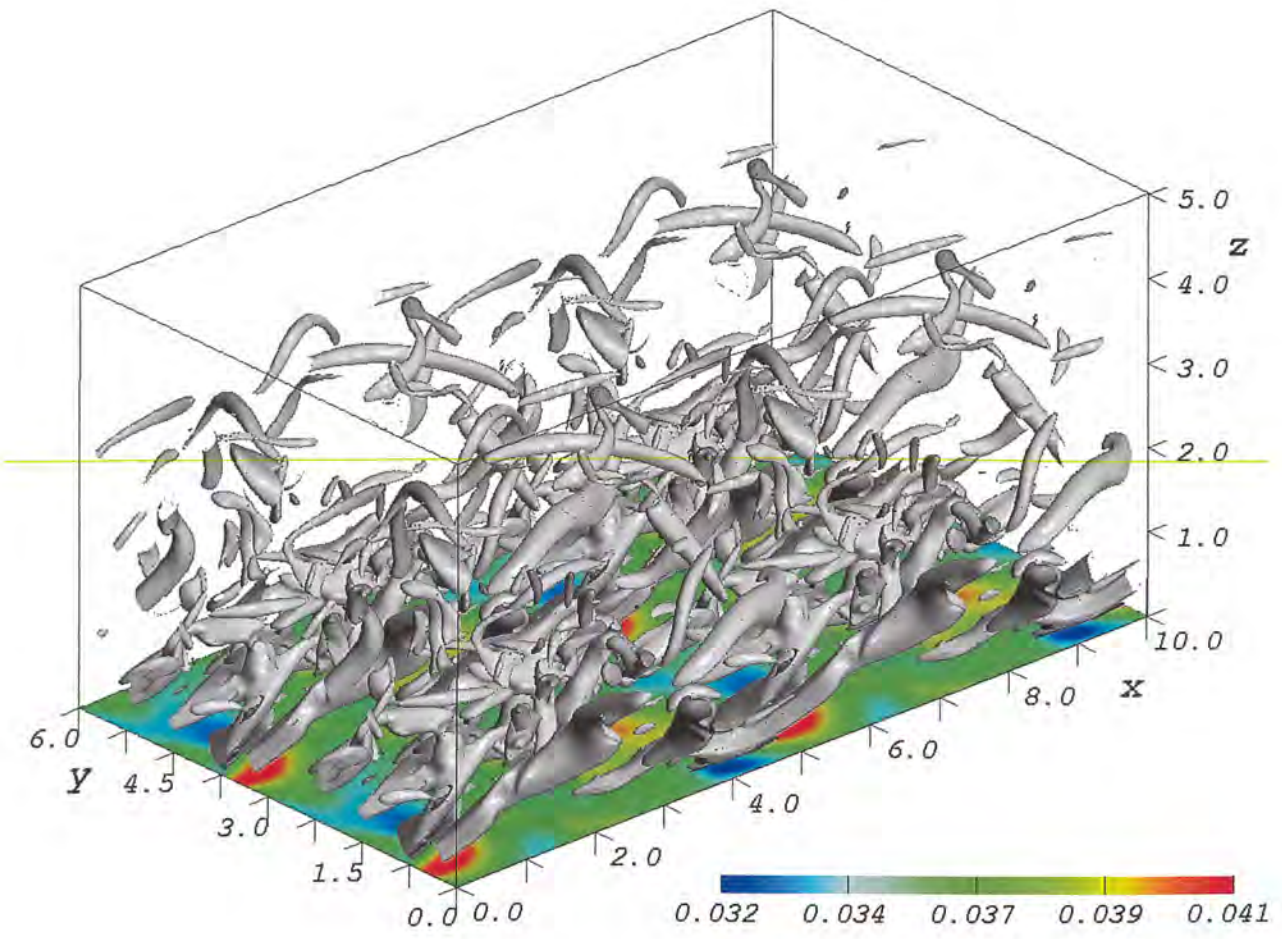

Figure 3: Visualization of vortical structures in a compressible turbulent boundary layer at time t = 655. The wall pressure distribution is shown by colour coding.

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User support interface; SeTO

Müller, Dr. Andreas
Software R&D; SeRD

Pagny, Pascal
Application software; SeSAM

Parini, Carla
Personnel administration; CeF

Paschedag, Norbert
Application software; SeTO

Pedrozzi, Nicola
Application software/system management; SeSAM/SeTO

Peyer, Mike
Network management; SeTO

Rosario Lorenzo, Paulo
Software R&D; SeRD

Rehmann, Dr. René
Software R&D; SeRD

Rühl, Dr. Roland
Software R&D; SeRD

Sawyer, William B.
Software R&D; SeRD

Schaidl Meyer, Elena
Library; CeF

Suter, Dr. Hans U.
Application software; SeTO

Tomassini, Marco
Application software; SeSAM (on leave of absence)

Valerioti, Remo
System management; SeTO

Vecchi, Nicole
Publications; CeF

Walther, Silvia
Publications; CeF

Wylie, Dr. Brian
Software R&D; SeRD

Zumthor, Bernardo
Central services; CeF

NEC Collaborators

Endo, Akiyoshi
R&D, Joint CSCS/NEC Collaboration

Hirano, Kinya
HW maintenance

Kenji, Tsuruta
HW maintenance

Masuda, Norio
R&D, Joint CSCS/NEC Collaboration

Zimmermann, Dr. Frank
R&D, Joint CSCS/NEC Collaboration

Visitors

Ackermann, Philipp–Institut für Informatik, Universität Zürich
Human Capital and Mobility Program

Aiex, Renata–Department of Computer Science, Catholic University of Rio de Janeiro (Brazil)
SSIP participant: Parallel Search Algorithm for the Detection of Irregular Structures
(July 17–October 13, 1995)

Anastopulous, Giorgio–Département d'Informatique, EPFL
Internship; SeSAM
(November 1, 1995–continuing)

Ardelea, Alexandre–CRPP-EPFL
Collaboration: Plasma Physics Program Environment
(Multiple visits)

Barras, Jean-Luc–Institut de Chimie Inorganique, Université de Fribourg
PRSS participant: Modelling of Lithium-thin-film Batteries
(August 7–October 6, 1995)

Betta, Federico–Departement Elektronik, ETHZ
SNMPD & MIB
(July 17, 1995–October 12, 1995)

Bonapersona, Michele–Ammonia Casale S.A.
Collaboration: Simulation of Catalytic Effects in Chemical Reactors
(Multiple visits)

Britton, Christopher–Department of Mathematics, Auburn University, Alabama (U. S. A.)
SSIP participant: Data Modeling Programming Assistant Interface for Parallel Systems: Integration and GUI
(July 17–October 13, 1995)

Bröker, Oliver–Department of Computer Science, University of Colorado at Boulder (U. S. A.)
SSIP participant: Parallelization of a Finite Element Environment Solver
(July 17–October 13, 1995)

Chu, Ching-Ling Gina–Department of Computer Science, Stanford University (U. S. A.)
SSIP participant: Data Modeling Programming Assistant Interface for Parallel Systems: The Knowledge-based Part
(July 17–October 13, 1995)

Colombo, Dr. Luciano–Dipartimento di Fisica, Università degli Studi di Milano (Italy)
Discussions: Parallel Implementation of TBMD
(Multiple visits)

Cooper, Dr. Wilfred Anthony–CRPP-EPFL
Collaboration: Plasma Physics Program Environment
(Multiple visits)

Dongarra, Prof. Jack–Departement of Computer Science, University of Tennessee, Oak Ridge National Lab (U. S. A.)
Academic guest; collaborator in several projects on BLACS, ScaLAPACK and TEMPLATE
(May 29–July 27, 1995)

Egli, Dr. Walter–ABB
Collaboration: Simulation of Electrostatic Precipitator (Electrofilter)
(Multiple visits)

Eghtessad, Bahram–Passera & Pedretti S. A.
Collaboration: Animation of NEAT
(January 1–June 30, 1995)

Estreicher, Stefan K.–Department of Physics, Texas Tech University (U. S. A.)
PRDDO/M on the NEC SX-3: Applying Non-empirical Quantum Mechanics to Extremely Large Molecules;
PRSS Student Advisor
(June 1995)

Foletti, Alessandro–Pini & Associati SA
Collaboration: Archiving of Territorial Data
(February 1–July 31, 1995)

Geus, Roman–Departement Informatik, ETHZ
SSIP participant: Parallelization of a Classical Molecular Dynamics Code
(July 17–October 13, 1995)

Gutzwiller, Andreas–Departement Informatik, Universität Zürich
SSIP participant: Performance Analysis Display Development
(July 17–October 13, 1995)

Hanser, Christof–Organisch-chemisches Institut, Universität Zürich
PRSS participant: Software Development in Computational Chemistry
(September 18–October 20, 1995)

Hüsser, Peter–Physik-Institut, Universität Zürich
PRSS participant: Calculations on HTC Materials
(August 7–September 29, 1995)

Kogelschatz, Ulrich–ABB
Collaboration: Simulation of Electrostatic Precipitator (Electrofilter)
(Multiple visits)

Rosario Lorenzo, Paulo–Department of Computer Science, State University of Campinas, Sao Paulo (Brazil)
SSIP participant: Performance Comparison of the Message-Passing and the Data-Parallel Programming Paradigm Using Application
(July 17–October 13, 1995)

Messmer, Peter–Departement Physik, ETHZ
SSIP participant: Data Modeling Programming Assistant Interface for Parallel Systems: Template Programming
(July 17–October 13, 1995)

Meehan, Michael–Department of Computer Science, University of North Carolina (U. S. A.)
User Support for the NEC Cenju-3
(June 1–August 31, 1995)

Mombelli, Matteo–Institut de Physique, Université de Neuchâtel
PRSS participant: Dynamics of Disordered Josephson Junction Arrays
(September 4–October 31, 1995)

Mayor-Lopez, Maria-José–Département de Chimie Physique, Université de Genève
PRSS participant: Calculations of Transition Metal Compounds
(October 2–13, 1995)

Murakami, Yoshimichi–Department of Electrical and Computer Engineering, Kanazawa University (Japan)
SSIP participant: High Performance Fortran Interface for ScaLAPACK
(July 17–October 13, 1995)

Ohmura, Prof. Atsumu–Geographisches Institut, ETHZ
Present a Possible Future for the Climate Research in Switzerland
(September 6, 1995)

Pedretti Andrea
Collaboration Passera & Pedretti S.A.
(April 1–June 30, 1995)

Ryan, Timothy–English Department, Carnegie Mellon University (U. S. A.)
Technical Editing
(June 1–August 30, 1995)

Sampath, Ramprasad–Department of Computer Science, University of South Carolina (U. S. A.)
SSIP participant: Porting Annai to Clusters of Workstations
(July 17–October 13, 1995)

January 1995

Wylie, Brian–CSCS
"Annai: An Integrated Programming Environment for Multicomputers."
HICSS-28 Hawaii International Conference on System Sciences
Maui, Hawaii (U. S. A.); January 4, 1995

Sawyer, William–CSCS
"Parallel Application and Algorithm Research at CSCS."
First High Performance Computing Symposium
Parallel Processing Center (PPC), NEC, Kanagawa (Japan); January 25, 1995

Müller, Andreas–CSCS
"Extending High Performance Fortran for the Support of Unstructured Computations."
High Performance Fortran Forum, Kick-Off Meeting
Houston, Texas (U. S. A.); January 30, 1995

March 1995

Sawyer, William–CSCS
"Parallel Library for Unstructured Mesh Problems."
Parallel CFD Day '95
ETHZ, Zurich; March 13, 1995

Decker, Karsten M.–CSCS
"Problem-Solving Environments: Methodologies and Basic Techniques."
17th SPEEDUP Workshop on Vector and Parallel Processing
Lugano; March 17, 1995

Schenfeld, Eugen–NEC Research Institute, Inc. (U. S. A.)
"MICA—Map-Interconnected Cache Architecture."
Swiss High Performance Computing Seminar
CSCS, Manno; March 20, 1995

April 1995

Tomassini, Marco–CSCS
"La théorie des systèmes: une approche inter- et transdisciplinaire."
Colloque d'inauguration officielle de l'Institut universitaire Kurt Boesch
Sion; April 4–6, 1995

May 1995

Decker, Karsten M.–CSCS
"Satisfying Application User Requirements: A Next-Generation Tool Environment for Parallel Systems."
International Conference and Exhibition on High-Performance Computing and Networking (HPCN Europe)
Milan (Italy); May 3, 1995

Tomassini, Marco–CSCS
"Evolutionary Approaches to Search and Optimization Problems."
General Assembly of the Swiss Society for Operations Research
Bern; May 5, 1995

Richter, Harald–Lehrstuhl für Rechnertechnik und Rechnerorganisation TU, München (Germany) and Max-Planck-Institut für Plasmaphysik (IPP), Garching (Germany)
"Interconnection Structures for Multiprocessors and Multicomputers."
Swiss High Performance Computing Seminar
CSCS, Manno; May 8, 1995

Decker, Karsten M.–CSCS
"How to Match User Requirements in Parallel Programming."
Fifth NEC-ETHZ Joint Workshop on Parallel Processing and Computational Science
NEC Corporation, Tokyo (Japan), May 11, 1995

Rühl, Roland–CSCS
"Tool Support for the Parallelization of Applications on Distributed-Memory Machines."
CSRD, Rice University, Houston, Texas (U. S. A.);
May 19, 1995

Müller, Andreas–CSCS
"Results of the Joint CSCS-ETH/NEC Collaboration in Parallel Processing."
Forschungszentrum Juelich, Zentralinstitut für Angewandte Mathematik, Juelich (Germany);
May 22, 1995

Rühl, Roland–CSCS
"Tool Support for the Parallelization of Applications on Distributed-Memory Machines."
NECI (NEC Research Institute), Princeton, New Jersey (U. S. A.); May 25, 1995

Sawyer, William–CSCS
"Parallel Library for Unstructured Mesh Problems."
University of Greenwich, Greenwich (England); May 26, 1995

June 1995

Zimmermann, Frank–NEC/CSCS
"PRNGlib: A Library of Parallel Random Number Generators."
PHYSICS COMPUTING '95 (Annual Meeting of the APS Division of Computational Physics)
Pittsburgh, Pennsylvania (U.S.A.); June 5–8, 1995

Taylor, P. R.–San Diego Supercomputer Center (U. S. A.)
"Computational Science Research at the San Diego Supercomputer Center."
Swiss High Performance Computing Seminar
CSCS, Manno; June 7, 1995

Sawyer, William–CSCS
"Parallelization of Applications on Distributed-Memory Machines."
Swiss High Performance Computing Seminar
CSCS, Manno; June 14, 1995

Dongarra, Jack–University of Tennessee and Oak Ridge National Laboratory (U. S. A.)
"Overview of the Innovative Computer Lab."
Swiss High Performance Computing Seminar
CSCS, Manno; June 21, 1995

Govaerts, Yves–Commission of the European Communities Joint Research Centre, Institute for Remote Sensing Applications, Ispra (Italy)
"Modelling the Scattering of Light in Three-dimensional Vegetated Target: a Monte Carlo Ray Tracing Approach."
Swiss High Performance Computing Seminar
CSCS, Manno; June 28, 1995

July 1995

Müller, Andreas–CSCS
"Extending High Performance Fortran for the Support of Unstructured Computations."
1995 International Conference on Supercomputing
Barcelona (Spain); July 4, 1995

Clémençon, Christian–CSCS
"Presentation of the CSCS-ETH/NEC Collaboration Project."
Institute for Computer Science, GeorgiaTech, Atlanta, Georgia (U. S. A.); July 5–7, 1995

Clémençon, Christian–CSCS
"Visualization, Execution Control, and Replay of Massively Parallel Programs with Annai's Debugging Tool."
High Performance Computing Symposium (HPCS'95)
Montreal (Canada); July 10–12, 1995

Philbin, James–NEC Research Institute (U. S. A.)
"The Design of an Operating System for Local Area Multi-Processor."
Swiss High Performance Computing Seminar
CSCS, Manno; July 11, 1995

Fuelscher, M. P.–Department of Theoretical Chemistry, Chemical Centre (Sweden)
"An Introduction to MOLCAS."
Swiss High Performance Computing Seminar
CSCS, Manno; July 11, 1995

Wylie, Brian–CSCS
"Tool Support for the Parallelization of Applications on Distributed-Memory Computer Systems."
2ème Séminaire du GRIP: "Outils pour la Programmation Parallèle"
Université de Neuchâtel, July 13, 1995

Wylie, Brian–CSCS
"Tool Support for the Parallelization of Applications on Distributed-Memory Computer Systems."
Seminario d'Informatica
Dipartimento di Informatica e Sistematica, Università degli Studi di Pavia, Pavia (Italy); July 21, 1995

August 1995

Dongarra, Jack–University of Tennessee and Oak Ridge National Laboratory (U. S. A.)
"Recent Work with Templates and Client Server Computing for Linear Algebra."
Swiss High Performance Computing Seminar
CSCS, Manno; August 2, 1995

Alippi, Cesare–Politecnico di Milano (Italy)
"Prediction and Identification with Neural Networks."
Swiss High Performance Computing Seminar
CSCS, Manno; August 9, 1995

Grote, Marcus–Stanford University (U. S. A.)
"Parallel Preconditioning with Sparse Approximate Inverses."
Swiss High Performance Computing Seminar
CSCS, Manno; August 21, 1995

Fritscher, Josef–CSCS
"An Implementation of Race Detection and Deterministic Replay with MPI."
EURO-PAR'95 Conference
Stockholm (Sweden); August 29–31, 1995

September 1995

Bhatt, Pramod–Indian Institute of Technology, Dehli (India)
"Co-operative Computing Platform and GIS Application."
Swiss High Performance Computing Seminar
CSCS, Manno; September 6, 1995

Bhatt, Pramod–Indian Institute of Technology, Dehli (India)
"Parallel and Distributed Simulation Platform and Application."
Swiss High Performance Computing Seminar
CSCS, Manno; September 7, 1995

October 1995

Sawyer, William–CSCS
"Prototype Parallelization—DREAMS Atmospheric Code."
MPI-ETH Information Exchange Seminar
ETHZ, Zurich; October 2, 1995

Aiex, Renata–Department of Computer Science, Catholic University of Rio de Janeiro (Brazil)
"Asynchronous Strategies for the Parallelization of Tabu Search Applied to the Logical Test of VLSI Circuits."
SIPAR Workshop on Parallel and Distributed Systems
Ingenieurschule, Biel, October 6, 1995

Geus, Roman–Departement Informatik, ETHZ
"Parallelization of a Classical Molecular Dynamics Code."
SIPAR Workshop on Parallel and Distributed Systems
Ingenieurschule, Biel, October 6, 1995

Messmer, Peter–Departement Physik, ETHZ;
Chu Gina–Department of Computer Science, Stanford University (U. S. A.);
Chris Britton–Department of Mathematics, Auburn University, Alabama (U. S. A.)
"Data Modeling Programming Assistant Interface for Parallel Systems."
SIPAR Workshop on Parallel and Distributed Systems
Ingenieurschule, Biel, October 6, 1995

Murakami, Yoshimichi–Department of Electrical and Computer Engineering, Kanazawa University (Japan)
"High Performance Fortran Interface for ScaLAPACK."
SIPAR Workshop on Parallel and Distributed Systems
Ingenieurschule, Biel, October 6, 1995

Rosario Lorenzo, Paulo-Department of Computer Science, State University of Campinas, Sao Paulo (Brazil)
"Perfomance Comparison of the Message-passing and the Data-parallel Programming Paradigms Using Application Kernels."
SIPAR Workshop on Parallel and Distributed Systems
Ingenieurschule, Biel, October 6, 1995

Prins, Jan–Computer Science Department, University of North Carolina (U. S. A.)
"High-Performance Irregular Computation using High-level Programming Models and Novel Compilation Techniques."
Swiss High Performance Computing Seminar
CSCS, Manno; October 6, 1995

Müller, Andreas–CSCS
"Extending High Performance Fortran for the Support of Unstructured Computations."
PARS Workshop
Stuttgart (Germany); October 9, 1995

Sawyer, William–CSCS
"Applications on Massively Parallel Systems."
Second GMD-NEC Workshop on Scientific Parallel Computing
GMD, Schloss Birlinghoven, Sankt Augustin (Germany); October 11, 1995

Wylie, Brian–CSCS
"Annai: An Integrated Programming Environment for Distributed-Memory Parallel Computers."
Second GMD-NEC Workshop on Scientific Parallel Computing
GMD, Schloss Birlinghoven, Sankt Augustin (Germany); October 12, 1995

November 1995

Decker, Karsten M.–CSCS
"The Swiss Scientific Computing Center (CSCS): Adding Value Between Universities and Industry."
Asian Technology Information Program (ATIP)
Tokyo (Japan); November 15, 1995

Decker, Karsten M.–CSCS
"Effective Parallel Computing for Application Users Systems Engineering Research Institute."
Korea Institute of Science & Technology, Taejeon (Korea); November 17, 1995

Decker, Karsten M.–CSCS
"Satisfying Application User Requirements in Parallel Computing Department of Electronic Engineering."
National Yunlin Institute of Technology, Yunlin (Taiwan); November 20, 1995

Decker, Karsten M.–CSCS
"Transforming Parallel Computing into an Effective Tool for Application Users."
Department of Information Systems and Computer Science, National University of Singapore, Singapore (Singapore); November 24, 1995

Sawyer, William–CSCS
"A Parallel Implementation of Tight-binding Molecular Dynamics Based on Reordering of Atoms and the Lanczos Eigen-solver."
Materials Research Society 1995 Fall Meeting
Boston, Massachusetts (U. S. A.); November 28, 1995

December 1995

Sawyer, William–CSCS
"Parallel Numerical Library Development at CSCS."
Vektorielles und Paralleles Rechnen, ETHZ
ETHZ, Zurich; December 12, 1995

Deshpande, Vaibhav–CSCS
"Parallelization of Applications on Distributed Memory Machines."
Centre for Development of Advanced Computing (C-DAC), Pune (India); December 13, 1995

Masuda, Norio–NEC/CSCS
"Progress of Algorithms and Applications group in the Joint CSCS/NEC Collaboration in Parallel Processing."
2nd NEC-HPC Workshop
The NEC headquarters, Tokyo (Japan); December 19, 1995

Curriculum Development Courses for Ticino Teachers

CSCS, Manno; January 25, February 9 and 16, 1995.
Organized by CSCS and Dr. G. Ravano (STS/DIC).
Introductory courses about Molekel, AVS, X-Windows/Motif, and Maple Mathematica for Ticino high-school teachers for the curriculum project of CSCS.

Cellular Networks

Computer Science Department, EPFL, Lausanne; April–June 1995.
Dr. M. Tomassini (CSCS), lecturer.

Introduction to Internet

CSCS, Manno; May 8 and September 12, 1995.
Organized by CSCS and the Istituto Svizzero di Pedagogia per la Formazione Professionale (Lugano).
Introductory course about Internet services for teachers of Ticino's professional schools.

Workshop on Mass Storage Products

Cadro; May 22–23, 1995.
Organized by CSCS and H. Fichtel (UniTree Users Group).
A collection of talks by the major players in the mass storage arena focused on technology developments and future trends.

UniTree Users Group Meeting

Cadro; May 23–24, 1995.
Organized by CSCS and H. Fichtel (UniTree Users Group).
A meeting among the UniTree HSM users, the system suppliers and archiving subsystems vendors. Major topics: users requirements and product development.

Project Related Student Stages (PRSS '95)

CSCS; June–October, 1995.
Organized by CSCS.
Block courses in programming environment and visualization-/animation-related topics, followed by 1–2 months project-related work for young researchers from Swiss Universities.

Computing and Communications Camp (C^3 '95)

CSCS, Manno; July 17–August 24, 1995 (three sessions).
Organized by CSCS, Dr. G. Ravano (DIC/STS) and M. de Senarclens (INGCH).
The two-week Computing and Communications Camp C^3 offers camps in applied computing and computer communication to talented students.
A practical approach to computer applications (computational science, simulations, visualization) and an access to the world of technology and science.

Summer Student Internship Program 1995 (SSIP '95)

CSCS, Manno; July 17, 1995–October 13, 1995.
Organized by CSCS.
Two-week initial course in Parallel Computation followed by an eleven-week research project conducted together with an advisor.

Annai Technical Tutorial

Fuchu, Tokyo; September 7–13, 1995.
Organized by CSCS.
Invited presentations for NEC tool development team, hosted by NEC Fuchu.
Presentation of Annai tool environment design, implementation details of the Annai components (framework, TSA, PST/PSTlib, PDT/PDTlib, PMA/PMAlib & UI) and their integration and synergetic interaction, and including demonstrations and discussion sessions.

Vector Programming Course

CSCS, Manno; September 28–October 26, 1995 (five sessions).
Organized by CSCS.
The course covered scientific applications, vector architecture, an introduction to Fortran programming, vectorization, elements of vector compilation and optimization; two sessions were devoted to hands-on exercises on the NEC SX-3/24R.

CSCS Education Program: School Visits

CSCS, Manno; October 20, 1995.
Organized by CSCS.
Trial visit of a primary school class for testing the new visits program for schools. Besides the visit, the pupils made some interactive exercises using simulated and visualized data of the region of Ticino and Greece.

International Workshop: "Towards Evolvable Hardware"

EPFL, Lausanne; October 2–3, 1995.
Organized by Dr. M. Tomassini (CSCS) and E. Sanchez.

Parallel Programming Courses

CSCS, Manno; November 9–December 21, 1995 (seven sessions).
Organized by CSCS.
The course examined "Ordinatori paralleli e reticoli d'interconnessione", communications, models for parallel programming, hardware platforms and software for practical work; three sessions were devoted to hand-on exercises.

Articles

(CSCS members are indicated in bold type).

Ankembrand, T. and **M. Tomassini**. 1995. Multivariate time-series modelling of financial markets with artificial neural networks. In *Proceedings, International Conference on Artificial Neural Networks and Genetic Algorithms ICANNGA95*. D. W. Pearson, N. C. Steele and R. F. Albrech Editors, Springer-Verlag: 257–260.

Ankembrand, T. and **M. Tomassini**. 1995. Neural network and statistical forecasting of multivariate economical and financial time series. *Neural Network World*: 365–369.

Azhari, A.-A and **H. U. Suter**. 1995. Correlated ab initio force fields and vibrational analysis of the spectra of isoxazole and isothiazole. *Journal of Physical Chemistry* Vol. 99: 12751–12758.

Beg, I., W. Ling, **A. Müller**, P. Przybyszewski, **R. Rühl** and **W. Sawyer**. 1995. PLUMP: Parallel Library for Unstructured Mesh Problems. *Parallel Algorithms for Irregular Problems: State of the Art*. Edited by A. Ferreira and J. D. P. Rolim. Dordrecht, The Netherlands: Kluwer Academic Publishers [ISBN: 07923-3623-2]: 45–67.

Chopard, B., M. Oussaidene and **M. Tomassini**. 1995. Programmation évolutionniste parallèle. In *Proceedings, RenPar'7, Rencontres Francophones du Parallélisme*. G. Libert, J.-L. Dekeyser and P. Manneback Editors, P. I. P. Mons: 221.

Clémençon, C., A. Endo, J. Fritscher, A. Müller, R. Rühl and **B. J. N. Wylie**. 1995. The 'Annai' environment for portable distributed parallel programming. In *Proceedings, 28th Hawaii International Conference on System Sciences (HICSS-28)*, Maui, Hawaii. Vol II. Edited by H. El-Rewini and B. Shriver. IEEE Computer Society Press [HICSS28] : 242–251.

Clémençon, C., J. Fritscher, M. J. Meehan and **R. Rühl**. 1995. An implementation of race detection and deterministic replay with MPI. In *Proceedings, EURO-PAR'95*, Stockholm, Sweden. Edited by S. Haridi, K. Ali and P. Magnusson. Lecture Notes in *Computer Science* vol 966, Springer-Verlag [ISBN: 3-540-620247-X]: 155–166.

Clémençon, C., J. Fritscher and **R. Rühl**. 1995. Visualization, execution control and replay of massively parallel programs within Annai's debugging tool. In *Proceedings, High Performance Computing Symposium (HPCS'95)*, Montreal, Canada. Edited by V. Van Dongen [ISBN: 2-921316-12-9]: 393–404.

Colombo, L. and **D. Maric**. 1995. Defect-induced amorphization in silicon. *Europhysics Letters* 29: 623.

Colombo, L., **W. Sawyer** and **D. Maric**. 1995. A parallel implementation of tight-binding molecular dynamics based on reordering of atoms and the Lanczos Eigensolver. *Proceedings, Materials Research Society Fall Meeting*, Boston, U. S. A.

Colombo, L. and **W. Sawyer**. 1995. A parallel implementation of tight-binding molecular dynamics. In *Proceedings, E-MRS 1995 Spring Meeting*, Strasbourg, France.

Dacorogna, M., O. Pictet, B. Chopard, R. Schirru and **M. Tomassini**. 1995. Using evolutionary algorithms for robust optimization in financial applications. *Neural Network World*: 573–587.

Decker, K. M. 1995. CSCS's artificial intelligence competence center. *CROSSCUTS* 4(2): 16–17.

Decker, K. M. 1995. CSCS at HPCN Europe 1995. *CROSSCUTS* 4(2): 18.

Decker, K. M. 1995. Problem-solving environments: Methodologies and basic techniques. *SPEEDUP* 9(1): 58–63.

Decker, K. M. 1995. 17th SPEEDUP Workshop on hardware and software trends in high-performance computing. *CROSSCUTS* 4(2): 19.

Decker, K. M., J. J. Dvorak, R. M. Rehmann and **R. Rühl**. 1995. Satisfying application user requirements: A next-generation tool environment for parallel systems. In *Proceedings, International Conference and Exhibition on High-Performance Computing and Networking (HPCN Europe'95)*, Milan, Italy, May 3–5, 1995. Edited by R. Hertzberger and G. Serazzi. Lecture Notes in *Computer Science* vol. 919, Springer-Verlag [ISBN: 3-540-59393-4]: 206–228.

Degtyarev, L., S. Medvedev, V. D. Shafranov, **M. Ballabio**, W. A. Cooper and **R. Gruber**. Three-dimensional model of plasma equilibrium based on poloidal representation of a magnetic field. Submitted to *Plasma Physics Reports* (in Russian).

Grossetie, J. C. and **M. C. Hohenadel**. 1995. Eléments d'analyse du signal par ondelettes. *Rapport EUR 16250 FR.*

Gruber, R., W. Egli, **E. Gerteisen, G. Jost** and S. Merazzi. 1995. Problem-solving environments: Towards an environment for engineering applications. *SPEEDUP* 9(1): 41–45.

Gruber, R., J. Brunson and **M. Hodous**. 1995. Benchmark measurements on the SX-4. *SPEEDUP* 9(2): 76–79.

Huan, M.-B., **H. U. Suter**, B. Engels, S. D. Peyerimhoff and S. Lunell. 1995. A multireference configuration interaction study of the Azetidine radical cation and the neutral Azetidin-1-yl radical. *Journal of Physical Chemistry* Vol. 99: 9724–9729.

Loraschi, A., A. Tettamanzi, **M. Tomassini** and P. Verda. 1995. Distributed genetic algorithms with an application to portfolio selection problems. In *Proceedings, International Conference on Artificial Neural Networks and Genetic Algorithms ICANNGA95*. D. W. Pearson, N. C. Steele and R. F. Albrech Editors, Springer-Verlag: 384–387.

Luchsinger, R., P. F. Meier, **N. Paschedag, H. U. Suter** and Y. Zhou. 1995. Computational studies of hydrogen-related complexes in semiconductors. *Philosophical Transactions of the Royal Society* Vol. A350: 203–214.

Maric D. and **C. Moor-Häberling**. 1995. Centro Svizzero di Calcolo Scientifico. *Chimia* 49: 124.

Marinucci, M. R., F. Giorgi, M. Beniston, M. Wild, P. Tschuck, A. Ohmura, and **A. Bernasconi**. 1995. High resolution simulations of January and July climate over the western Aline region with a nested regional modeling system. *Theoretical and Applied Climatology* Vol. 51, No. 3.

Miccio, C., E. Sanchez and **M. Tomassini**. 1995. Parallel genetic programming induction of binary decision diagrams. *EPFL Supercomputing Review* 7: 37–41.

Müller, A. and **R. Rühl**. July 1995. Extending high performance Fortran for the support of unstructured computations. In *Proceedings, 9th International Conference on Supercomputing '95*, Barcelona, Spain. ACM [ISBN: 0-89791-728-6]: 127–136.

Müller, A. and **R. Rühl**. 1995. Communication-buffer organization and performance of data-parallel unstructured computations. *Languages, Compilers and Run-Time Systems for Scalable Computers*. Edited by B. K. Szymanski and B. Sinharoy. Kluwer Academic Publishers [ISBN: 0-7923-9635-9].

Müller, A. and **R. Rühl**. 1995. Extending high performance Fortran for the support of unstructured computations. In *Proceedings, PARS Workshop*, Stuttgart, Germany. Gesellschaft für Informatik, Erlangen, Germany.

Rehmann, R. M. 1995. Computing and Communication Camp C3. *CROSSCUTS* 4(3): 12.

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