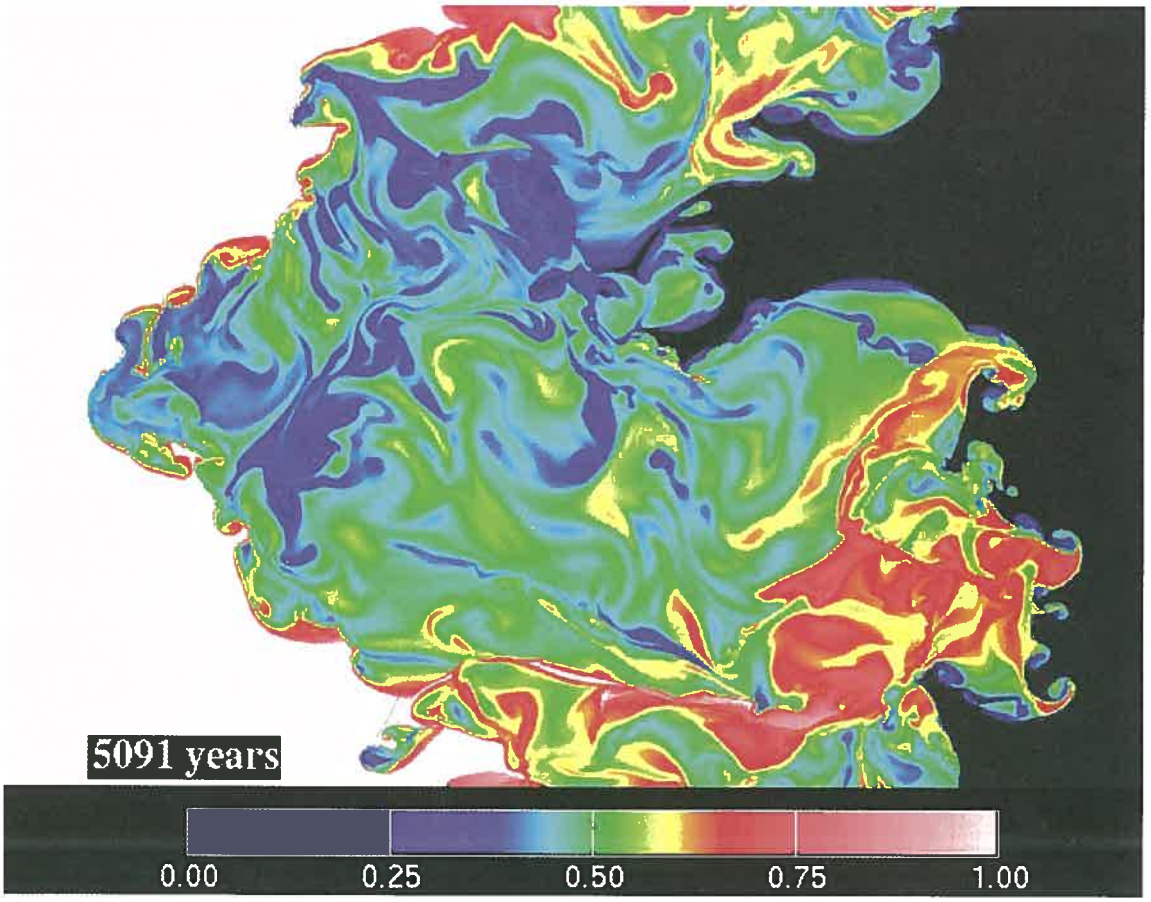
CSE

Computational Science and Engineering

Annual Report
2000/2001



ETH Eidgenössische Technische Hochschule Zürich

CSE

Computational Science and Engineering

Annual Report 2000 / 2001

July 2000 to July 2001

Impressum:

Eidgenössische Technische Hochschule (ETH) Zürich
Switzerland

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Diploma studies in CSE at the ETH Zürich on the internet:

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Cover:

Supersonic turbulent mixing within the interaction zone of colliding stellar winds. The mixing zone of the two colliding Mach-20 flows is confined by two strong shocks. The patchy appearance and further shocks within the zone are typical for strongly compressible turbulence. Shown is a passive scalar transported with the left wind, color-coded in red-white, normalized to 1. The absence of the passive scalar, 0, is color-coded in blue-black. (Computation by Rolf Walder, Institute of Astronomy, ETH Zürich, and Doris Folini, Observatoire de Strasbourg, France.)

Printing:

Fröhlich Druck AG, www.froehlich.ch

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1
Introduction

Here it is, the first Annual Report of Computational Science and Engineering at ETH! In this Annual Report you find the first map on what is done in research and education in the area of Computational Science and Engineering (CSE) at ETH.

Why should one make such a report?

Traditionally, ETH has been strong in computing. It was the first university institution in Europe to install a computer. The Z4, a Zuse computer, was already rented in 1949. In the 50-ies, ETH was one of the places world wide where numerical analysis and computing were done. Unfortunately, in the 70-ies and 80-ies ETH got behind in computing: it failed to hire young blood and to jump onto the high performance computing track. Fortunately, this picture was changed in the late 80-ies and 90-ies: the Interdisciplinary Project Center for Supercomputing (IPS) and later the CSCS in Manno were established. In addition, in many different areas and departments professors who use computers as a major tool for their investigations were hired. This led to an initiative to introduce a new curriculum in Computational Science and Engineering. The brain storming started in 1995 and the first students were enrolled in this program in 1997. Unfortunately, the name had to be teutonic and the words "Rechnergestützte Wissenschaften (RW)" were chosen. In the year 2000, CSE was chosen as a "Strategische Erfolgs-Position (SEP)". The ETH-Rat approved the hiring of three professors in CSE, the first one being Petros Koumoutsakos. In 2001, the steering committee CSE, in German "Ausschuss RW", submitted to the rector a detailed proposal to introduce Bachelor and Master degrees in CSE.

The aim of this first Annual Report CSE is to give an overview of CSE activities at the ETH. It gives a view on the curriculum in CSE, its students and a glimpse of the future. It is meant to serve as a source of information about research and education in CSE at ETH, not only to the outside world and new members of the ETH CSE community but also for the non-CSE part of the ETH.

At this point, we thank the Vice-president Research, Prof. Albert Waldvogel, for his moral support to produce such a report. Our thanks for the financial support go to the rector, Prof. Konrad Osterwalder, and the Vice-president Research, Prof. Albert Waldvogel. We thank all at ETH who have contributed to this report. As with any report, it may not be complete, especially since it is the first one produced at ETH.

Zürich, October 20, 2001
Rolf Jeltsch, Fachberater Rechnergestützte Wissenschaften

2
Education

The curriculum in Computational Science and Engineering (CSE) at ETH was started in the winter semester 1997/1998. The German name is 'Studiengang Rechnergestützte Wissenschaften (RW)'. The CSE curriculum provides an interdisciplinary, application-oriented and problem-solving education and was one of the first of its kind to be established in Europe. It is to mention that in a recent SIAM report (Graduate Education in Computational Science and Engineering, SIAM Rev. 43 (2001), 163-177) attempting to give the core areas and the scope of CSE the definition of a model CSE curriculum is completely along the lines of the existing CSE curriculum at ETH.

CSE means mathematical modelling, scientific computing and the use of computers for analysing scientific and technical problems. CSE is different from computer science but also from theory and experiment, the traditional ways of studying processes in science and engineering. CSE represents a third scientific way in addition to theory and experiment. Graduates of the CSE curriculum should be able to work on interdisciplinary problem solving in an application area, making use of a profound knowledge in mathematics and computer science. They are trained to communicate and collaborate with engineers, physicists, computer scientists and/or mathematicians to solve difficult practical problems.

The CSE curriculum is under the guidance of the Studies Adviser (Fachberater) and of the CSE committee (Ausschuss RW). Formally, it is attached to the Interdepartemental Diploma Studies of the Departments of Mathematics and of Physics (Diplomstudienbereich der Departemente Mathematik und Physik). Instead of the usual 4.5 years (9 semesters) of diploma studies at ETH, the CSE curriculum takes only 2.5 years and builds upon knowledge acquired in the first two years of a classical discipline. Candidates for the CSE curriculum have to take two years of basic studies; this can be done in mechanical or electrical engineering, computer science, chemistry, mathematics, physics at ETH, or elsewhere.

For the winter semester 2002/2003 it is planned to establish a CSE Bachelor/Master program. A request by the Ausschuss RW has been made to the Rektorat and the Schulleitung of ETH in the summer semester 2001. The Bachelor of Science in CSE will be received after 1 year of CSE studies, and the Master of Science in CSE, which is equivalent to the Diploma, after 2.5 years. The main reason for introducing the Bachelor/Master system is to attract excellent students from abroad with a Bachelor degree to the CSE Master program at ETH in order to enhance the number of CSE students.

In the past academic year 12 new students have started their CSE studies at ETH; 11 students took their basic studies at ETH and 1 at the University of Berne in the following branches: Mathematics 4 students, Physics 3, Mechanical Engineering 2, Environmental Sciences 2, Chemical Engineering 1. The presentation of the CSE curriculum for ETH students of the 4-th semester of June 19 attracted around 60 persons. It is hoped that a fair number of those will start with the CSE studies this fall.

In the past academic year 10 students have very successfully finished their CSE studies and have received a CSE diploma. They chose the following application areas: Numerical Fluid Dynamics 4 students. Robotics 4, Theoretical Physics 1, Physics of the

Atmosphere 1. In the following list we give the name of the students, the title of the diploma thesis and the name and the institute of the adviser.

Diploma Theses

G. Bleiker	Interpolatory adaptive multi-resolution scheme for conservation laws (L. Kleiser, Fluid Dynamics)
M. DiMinno	Optimierung der Kommunikationsroutinen für Large-Eddy- Simulation unter Verwendung dynamischer Feinstrukturmodelle (L. Kleiser, Fluid Dynamics)
D. Hoch	High-order finite-element method for time-dependent scattering in complex geometry (M. Grote, Mathematics)
D. Leuenberger	Anew terrain-following coordinate for high-resolution atmospheric models (C. Schär, Atmospheric and Climate Science)
M. Lüscher	Implementierung eines Multirate-Verfahrens für ein einfaches technisches System (G. Schweitzer, Robotics)
F. Mohamed	Simulation of the vortex texture in a superconductor with $\kappa \approx 1/sqrt(2)$ (J. Blatter, Theoretical Physics)
B. Müller	Dampftransport in einem operationellen Schneedeckenmodell (E. Anderheggen, Structural Engineering)
A. Rüegg	Verallgemeinerte Finite-Elemente-Methoden für Multiskalenprobleme (C. Schwab, Applied Mathematics)
R. Schorno	Bewegungssteuerung redundanter Manipulatoren mit Hilfe von Manipulierbarkeits-Ellipsoiden (G. Schweitzer, Robotics)
M. Stoffel	Design of a real-time sensory and control system for a destroyer model (T. Rösgen, Fluid Dynamics)

The total number of CSE students enrolled in the past academic year was 27. Listed below are the term papers written by the CSE students in the past two semesters.

Term Papers

S. Benkler	Absorbing boundary conditions for time dependent electromagnetic scattering (M. Grote, Mathematics)
P. Häfliger	Application of a convolutional multilayer perceptron to object recognition with contrast pictures: Network architecture and training strategies (J. Bernasconi, ABB)
P. Häfliger	Animierte Datenstrukturen in Java (P. Widmayer, Theoretical Computer Science)

A. Jost	Integration einer virtuellen Trainigsumgebung (M. Gross, Scientific Computing)
K. Meyer	Axialsymmetrische Wellenausbreitung in elastischen und viskoelastischen Materialien (J. Dual, Mechanics)
G. Stark	Face space (L. Van Gool, Communication Technology)

Each semester on Thursdays, 15 - 17 hours, the CSE Case Studies Seminar takes place. Speakers from ETH, from other universities as well as from industry are invited to give a 2x45 minutes talk on an applied topic. The idea is to show the students a case study of an application problem containing the problem setting, the modelling, the mathematical approach and the simulation on a computer. Such a case study should also show what is going on in the field of CSE or what are the job perspectives for a CSE engineer. The seminar talks of the past academic year are listed in Chapter 3 of the report. Beside the scientific talks the CSE students are asked to give short presentations (10 minutes) on published papers out of a list (containing articles from, e.g., Nature, Science, Scientific American, etc.). These presentations help the students to practise giving talks. Students are also asked to give talks on their term papers and voluntarily on their diploma theses (if there are free time slots).

Zürich, October 3, 2001
Kaspar Nipp, Mitglied des Ausschusses Rechnergestützte Wissenschaften

For detailed information on the Diploma Studies in CSE at the ETH Zürich see:
http://www.cse.ethz.ch

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CSE Case Studies Seminar

The CSE Case Studies Seminar takes place each semester on Thursdays, 15 - 17 hours. Speakers from ETH, from other universities as well as from industry are invited to give a 2x45 minutes talk on an applied topic. The idea is to show the students a case study of an application problem containing the problem setting, the modelling, the mathematical approach and the simulation on a computer. In addition, such a case study should show what is going on in the field of CSE and what are the job perspectives for a CSE engineer. The seminars of the past academic year are given in the two following lists.

Case Studies Seminar WS00/01

2. 11. 00	T. Rösgen, R. Totaro, Fluiddynamik Numerische Bildanalyse in der Strömungsmesstechnik
9. 11. 00	C. Frouzakis, Combustion Research Lab, PSI Simulation of Chemically Reactive Flows
16. 11. 00	A. Sebestyen, VA Tech Escher Wyss AG CFD im industriellen Einsatz
23. 11. 00	P. Arbenz, Wissenschaftliches Rechnen Zum Entwurf von Hochfrequenzkavitäten bei Teilchenbeschleunigern
7. 12. 00	E. Windhab, Lebensmittelverfahrenstechnik Simulation und experimentelle Besätigung von Dispergier- strömungsfeldern fr nicht Newtonsche Fluidsysteme
11. 1. 01	R. Jeltsch, SAM Simulation von Protonenstrahlen hoher Intensität in Beschleunigern
18. 1. 01	Ph. Hünenberger, Physikalische Chemie Electrostatic Interactions in Computer Simulations of (Bio-)Molecular Systems
25. 1. 01	R. Schlegel, Sulzer Markets and Technology Ltd. Numerische Simulation und Analyse laminarer Mischvorgaenge

Case Studies Seminar SS01

12. 4. 01 U. Schmock, Risklab
A Case Study in Financial Engineering: Securitization of Insurance Risk

19. 4. 01 K. Binder, Physik, Uni Mainz
Finite Size Scaling: Ein Werkzeug zur Untersuchung von Phasenübergängen mittels Computersimulation

26. 4. 01 A. Saxer, Alstom Power, Baden
Turbomachinery Design System: A Mixture of Engineering and Computational Science

3. 5. 01 A. Reischke, G. Mundinger, ABB Turbo Systems AG, Baden
1) Axialventilator: Untersuchung mit Q3D
und 3D CFD Verfahren
2) Turbinenaustrittsgehuse: Untersuchung mit Q3D
und 3D CFD Verfahren (instationre Strmung)

10. 5. 01 R. Westermann, RWTH Aachen
Hardware untersttzte Volumenvisualisierung

14. 6. 01 K. Nagel, Wissenschaftliches Rechnen
Stadtplanung als Videospiel: Grosse Verkehrssimulationen

21. 6. 01 J. Quiby, Meteo Schweiz
Die wichtigsten Methoden in der numerischen Meteorologie

4
Computational Highlight

High-Resolution Weather Prediction in the Alps

Christoph Schär, Huw Davies, Oliver Fuhrer, Daniel Lüthi, Michael Sprenger, André Walser
Institute for Atmospheric and Climate Science ETH, Zürich, Switzerland

Peter Binder
Meteo Swiss, Zürich, Switzerland

Robert Benoit
Recherche en Prévision Numérique, Environment Canada, Dorval, Canada

Djordje Maric
Swiss Center for Scientific Computing CSCS, Manno, Switzerland

1. Introduction

Weather prediction is increasingly based on numerical models of the atmosphere. These integrate a complex set of governing equations forward in time, based upon initial condition as derived from operational meteorological networks. Typically, forecasts are conducted using a series of nested models of increasing resolution. For instance, current operational weather prediction in Switzerland involves both global models with horizontal resolutions around 40 km, and a limited-area model with a corresponding resolution of ~7 km (run at CSCS by MeteoSwiss). The computational needs for such forecasting is huge, and represents one of the largest computational tasks performed on a day-to-day operational basis.

The further development of forecasting models is well underway, and it is currently expected that the feasible horizontal resolution will go on increasing at a rate similar to that in the past. Thus, limited-area numerical models will reach a resolution of ~1 km within a few years. Such a high resolution has major advantages and offers exciting prospects. In particular, it will become feasible to dramatically improve the representation of the terrain and thereby to resolve major valleys and massifs of the Alpine topography. Furthermore, kilometer-scale resolution will for the first time allow explicit simulation of convective precipitation events. This kind of precipitation is characterized by deep and narrow ascent of moist warm air over a depth of many kilometers, a process which has been parameterized rather than simulated in the past, due to the lack of appropriate computational resolution. It is expected that the gain in resolution will improve the prediction of precipitation, including the occurrence of heavy events, and thereby contribute towards better prediction of runoff and flash flood events.

These developments are of considerable economic value since major flooding events can cause significant loss of life and large property damage. Indeed the southern side of the Alps is frequently affected by such events. The most recent of these, the devastating Gondo / Ticino / Piedmont flood of October 2000, resulted in 37 casualties and, according to SwissRe estimates, an insured property damage of ~450 million US$. The timely numerical prediction of heavy precipitation and runoff events in combination with real-time information from in-situ and remotely sensed observations could substantially mitigate these effects. An improved understanding of heavy precipitation events is also of considerable interest for the current

research on anthropogenic climate change, as the frequency of heavy precipitation events is one of the most pertinent, influential and sensitive characteristics of our climate.

The effective exploitation of the foregoing computational developments poses substantial challenges for the scientific community. First, the development of high-resolution models will need to be supplemented by accurate high-resolution observational data sets to provide initial conditions and to serve for forecast validation. Currently the operational meteorological data in the free Alpine atmosphere has a resolution of ~100 km. Second, the increase in resolution will need to be matched by the introduction of a new generation of atmospheric forecasting models. In the past, most forecasting models were based on the so-called hydrostatic approximation that becomes invalid at resolutions below ~10 km. The development and validation of non-hydrostatic numerical models requires a major effort. Third, there is a need to undergird these technical developments with a better understanding of the dynamical, physical and microphysical processes at scales below ~100 km.

In response to these challenges, the atmospheric and hydrologic scientific community are currently undertaking a major international research initiative. The Mesoscale Alpine Programme (MAP) was founded in 1994, and involves scientists from Europe and further abroad. MAP includes numerical, theoretical, and observational activities, and a major focus

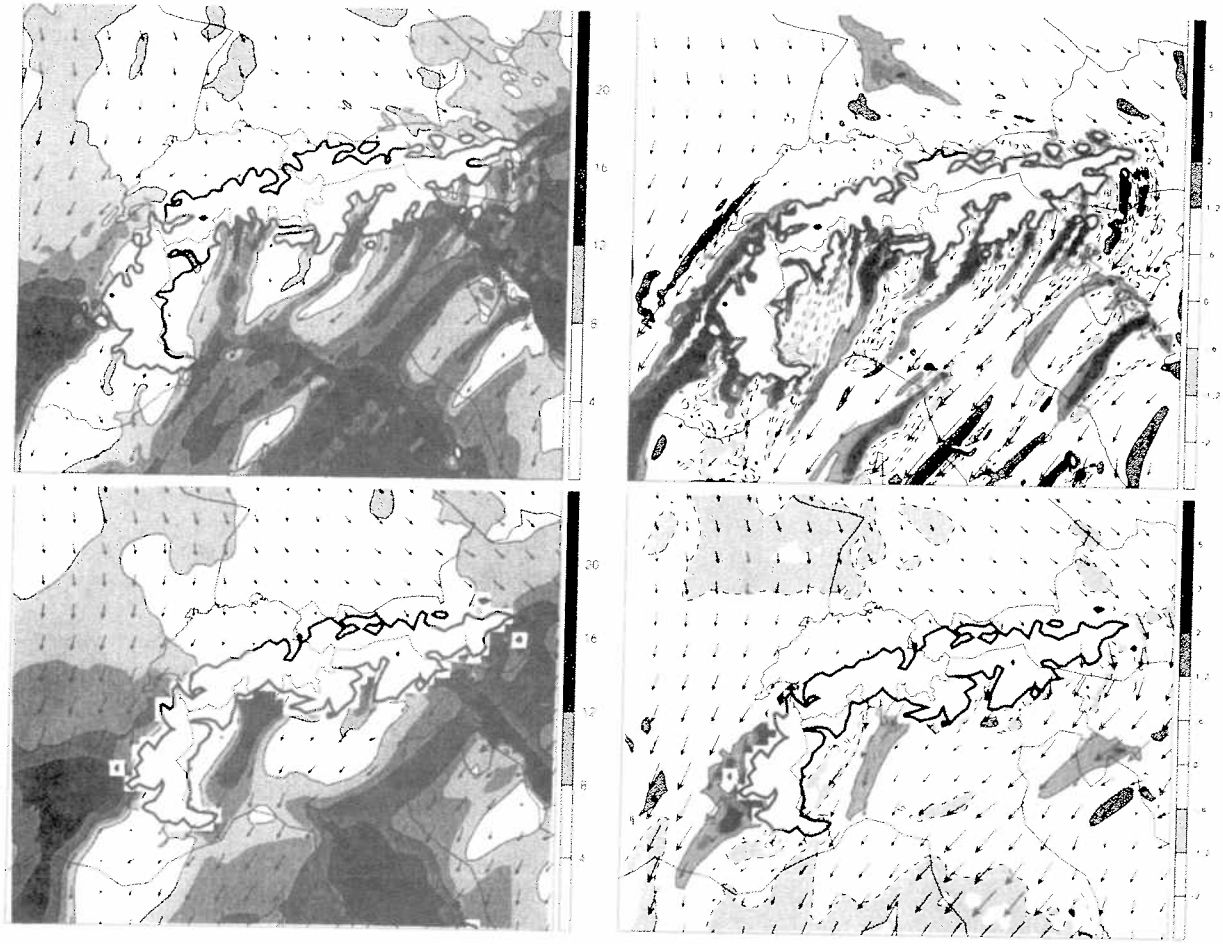

Fig.1: Numerical simulation of the Alpine wake. Horizontal wind velocity and vectors (left-hand panels, m/s) and potential vorticity PV (right-hand panels, pvu) on the 850 hPa level (approximately 1.5 km a.s.l.) on November, 8, 1999, 15 UTC. Upper and lower panels display, respectively, simulation results of the 3 km resolution MC2 model, and the 14 km resolution SM model.

was a large-scale international field campaign held in the autumn of 1999 (Binder and Schär 1996; Bougeault et al. 2001). This campaign was highly successful in monitoring several Alpine flow and precipitation events with unprecedented accuracy and resolution. During the field phase from September 7 to November 15, 1999, the standard meteorological monitoring was enhanced by the deployment of remote sensing instruments (surface-based Doppler radar networks, airborne dual-Doppler radar, Lidar and wind profilers) and the collection of in-situ data (both from surface-based and airborne observing system). Currently the data assembly and screening has largely been completed and data is available from the MAP data center run by the Institute for Atmospheric and Climate research of ETH (http://www.map.ethz.ch/).

2. High-resolution forecasting during the MAP field phase

In the context of MAP, the emergence of a new generation of high-resolution non-hydrostatic numerical weather prediction models was not only a key motivation, but also computer simulations undertaken at unprecedented resolution played a crucial role in the day-to-day organization of the scientific activities during the field experiment. Such simulations were used to provide timely warnings for the activation of measurement systems, and to gain early experience with a next-generation forecasting tool. The highest resolution model utilized in real time during the field phase was the Canadian MC2 code, one of the aforementioned advanced non-hydrostatic weather prediction models. During the MAP field phase, it was run in a collaborative effort between ETH Zürich, Environment Canada, and MeteoSwiss on the 12-CPU NEC SX-4 parallel-vector supercomputer at CSCS. Every night from 11 PM to 4 AM, the model was run in a dedicated mode and produced a daily forecast at a horizontal resolution of 3km, compared to the 14 km of the MeteoSwiss model that was operational at the time.

The real-time operations of the MC2 model were carefully validated against observational data (e.g., Benoit et al. 2001). Here we present some results pertaining to the dynamical effects of the Alps. Fig.1 presents a comparison of simulation results from the MC2 model with 3 km horizontal resolution against the SM forecasting model with 14 km resolution. The panels depict the Alpine wake in terms of horizontal wind velocity and potential vorticity fields on the 850 hPa level (approximately 1.5 km a.s.l.). The prevailing situation is one of strong northerly flow towards the Alps, leading to the onset of Mistral (to the southwest of the Alps), Bora (to the southeast) and north Föhn (over the major Alpine passes). The increased resolution of the 3 km simulation provides a highly detailed view of the Alpine

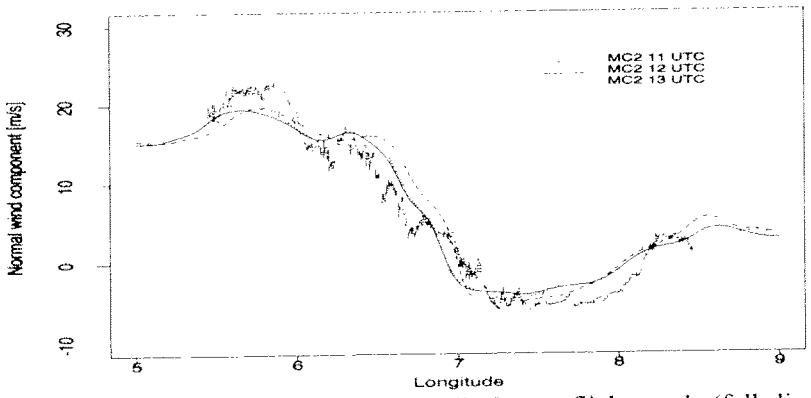

Fig.2: Comparison of in-situ wind observations perpendicular to flight track (full line) with respective prediction of the MC2 model (dashed line) at a pressure altitude of 3000 ft (about 900 m) across an Alpine shear line to the south of Nice (IOP 4, October 1, 12 UTC). The MC2 simulation results are plotted for the three consecutive times 11, 12, and 13 UTC.

wake. It is characterized by numerous narrow shear lines. In-situ observational data from two research aircraft were used to validate the numerical simulations. With respect to the dynamical fields, the higher-resolution MC2 model was often able to capture the structure of the observed fields with notable accuracy (see Fig.2, Schär et al. 2000).

3. Predictability of precipitation events

The atmosphere is a chaotic system. Thus, a numerical weather forecast, irrespective of its computational resolution, can only be skillfull for a limited time period, until the predictability is lost due to the growth of uncertainties in the initial conditions. To estimate the associated implications for weather forecasting, a PhD project is devoted to conducting so-called ensemble integrations. The members of an ensemble pertain to the same weather evolution but differ slightly in their initial conditions. The degreee of spread among the different forecasts can then be used as a measure of the predictability of the atmospheric state. On the synoptic scale (>1000 km), this technique is operationally used and was further refined during MAP (Fehlmann et al. 2000), but here consideration is given to the role of uncertainties with horizontal scales smaller than a few hundred kilometers.

To investigate the predictability of precipitation in different regions, selected weather situations are investigated using 24-hours ensemble simulations. Each ensemble contains six members. We use the MC2 model with 50 computational levels in the vertical, 3 km grid-spacing in the horizontal, and a domain of 1030 km x 880 km covering the European Alps. The simulations are conducted with a timestep of 30 seconds on the super-computer NEC-SX5/10 at the CSCS in Manno. First results of the study suggest that the predictability of precipitation differs strongly depending upon the weather type and the underlying terrain under consideration. In cases with strong convection, the limited predictability can invalidate a forecast on scales of O(100 km), even for short-term forecasting up to 24 hours. For illustration, the simulated hourly precipitation on 25 September 1999, 19 UTC is shown for three members of a 24 h ensemble simulation in Fig.3. The differences between the three patterns point towards the large uncertainties in simulations of heavy precipitation with strong embedded convection. While all ensembles members generate substantial precipitation in the Ticino region, there are appreciable differences concerning the distribution of precipitation into different catchments.

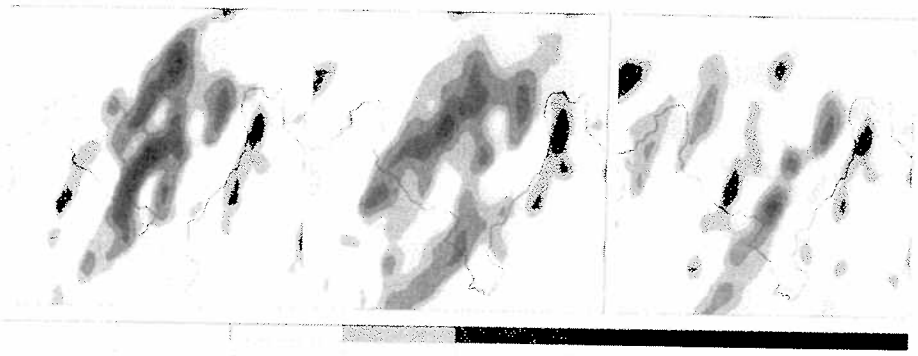

Fig.3: Inherent limitations to atmospheric predictability due to the chaotic nature of the atmospheric dynamics. Simulated hourly precipitation rate [mm/h] over the Ticino area on 25 September 1999, 19 UTC for three members of an ensemble simulation. The initial states of the ensemble members are barely distinguishable with today's operational data assimilation systems.

4. Idealized simulations of stratiform and convective precipitation

A particularly promising feature of high-resolution atmospheric simulations is the explicit representation of moist convection. Atmospheric convection is distinct from convection in classical fluid dynamics due to the driving role of the latent heat release in saturated updraughts, and is still poorly understood. In current weather prediction models, atmospheric convection is parameterized due to the smallness of the horizontal scales involved. A PhD project at our institute is devoted to the investigation of such processes with explicit convection-resolving integrations. To this end, idealized simulations are performed using the MC2 model running on the NEC-SX5 at the CSCS. The simulations employ a three-dimensional domain with a prescribed stably stratified flow profile directed perpendicular towards a two-dimensional ridge. The computational domain has a size of 490 km x 50 km with a gridspacing of 1 km in the horizontal. In the vertical, 65 model levels with a spacing between 80 m to 400 m are used.

Fig.4 shows a comparison of two simulations with different flow and precipitation regimes. In panel (a), the incoming flow is comparatively cold such as to yield a stably stratified flow. The response in the vertical motion field is characterized by vertically propagating atmospheric gravity-waves (see wave-train over obstacle), which form in response to the vertical density gradient. This flow regime leads to quasi-stationary clouds upstream and over the ridge, and to small and quasi-stationary stratiform precipitation rates over the obstacle. The flow in panel (b) is warmer, moister and more unstable. As a result, small-scale

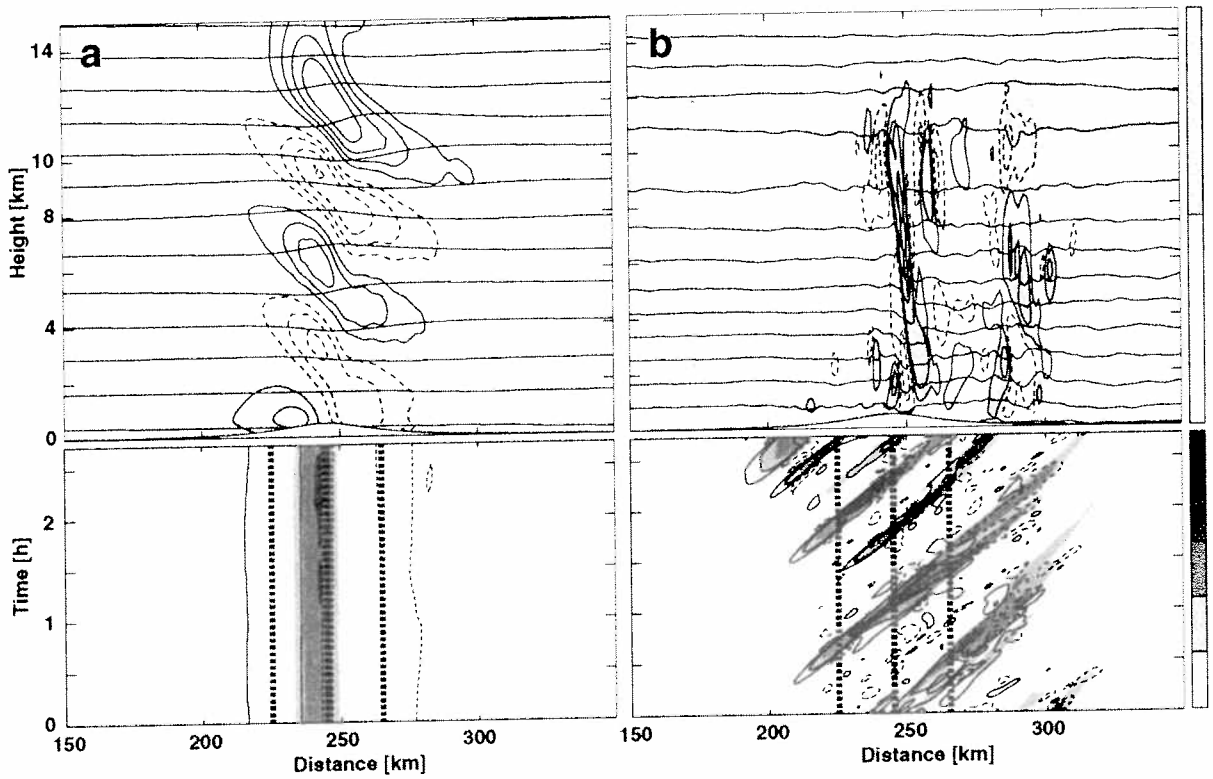

Fig.4: Moist airflow over an idealized two-dimensional ridge in the presence of (a) stratiform and (b) convective precipitation. The flow is from left to right. The upper panels show vertical x-z-sections, presenting vertical motion (contours, dashed for downward motion), clouds (shading) and potential temperature (thin contours). Note that the potential temperature is directly related to density. The lower panels present x-t-diagrams close to the surface with precipitation rates (shaded) and vertical motion (contours, dashed for downward motion). The bold dotted lines in the lower panels denote the topography at altitudes of 250 m and 500 m.

convective cells with strong updraughts are formed. These disrupt the propagating gravity waves of the stratiform flow regime and dominate the flow response. The corresponding *x-t*-diagram in panel (b) shows the respective formation of convective cells upstream of the obstacle, their propagation downstream and finally their decay some 50 km downstream of the ridge. The vertical winds and precipitation rates are much higher in this convective case than in the stratiform case shown in panel (a).

5 Outlook

Numerical weather prediction models with kilometer-scale resolution offer major advantages and exciting prospects for the prediction of flow and precipitation phenomena in mountainous regions. Successful implementation of this strategy will, however, require major efforts in wide range of aspects including data assimilation, dynamical model formulation, cloud microphysics and other parameterization schemes and model validation. In the medium term, it would also be desirable to replace the current limited-area deterministic forecasting procedures by probability forecasts.

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Walser, A., D. Lüthi, C. Schär, 2001: Predictability issues in high-resolution numerical modelling of stratiform and convective precipitation. MAP newsletter, 15, 235-241

5
CSE Research Projects

Title: Vortices in superconductors

Researchers: M. Bou-Diab, F. Mohamed, M. Troyer, G. Blatter [*]
I. Luk'yanchuk [**]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Landau Institute, Moscow, Russia

Description:

Vortices in type-II superconductors, caused by the intrusion of a magnetic field, form a new and unusual form of matter, so-called "vortex matter". Using numerical simulations we investigate two aspects in particular. The first are equilibrium ground state vortex configurations close to the quantum phase transition between type-I and type-II superconductors at $\kappa=1/\sqrt{2}$. The second project concerns the dynamics of vortex collisions, as a basis of a microscopic description of vortex lattice melting. Numerical simulations show that when two vortices collide, they recombine twice, and thus effectively cross.

References:

- M. Bou-Diab and G. Blatter, Phys. Rev. Lett. **86**, 5132 (2001).
- F. Mohamed, M. Troyer, G. Blatter and I. Luk'yanchuk, Preprint, submitted to Phys. Rev. B.

Title: Topologically protected quantum bits

Researchers: D. Ivanov, M. Troyer, G. Blatter [*]
L. Ioffe [**]
M.V. Feigel'man, A. Ioselevich [***]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Rutgers University, USA
[***] Landau Institute, Moscow, Russia

Description:

We propose an implementation of a topologically protected quantum bit based on Josephson junction arrays. A topologically protected quantum bit has the huge advantage that no error correction is needed, since it is stable to disorder because of its topological nature. Unfortunately the implementation of a topologically protected quantum bit has remained unclear so far. Based on numerical investigations of strongly correlated systems, we show how their developing an isolated two-fold degenerate quantum dimer liquid groundstate can be used in the construction of topologically stable qubits and discuss their implementation using Josephson junction arrays

References:

- L. Ioffe, M.V. Feigel'man, A. Ioselevich, D. Ivanov, M. Troyer and G. Blatter
Preprint, submitted to Nature

Title: Direct Numerical Simulation of Chemically Reactive Flows

Researchers: Christos E. Frouzakis*
Jerry Lee**
Ananias G. Tomboulides**
Konstantinos Boulouchos**

Institute/ Group: * Paul Scherrer Institute
** I.C. Engines and Combustion Technology Laboratory

Description:

Direct Numerical Simulation (DNS), although still severely limited by the availability of resources for application in turbulent reactive flows, can provide in-depth knowledge of fundamental problems in combustion. In addition, DNS results are of direct relevance to the proper modeling of turbulence and chemistry. Our DNS code is based on a high-order time splitting scheme and the spectral element method for the time-accurate integration of the low Mach number form of the conservation equations. It is capable of incorporating chemical kinetics and transport models of various complexities. Recently, the code was used to study diffusion flame-vortex interactions and edge flames in a hydrogen/air opposed-jet burner. The aim of both studies was to improve our understanding of turbulent reactive flows as described by flamelet theory. In addition to the application of the code in the detailed study of problems of fundamental interest in laminar combustion, we are extending its capabilities to the study of phenomena in the transitional/early-turbulent regime.

References:

C. E. Frouzakis, A. G. Tomboulides, J. Lee, K. Boulouchos, From diffusion to premixed flames in an H_2/air opposed-jet burner: the role of edge flames, *Combust. Flame*, submitted, (2001)

C. E. Frouzakis, Y. Kevrekidis, J. Lee, K. Boulouchos, A. Alonso, Proper Orthogonal Decomposition of Direct Numerical Simulation data: data reduction and observer construction, *Proc. Combust. Inst.*, **28**, pp. 75-81, (2000).

J. Lee, C. E. Frouzakis, and K. Boulouchos, Two–Dimensional Direct Numerical Simulation of Opposed-Jet Hydrogen/Air Flames: Transition from a Diffusion to an Edge Flame, *Proc. Combust. Inst.*, **28**, pp. 801-806, (2000).

J. Lee, C. E. Frouzakis, and K. Boulouchos Numerical Study of Opposed-jet H_2/air Diffusion Flame - Vortex Interactions, *Combust. Sci. Techn.*, **158**, pp. 365-388, (2000).

A. Tzannis, J. Lee, P. Beaud, H. Frey, T. Greber, B. Mischler, P. Radi, K. Boulouchos, Application of Resonant Holographic Interferometry to OH Concentration Measurements in a two-dimensional CO-Flow H2/Air Diffusion Flame and Comparison with Direct Numerical Simulations, *Flow Turb. Combust.*, **64**, p. 183-196, (2000).

J. Lee, R. A. Yetter, S. A. Orszag, F. L. Dryer. Simulation and Analysis of Laminar Flow Reactors, *Combust. Sci. Techn.*, **159**, pp. 199-211, (2000)

Title:	Numerical modelling of extratropical weather systems
Researchers:	Huw C. Davies Heini Wernli Cornelia Schwierz Sebastien Dirren, Patrick Koch, Mark Liniger, Matthias Zillig
Institute/ Group:	Institute for Atmosphere and Climate Group for dynamic meteorology

Description:

A state-of-the-art numerical weather prediction model (the HRM from the German Weather Service) is used to investigate the detailed dynamical and physical processes that determine the evolution of various extratropical weather systems, including storms, severe precipitation events and anticyclonic blockings. The numerical simulations serve on the one hand to obtain a detailed data set used for the investigation of the system, and on the other hand to determine the impact of distinct features/processes by performing sensitivity experiments with changed initial conditions or model parameterizations. Particular consideration has been given to (i) the flash-floods of Brig (1993) and Piedmont (1994), (ii) the interaction of moist diabatic processes and the Greenland orography for the formation of the North Atlantic blocking, and (iii) a mesoscale investigation of the life-cycle of the extreme winter storm 'Lothar'.

References:

Fehlmann, R., C. Quadri und H. C. Davies, 2000. An Alpine rainstorm: Sensitivity to the mesoscale upper-level structure. *Wea. Forecasting,* **15,** 4-28.

Massacand, A. C., H. Wernli und H. C. Davies, 2001. Influence of upstream diabatic heating upon an Alpine event of heavy precipitation. *Mon. Wea. Rev.,* in press.

Rossa, A. M., H. Wernli und H. C. Davies, 2000. Growth and decay of an extra-tropical cyclone's PV-tower. *Meteorol. Atmos. Phys.,* **73,** 139-156.

Wernli, H., S. Dirren, M. A. Liniger und M. Zillig, 2001. Dynamical aspects of the life-cycle of the winter storm 'Lothar' (24-26 December 1999). *Quart. J. Roy. Meteor. Soc.,* in press.

Title:	Temperature, ozone and denitrification in the Arctic winter stratosphere
Researchers:	Thomas Peter Sandro Buss, Stefan Füglistaler Heini Wernli
Institute/ Group:	Institute for Atmosphere and Climate Groups for dynamic meteorology and atmospheric chemistry

Description:

Stratospheric ozone loss in the Arctic winter shows a large year-to-year variability. For instance in 1999/2000, which was an extremely cold winter (in the stratosphere), the Arctic ozone loss was extremely large (up to 70% at altitudes of ~20 km), whereas one year earlier temperatures were much warmer and practically no ozone loss occurred. The reason for this drastic sensitivity to temperature of stratospheric ozone depletion is the necessity of very cold temperatures for the formation of polar stratospheric clouds and subsequent ozone activation. Dynamical processes like the vertical propagation of gravity waves above the Arctic mountains (Greenland and Scandinavia) can lead to transient mesoscale cooling events and stratospheric cloud formation. Our investigations are based upon (i) high-resolution numerical model simulations for the gravity wave propagation, (ii) detailed analyses of observational and global data sets and (iii) comprehensive Lagrangian transport calculations for the issue of denitrification. The results indicate the importance of mesoscale dynamical processes for the understanding of Arctic ozone loss.

References:

Buss, S., H. Wernli, T. Peter, R. Kivi, P. T. Bui, A. Kleinböhl and C. Schiller, 2001. Arctic stratospheric temperature in the winters 1999/2000 and 2000/2001: a quantitative assessment and microphysical implications. *J. Geophys. Res.*, submitted.

Title: Computational Solid State Electronics

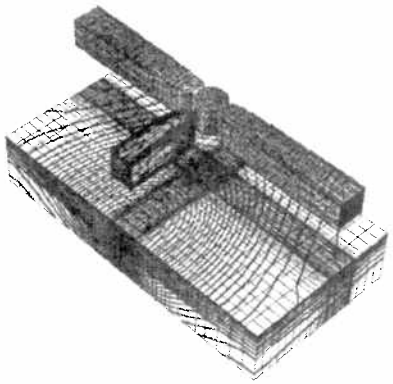
Researchers: Wolfgang Fichtner
Andreas Schenk
Andreas Witzig
Jens Krause
Eduardo Alonso
Dölf Aemmer

Institute/ Group: Integrated Systems Laboratory/
Technology Computer Aided Design (TCAD) Group

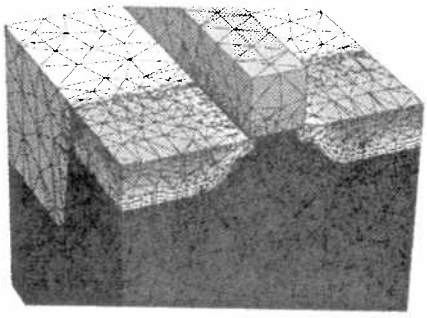
Description:

For the development of novel micro- and opto-electronic processes, devices and circuits, the use of advanced numerical simulation tools has become indispensable. With the continuing advances in semiconductor technology, and the trend to further scaling of the active device dimensions, computational solid state electronics has reached an extremely high level of physical and numerical sophistication. As we are rapidly approaching nanoscale dimensions, effects at the atomistic or quantum-mechanical level are becoming dominant.

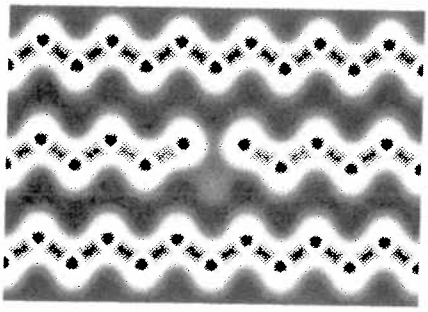
We are performing research in a variety of fields in the computational solid state electronics domain. Current projects include the development and utilization of new simulations tools for molecular dynamics studies in material diffusion, novel devices such as single-electron transistors, and optoelectronic devices such as LEDs and laser diodes. For all of our projects, the main emphasis lies in the exploration how accurate physical models can be pragmatically combined with state-of-the-art numerical algorithms. The following pictures illustrate some of our activities:



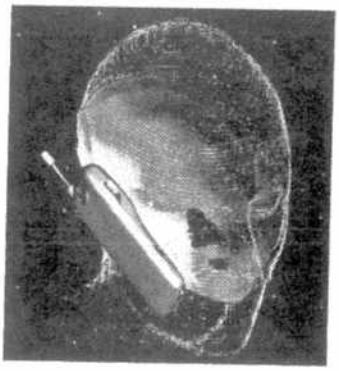
Quantum mechanical simulation of a single electron transistor in Silicon-on-Insulator technology.



Mesh generation of a trench isolated MOS transistor created by Normal Offsetting algorithm.



Electron density simulation of a single vacancy in silicon using LDA (Local Density Approximation) with VASP.



Simulation of electromagnetic fields for EMC, antenna design and dosimetry using SEMCAD.

Title: Solitons in the nonlinear Hartree Equation

Researchers: W.H Aschbacher, J. Fröhlich, G. Interlandi, M. Troyer,

Institute/Group: Theoretische Physik, ETH Zürich

Description:

This project concerns minimizers (lowest energy eigenfunctions) of the Hartree energy functional with attractive Hartree interaction. Among the most important findings is a symmetry breaking of the ground state wave function when the interaction is sufficiently strong. We also investigate the time evolution of such soliton-like minimizers in an external potential. As a particular application of these results and as a motivation for the investigation of the Hartree functional, we propose a generalization of the Gross-Pitaevskii functional of Bose-Einstein condensation for *attractive* interatomic forces that overcomes the breakdown of this theory at the collapse point of the condensate.

References:

- W.H. Aschbacher, PhD Thesis (ETH Zürich, 2001)
- G. Interlandi, Diploma thesis (ETH Zürich, 2000)
- W.H. Aschbacher, J. Fröhlich, G.M. Graf, K. Schnee, M. Troyer, Preprint

Title: A strategy for analysis of (molecular) equilibrium simulations: Configuration space density estimation, clustering, and visualization

Researchers: Fred A. Hamprecht
Christine Peter
Xavier Daura
Walter Thiel*
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie
*Max-Planck-Institut für Kohlenforschung
Mülheim, Germany

Description:

We propose an approach for summarizing the output of long simulations of complex systems, affording a rapid overview and interpretation. First, multidimensional scaling techniques are used in conjunction with dimension reduction methods to obtain a low-dimensional representation of the configuration space explored by the system. A nonparametric estimate of the density of states in this subspace is then obtained using kernel methods. The free energy surface is calculated from that density, and the configurations produced in the simulation are then clustered according to the topography of that surface, such that all configurations belonging to one local free energy minimum form one class. This topographical cluster analysis is performed using basin spanning trees which we introduce as subgraphs of Delaunay triangulations. Free energy surfaces obtained in dimensions lower than four can be visualized directly using iso-contours and -surfaces. Basin spanning trees also afford a glimpse of higher-dimensional topographies. The procedure is illustrated using molecular dynamics simulations on the reversible folding of peptide analoga. Finally, we emphasize the intimate relation of density estimation techniques to modern enhanced sampling algorithms.

References: J. Chem. Phys. **114** (2001) 2079-2089

Title: Comparison of different schemes to treat long-range electrostatic interactions in molecular dynamics simulations of a protein crystal

Researchers: Regula Walser
Philippe H. Hünenberger
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie

Description:

Eight molecular dynamics simulations of a ubiquitin crystal unit cell were performed in order to investigate the effect of different schemes to treat the long-ranged electrostatic interactions as well as the need to include counter ions. A crystal system was chosen as the test system, since the higher charge density compared to a protein in solution makes it more sensitive to the way of treating the electrostatic interactions. Three different schemes of treating the long-ranged interactions were compared: straight cut-off, reaction-field approximation and a lattice-sum method (P^3M). For each of these schemes two simulations were performed, one with and one without the counter ions. Two additional simulations with a reaction-field force and different initial placements of the counter ions were performed in order to examine the effect of the initial positions of the ions. The inclusion of long-range electrostatic interactions using either a reaction-field or a lattice-sum method proved to be necessary for the simulation of crystals. These two schemes did not differ much in their ability to reproduce the crystallographic structure. The inclusion of counter ions on the other hand seems not necessary for obtaining a stable simulation. The initial positions of the ions have a visible but small effect on the simulation.

References: Proteins **44** (2001) 509-519

Title: An improved GROMOS96 force field for aliphatic hydrocarbons in the condensed phase

Researchers: Lukas D. Schuler
Xavier Daura
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie

Description:

Over the past four years the GROMOS96 force field has been successfully used in biomolecular simulations, e.g. in peptide folding studies and detailed protein investigations, but no applications to lipid systems have been published yet. Here we provide a detailed investigation of aliphatic liquid systems. For liquids of larger aliphatic chains, *n*-heptane and longer, the standard GROMOS96 parameter sets 43A1 and 43A2 yield a too low pressure at the experimental density. Therefore, a reparametrisation of the GROMOS96 force field regarding aliphatic carbons was initiated. The new force field parameter set 45A3 shows considerable improvements for *n*-alkanes, cyclo-, iso- and neoalkanes and other branched aliphatics. Liquid densities and heat of vaporisation are reproduced for almost all of these molecules. Excellent agreement is found with experiment for the free energy of hydration for alkanes. The GROMOS96 45A3 parameter set should therefore be suitable for application to lipid aggregates such as membranes and micelles, for mixed systems of aliphatics with or without water, for polymers and other apolar systems that may interact with different biomolecules.

References: J. Comput. Chem. **22** (2001) 1205-1218

Title: A comparison of seven fast but approximate methods to compute the free energy of deprotonation for amino acids in aqueous solution

Researchers: Roland Bürgi
Florian Läng
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie

Description:

In recent years, a variety of methods based on statistical mechanics have been successfully applied to calculate free energy differences of chemical reactions from molecular simulation. The accuracy and computational efficiency vary strongly between these methods. Seven approximate but fast methods to calculate free energy differences are compared in terms of accuracy and efficiency with the accurate but expensive thermodynamic integration method as reference, using 28 protonation and deprotonation reactions of aspartic acid in aqueous solution as test cases. At least two simulations are required to obtain an accurate free energy difference between two states of the system. Both, the averaged one-step perturbation method and the linear response method yield the most accurate results, while the latter method shows the fastest convergence.

References: Mol. Simulation (2001) in press

Title: Chemical library subset selection algorithms: A unified derivation using spatial statistics

Researchers: Fred A. Hamprecht
Walter Thiel*
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie
*Max-Planck-Institut für Kohlenforschung
Mülheim, Germany

Description:

If similar compounds have similar activity, rational subset selection becomes superior to random selection in screening for pharmacological lead discovery programs. Traditional approaches to this experimental design problem fall into two classes: (i) a linear or quadratic response function is assumed; (ii) some space filling criterion is optimized. The assumptions underlying the first approach are clear but usually not defendable; the second approach yields more intuitive designs, but lacks a clear theoretical foundation. We model activity in a bioassay as realization of a stochastic process and use the best linear unbiased estimator to construct spatial sampling designs that optimize the integrated mean square prediction error, the maximum mean square prediction error or the entropy. We argue that our approach constitutes a unifying framework encompassing most proposed techniques as limiting cases and sheds light on their underlying assumptions. We suggest to use either the integrated mean square prediction error or the entropy as optimization criteria rather than approximations thereof, and propose a scheme for direct iterative minimization of the integrated mean square prediction error. Finally, we discuss how the quality of chemical descriptors manifests itself and clarify the assumptions underlying the selection of diverse or representative subsets.

References: submitted to J. Chem. Inf. Comput. Sci. (2001)

Title: Water in protein binding cavities: Implementation of a method to identify internal water and exchange pathways and application to fatty acid binding protein

Researchers: Dirk Bakowies
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie

Description:

A computational approach based on Delaunay triangulation is presented to identify internal water molecules in proteins and to capture pathways of exchange with the bulk. The implemented procedure is computationally efficient and can easily be applied to long molecular dynamics trajectories of protein simulations. In an application to fatty acid binding protein in *apo*-form and with bound palmitate, several protein orifices known from crystal structures have been confirmed to be major portals of solvent exchange. Differences between the two forms of the protein are observed and discussed.

References: submitted to Proteins (2001)

Title: One-step perturbation methods for solvation free energies of polar solutes

Researchers: Jed W. Pitera
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie

Description:

The one-step perturbation approach to free energy calculations permits the calculation of relative free energies for a number of end-states from a single simulation of a carefully-chosen reference state. This approach has successfully been used for the calculation of relative and absolute solvation free energies of nonpolar solutes in water, as well as relative binding free energies for a family of nonpolar protein ligands. We have investigated several possible approaches to extend one-step perturbation methods to also obtain accurate solvation free energies of polar species. A "soft dipole" reference state permits the determination of accurate relative solvation free energies for polar solutes (average unsigned error < 2.0 kJ/mol) but does not yield accurate absolute solvation free energies. However, contrary to expectations, simulations of a neutral reference state even yield accurate (average unsigned error < 2.9 kJ/mol) absolute solvation free energies for polar solutes when translational and rotational sampling of the solute is included. In general, the choice of an appropriate reference state for one-step perturbation is a challenge due to complex many-body effects. Nonetheless, the one-step perturbation method combined with an unphysical reference state yields accurate free energy estimates with an efficiency several times greater than traditional approaches.

References: submitted to J. Phys. Chem. A (2001)

Title: Simulating proteins at constant pH: An approach combining molecular dynamics and Monte Carlo simulation

Researchers: Roland R. Bürgi
Peter A. Kollman*
Wilfred F. van Gunsteren

Institute/ Group: Laboratory of Physical Chemistry
Gruppe für Informatikgestützte Chemie
*University of California
San Francisco, USA
(Peter Kollman deceased in spring 2001)

Description:

For the structure and function of proteins, the pH of the solution is one of the determining parameters. Current molecular dynamics (MD) simulations account for the solution pH only in a limited way by keeping each titratable site in a chosen protonation state. We present an algorithm that generates trajectories at a Boltzmann distributed ensemble of protonation states by a combination of MD and Monte Carlo (MC) simulation. The algorithm is useful for pH dependent structural studies and to investigate in detail the titration behaviour of proteins. The method is tested on the acidic residues of the protein hen egg white lysozyme. It is shown that small structural changes may have a big effect on the pK_A values of titratable residues.

References: submitted to Proteins (2001)

Title: Anisotropic photodissociation of $CH_3Cl^{+\cdot}$ radical cation

Researchers: T.-K. Ha
M.S. Kim*
D.S. Won*

Institute/ Group: Laboratory of Physical Chemistry
*Department of Chemistry, Seoul National University, Korea

Description:

Photodissociation of the methyl chloride ion has been investigated using mass-analyzed ion kinetic spectroscopy (MIKES). The MIKE spectrum for the chlorine atom loss from the methyl chloride ion has been measured as a function of the laser polarization angle at 357, 488 and 514 nm. The anisotropy parameters and kinetic energy release distributions have been determined.

At all the wavelength used , an anisotropic dissociation (β=1.2) in the repulsive excited electronic state has been observed. Results from quantum chemical calculations carried out at various levels suggest that the methyl chloride ion is excited to the first electronic excited state, A', and dissociates repulsively in this state.

References: D.S. Won, M.S. Kim and T.-K. Ha, J. Chem. Phys., in press (2001)

Title: A theoretical study of the anionic intermolecular hydrogen bonding between dihydroxy tetrahydrofuran and phosphate ions

Researchers: T.-K. Ha
O. Suleimenov
* M.J. Han

Institute/ Group: Laboratory of Physical Chemistry
*Ajou University, Suwon, Korea

Description:

The formation of strong hydrogen bonds between 3,4-cis-dihydroxy tetrahydrofuran (DHTHF) and diphosphate anion ($H_2PO_4^-$) and between DHTHF and phosphate dianion (HPO_4^{-2}) was detected by quantum chemical studies. Quantum chemical calculations done using the ab initio MP2 level of theory and using the density functional theory with the B3LYP/aug-cc-pVTZ basis set showed that the hydrogen bond distances are rather short,the dissociation energies of the hydrogen bonds are quite large, and the shifts of the OH-stretching frequencies of DHTHF in the adducts are very large. Based on these theoretical results, a mechanism has been proposed to interpret the catalytic activity of the ribose containing polymers for the cleavage of DNA.

References:

T.-K. Ha, O. Suleimenov and M.J. Han, J. Mol. Struct., (Theochem), in press (2001)
M.J. Han, K.S. Yoo, J.Y. Chang and T.-K. Ha, Angew. Chem. Int. Ed. Engl., 39, 347 (2000)

Title: Ab initio study of the open-shell van der Waals complex

Researchers: T.-K. Ha
M. Schaefer
A. Bauder

Institute/ Group: Laboratory of Physical Chemistry

Description:

The rotational spectrum of the open-shell complex argon-chlorine dioxide has been measured between 5-24 GHz with a pulsed nozzle Fourier transform microwave spectrometer. The complex displays a- and c-type spectra, the latter of which is shifted by internal motion of the ClO_2 unit. Structure information has been gained from the analysis of the rotational constants and of the fine and hyperfine structure parameters of the Ar-$^{35}ClO_2$ and Ar-$^{37}CO_2$ complexes. Changes of the electronic structure of ClO_2 upon complexation are shown to be small. The observed tunneling effect was analysed with a model of an internal rotation of the ClO_2 subunit around its axis. The complex structure has been explored by ab initio calculations. The equilibrium structure of the complex has been investigated at the second-order spin-unrestricted Möller-Plesset (UMP2) level of theory employing the aug-cc-pvTZ basis set. Similar ab initio studies have also been performed for some open-shell as well as closed-shell van der Waals complexes such as Ar-NO_2, Ar-O_3 and Ar-SO_2 in order to compare with the available experimental values.

References: M. Schaefer, T.-K. Ha and A. Bauder, J. Chem. Phys., in press (2001)

Title: Quantum chemical study of van der Waals complexes: CH_2XCH_2X . Ar

Researchers: T.-K. Ha
H.H. Gunthard

Institute/ Group: Laboratory of Physical Chemistry

Description:

The present investigation is directed towards an analysis of the interaction potential of Ar atoms and 1,2-difluoroethane as derived from high level quantum chemical calculations. The quantum chemical data will be used to derive atom pair interaction potentials (Lenard-Jones/Born-Buckingham) and electrostatic contributions based on a molecular multipole model including mutual polarization. These pair potentials will be compared with empirical pair potentials (used frequently in consistent force free models of matrix isolated molecules) with the aim to arrive at a more reliable parameters. Furthermore, the molecular multipole approach should be compared with the localized multipole approximation commonly used for interpretation of stability and molecular structure of rare gas-molecule van der Waals complexes

References: A manuscript is in preparation.

[1] T.-K. Ha and H.H. Gunthard, Chem. Phys., 134 (1989) 203-228
[2] R. Gunde, T.-K. Ha and H.H. Gunthard. Chem. Phys., 45 (1990) 37-65
[3] R. Gunde, H.J. Keller, T.-K. Ha and H.H. Gunthard, J. Phys. Chem., 95 (1991) 2802

Title: Interaction between torsional and vibrational degrees of freedom of simple molecules

Researchers: T.-K. Ha
H.H. Gunthard

Institute: Laboratory of Physical Chemistry
Group:

Description:

In quantum chemical studies of vibrational force fields of 1,2-difluoroethane and related molecules it was observed that the neglect of interaction constants between stretching or bending modes and the torsional mode introduces alterations of vibrational frequencies by up to 25 cm^{-1}. The present investigation relates to the analogous situation for matrix isolated molecules, basing on one hand on high level quantum chemical molecular potential functions, on the other hand, on extending existing computer programs for molecular mechanics of rare gas matrix-molecule systems (M_n – A, n>400) to allow use of the complete harmonic force fields. This should allow more exact estimation of matrix shifts, extrapolation to force free state spectra and exploration of the mechanism of conformer conversion by infrared radiation.

References: A manuscript is in preparation.

Title: Parallelization of a finite element code to simulate bulk forming processes

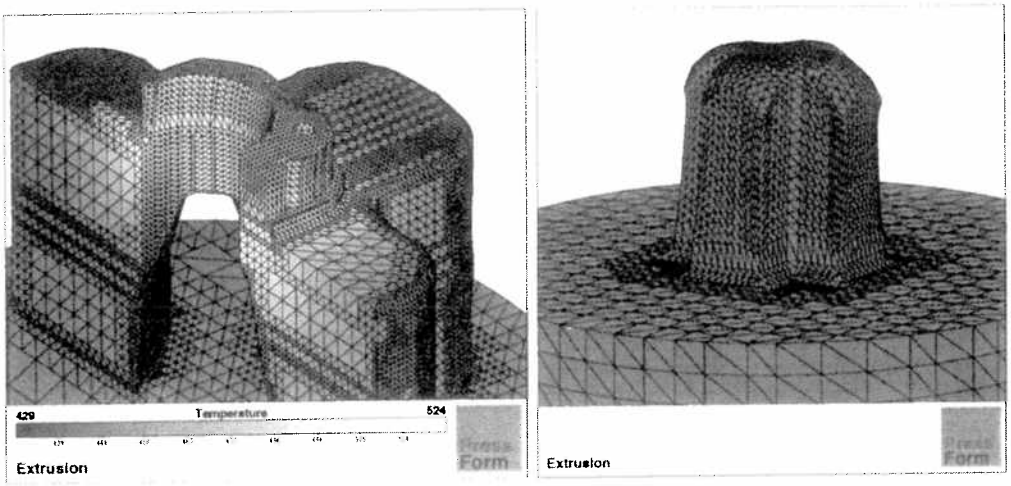
Researchers: Andreas Unterkircher
Longchang Tong
Pavel Hora
Josef Reissner

Institute/ Group: Institute of virtual production

Description:

For the planning of 3D bulk metal forming processes nonlinear finite element methods are used. Based on the code PressForm which has been developed at the institute the two most time consuming tasks have been parallized: assembling the stiffness matrix and solving the linear equations. Applying ideas from graph theory, a new algorithm for parallel assembling has been designed. Compared to existing solutions this algorithm is easy to implement as well as independent of dimension and element type. For equation solving we use the conjugate gradient method with all major tasks being done concurrently. In addition we developed a multiplicative Schwarz type preconditioner. This preconditioner reuses data structures from parallel assembling. As a result both the construction as well as the application of the preconditioner can be done in parallel. For the linear systems appearing in PressFrom this preconditioner exhibits a better efficiency than Jacobi and incomplete Cholesky methods.

References: A. Unterkircher, P. Berkes, J. Reissner: An efficient algorithm for parallel stiffness matrix assembling on shared memory machines. Simulation of Material Processing: Theory, Methods and Applications, K. Mori(ed.), Rotterdam: Balkema, 2001, 173-176.



Title: Simulations for tribology on different length scales

Researchers: Thomas Bonner
Reto Grüebler

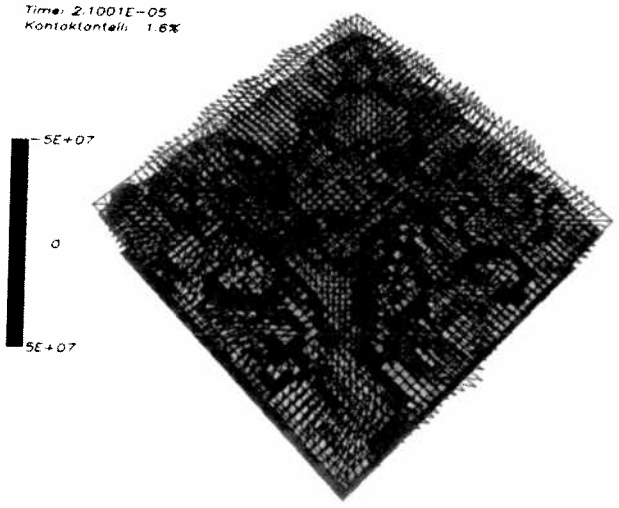
Institute/ Group: Institute for virtual manufacturing
Institut für virtuelle Produktion

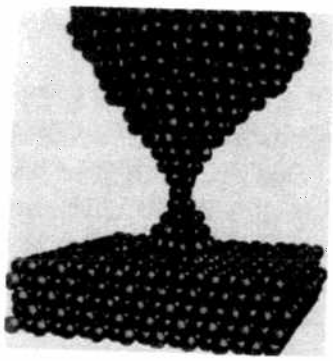
Description:

For the simulation of tribological systems relevant to the industrial manufacturing praxis different length scales are considered: While the hydrodynamic part of the friction, which is influenced mostly by the lubricant and the surface roughness, is modeled by means of finite element methods, molecular dynamics simulations are employed for the places where boundary lubrication occurs. For the latter three different regimes are identified: First a thin layering regime is reached, where the discretization by single molecules becomes apparent and the remaining layers inbetween show a solid-like behavior. Next, anti-wear additives with special head groups, to favor the adsorption onto the surface, are building up carpet-like protective layers on the surface. Finally, under severe conditions, extreme pressure additives come into play to react at the points with elevated temperatures (under optimum conditions this happens only at the asperities where friction is taken place) and to form very hard, protective EP-layers. They may be bad lubricants, but their function is to protect the surface against microwelding between the two surfaces.

References:

J. Reissner, R. Grüebler, Th. Bonner. Tribosimulation. in: Umformtechnik 2000 Plus, S. 245 - - 254, Festschrift zu Ehren von Professor Kurt Lange, Herausgeber: M. Geiger.





Title: Computational Analysis of PKA-Balanol Interactions

Researchers: Chung F. Wong[***]
Philippe H. Hünenberger[*]
Pearl Akamine[**]
Narendra Narayana[**]
Tom Diller[**]
J. Andrew McCammon[**,***]
Susan Taylor[**]
Nguyen-Huu Xuong[**]

Institute/ Group: [*] Laboratory of Physical Chemistry
[**] UCSD, Department of Chemistry & Biochemistry
[***] UCSD, Department of Pharmacology

Description :

Protein kinases are important targets for designing therapeutic drugs. This study illustrates a computational approach to extend the usefulness of a single protein-inhibitor structure in aiding the design of protein kinase inhibitors. Using the complex structure of the catalytic subunit of PKA (cPKA) and balanol as a guide, we have analyzed and compared the distribution of amino acid types near the protein-ligand interface for nearly 400 kinases. This analysis has identified a number of sites that are more variable in amino acid types among the kinases analyzed, and these are useful sites to consider in designing specific protein kinase inhibitors. On the other hand, we have found kinases whose protein-ligand interfaces are similar to that of the cPKA-balanol complex and balanol can be a useful lead compound for developing effective inhibitors for these kinases. Generally, this approach can help us discover new drug targets for an existing class of compounds that have already been well characterized pharmacologically. The relative significance of the charge/polarity of residues at the protein-ligand interface has been quantified by carrying out computational sensitivity analysis in which the charge/polarity of an atom or functional group was turned off/on, and the resulting effects on binding affinity have been examined. The binding affinity was estimated by using an implicit-solvent model in which the electrostatic contributions were obtained by solving the Poisson equation and the hydrophobic effects were accounted for by using surface-area dependent terms. The same sensitivity analysis approach was applied to the ligand balanol to develop a pharmacophoric model for searching new drug leads from small-molecule libraries. To help evaluate the binding affinity of designed inhibitors before they are made, we have developed a semiempirical approach to improve the predictive reliability of the implicit-solvent binding model.

References: Wong, C.F., Hünenberger, P.H., Akamine, P., Narayana, N., Diller, T., McCammon, J.A., Taylor, S. & Xuong, N.-H.
J. Med. Chem. **44** (2001) 1530-1539.

Title: Explicit-solvent molecular dynamics simulation at constant pH: methodology and application to simple amines

Researchers: Ulf Börjesson*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

A method is developed for performing classical explicit-solvent molecular dynamics (MD) simulation s at constant pH, where the protonation state of each ionizable (titratable) group in a simulated compound is allowe d to fluctuate in time, depending on the instantaneous system configuration and the imposed pH. In this method, each ionizable group is treated as a mixed state, *i.e.* the interaction-function par ameters for the group are a linear combination of those of the protonated state and those of the deprotonated stat e. Free protons are not handled explicitly. Instead, the extent of deprotonation of each group is relaxed towards its equilibrium value by weak-coupling to a "proton bath". The method relies on pre-calibrated empirical functio ns, one for each type of ionizable group present in the simulated compound, which are obtained through multiple MD simulations of monofunctional model compounds. In this study, the method is described in detail and its application illustrated by a series of co nstant-pH MD simulations of small monofunctional amines. In particular, we investigate the influence of the rel axation time used in the weak-coupling scheme, the choice of appropriate model compounds for the calibration of the required empirical functions, and corrections for finite-size effects linked with the small size of the simulation box.

References: Börjesson, U. & Hünenberger, P.H.
J. Chem. Phys. **114** (2001) 9706-9719.

Title: Comparison of four methods to compute the dielectric permittivity of liquids from molecular dynamics simulations.

Researchers: Tim N. Heinz*
Wilfred F. van Gunsteren*
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry

Description :

Four methods to compute the dielectric permittivity ϵ of a liquid from molecular simulations are compared in the context of the simple point charge (SPC) water model. In the first method (unrestrained method), ϵ is evaluated from the fluctuations of the box dipole moment M, monitored during a single equilibrium simulation. In the three other methods, ϵ is evaluated from the probability distribution $p(M)$ of the dipole moment norm. This distribution is itself evaluated in three different ways : (*i*) from multiple simulations involving a M-dependent biasing potential (umbrella-sampling method), (*ii*) from multiple simulations involving a constrained dipole moment norm (M-constraint method), or (*iii*) from fitting of incomplete $p(M)$ estimates to a Maxwell distribution (fitting method). The four methods are shown to converge to an identical estimate of $\epsilon = 61 \pm 1$ for SPC water (256 molecules, reaction-field electrostatics). The convergence properties, advantages, and drawbacks of the different methods are analyzed in detail.

References: Heinz, T.N., van Gunsteren, W.F. & Hünenberger, P.H. J. Chem. Phys. **115** (2001) 1125-1136.

Title: Calculation of the group-based pressure in molecular simulations : I. A general formulation including Ewald and particle-particle–particle-mesh electrostatics.
II. Numerical tests and application to liquid water.

Researchers: Baldomero Oliva**
Philippe H. Hünenberger*

Institute/ Group: * Laboratory of Physical Chemistry
** Institut de Biologia Fonamental, Universitat Autòma de Barcelona

Description :

A general formulation is given for the calculation of the isotropic or anisotropic group-based instantaneous pressure in molecular simulations under periodic boundary conditions. The equations, derived from the statistical mechanical definition of the pressure, apply to groups defined as single atoms (atomic pressure), whole molecules (molecular pressure), but also to any other arbitrary atom grouping. Different definitions lead to different pressure fluctuations, but to the same average pressure. Two sets of equations are derived for the calculation of the group-based virial. The "traditional" set, which is the one commonly used to compute molecular pressures in simulations, has two main drawbacks : (*i*) it requires bookkeeping of group definitions in the inner loop of the non-bonded interaction calculation ; (*ii*) it cannot be applied when electrostatic interactions are computed through lattice-sum methods. The "alternative" set is based on the remarkable result that any group-based virial can be computed from the atomic virial by adding a computationally inexpensive correction term to account for atom grouping. This new formalism presents the following advantages : (*i*) it requires no bookkeeping of group definitions in the inner loop of the non-bonded interaction calculation ; (*ii*) the isotropic virial corresponding to each homogeneous pairwise interaction term can be computed directly from the corresponding interaction energy contribution without knowledge of the pairwise forces ; (*iii*) application to lattice-sum electrostatics is straightforward. "Traditional" and "alternative" virial expressions are derived for all terms typical of interaction functions used in molecular simulations. The validity and consistency of the different equations derived are assessed through a series of numerical tests. In the case of P^3M electrostatics, a problem associated with the loss of accuracy of the force calculation due to volume fluctuations in constant-pressure simulations is also discussed. Finally, the new formalism is applied to constant-volume and constant-pressure simulations of systems containing 16 to 1024 simple-point-charge (SPC) water molecules.

References: (I) Hünenberger, P.H. and (II) Oliva, B. & Hünenberger, P.H. Submitted to J. Chem. Phys.

Title: A new Field Solver for Space Charge dominated Beams

Researchers: Andreas Adelmann*
Stefan Adam *
Rolf Jeltsch**
Ralph Eichler*

Institute/ Group: *Paul Scherrer Institut
Beam Dynamics Group
**D-MATH, Seminar for Applied Mathematics ETHZ

Description:

In the accelerator complex of the Paul Scherrer Institut PSI the properties of the high intensity particle beams are strongly determined by space charge effects.

The theoretical knowledge off these effects is barely sufficient to understand qualitatively the principal beam behavior, but it clearly lacks the level that would permit quantitative predictions. With the frame of this research project, a 3D code (Mad9p) is developed to simulate the beam behavior dominated by space charge. Based on that code it is planned to extend substantially the knowledge on properties of very high intensity beams at injection into a cyclotron and during acceleration.

Through numerical experiments the simulation code will allow to study in detail the effects of relevant parameters on the beam behavior. Reviewing the numerical results will then yield a better understanding of the phase space transformations that occur in high intensity beams. We use various high performance computing platforms namely: the *Asgard* Beowulf cluster at the ETH, *Nirvana Origin 2000* at Los Alamos and an IBM SP-2 cluster, *Seaborg* at Berkeley. Typical running times are from several hours to a couple of day's. A simulation run generates in the order of 2-3 Gbytes of raw data.

Comparing the simulation results to beam properties measured in the cyclotron will give two benefits: 1. it will be an excellent test of the quality of the simulation and 2. it may help to further increase the beam intensity in the PSI accelerators while reducing the beam losses.

Not just at PSI, but in the whole international community of accelerator specialists there is a strong demand for improved knowledge on the properties of high intensity beams. Increasing this knowledge is important for all the modern projects considering to use very high intensity particle accelerators for nuclear transmutation of radionucleides or for driving a subcritical reactor (energy amplifier).

References: A paper will be appear in the book series on Mathematics in Industry (ECMI Subseries)

Title: Inverse Design for Internal Flow Configurations

Researchers: Andrea Scascighini*
Andreas Troxler*
Rolf Jeltsch*

Institute/ Group: *Seminar for Applied Mathematics
ETH Zurich

Description:

The optimization of internal flow configurations such as diffusers or flow separators, can be based on the *target–pressure–problem* (or inverse design problem) which reads

> find the shape of a device which generates a given target pressure distribution along its walls.

Two approaches to the solution of the target–pressure–problem are investigated in this project.
In the first approach a numerical method for solving the Inverse Euler equations [J.J. Keller, Physics of Fluids **11** (1999) and ZAMP **49** (1998)] has been developed. The design tool is based on a finite difference discretization and a Newton–Krylov solver. Since the three dimensional inverse Euler equations hold only for complex lamellar flows, we extend the basic axis–symmetric flow model to handle viscous effects by means of a distributed loss model and to handle quasi–three-dimensional effects by deriving a quasi–three-dimensional formulation of the inverse Euler equations from the passage averaged 3D Euler equations. The coupling of the 2D inverse Euler equations with an integral boundary layer method has been investigated too. This method has been applied to the design or subsonic diffusers.
In the second approach, the Euler equations of fluid–dynamics are coupled with an elliptic system of equations for the generation of a grid. This extended system of equations is discretized by means the Jameson–Schmidt–Turkel scheme. An implicit pseudo–time stepping is applied to drive the solution to a steady state. The multi–block code has been applied to the redesign of diffusers, of nozzles with supersonic flows and shocks as well as flow separators.
This project is financed by Alstom Power (Switzerland) Ltd. and the Commission for Technology and Innovation (KTI) under grant nr. 4571.1 KTS.

References: A manuscript has been submitted to the *International Journal for Numerical Methods in Fluids*

Title: Genuine Multidimensional, Divergence-free Numerical Method for the Equations of Magnetohydrodynamics

Researcher: Manuel Torrilhon
Prof. Rolf Jeltsch

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

The equations of magnetohydrodynamics (MHD) describe the flow of plasmas in interaction with a magnetic field. MHD equations are relevant in investigations in several areas of engineering and astrophysical research.

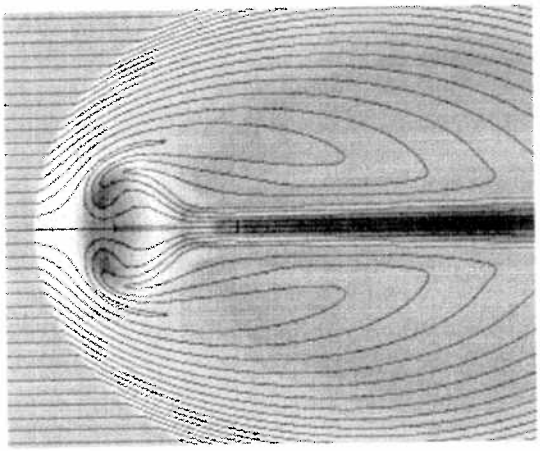


Fig. 1: Interaction of supersonic, magnetized flow with a dense cloud. Isocolor plot of density together with magnetic field lines

The MHD equations form a system of hyperbolic partial differential equations, which will be solved in this project by use of the numerical scheme 'Method of Transport' (MoT). The Method of Transport was developed as genuine multidimensional numerical scheme for the Euler equations. The ideas of MoT could also be adopted to other systems, for example the shallow water equations or turbulent flow. In MHD two new difficulties arise compared to the Euler or shallow water equations. First, the characteristic surfaces are no longer spheres. The influence of the magnetic field reduces the symmetry of the problem at least by one space dimension. Second, the divergence of the magnetic field has to be zero at any time, i.e. an additional constraint has to be imposed on the solution in each time step. Fortunately, these constraint is inherent to the equations, i.e. once fulfilled at the initial data it is fulfilled for all times. Thus this constraint does not change the character of the equations, as in the case of the incompressible Euler equations.

It could be shown, that the additional constraint may be incorporated into the numerical method by special 2-dimensional-flux formulations within the framework of MoT. This approach will be theoretically justified and extended to three dimensions. The large computations are parallelized and performed at the Beowulf cluster 'Asgard' at ETH Zürich.

Title: Finite volume dynamical core for decadal-scale climate simulations

Researchers: William Sawyer*
Shian-Jiann Lin**
Kevin Yeh++
Rolf Jeltsch***

Institute/ Group: *Institute for Atmospheric and Climate Research, ETHZ

**Data Assimilation Office, NASA Goddard Space Flight Center
++Earth and Space Science Interdisciplinary Center, Univ. of Maryland
***Seminar for Applied Mathematics, ETHZ

Description:

A central component of numerical weather prediction and climate simulation is the solver of the equations of atmospheric motion, also known as the "dynamical core." Recent research indicates that the schemes which conserve physical quantities, such as mass, consistently produce more accurate mid-term forecasts than non-conservative schemes. Several conservative dynamical cores have been proposed and implemented in recent years for atmospheric general circulation models employing orthogonal latitude-longitude grids.

Our project investigates conservative schemes for non-orthogonal grids, such as icosahedral grids. Such grids have a future in weather and climate simulation since, among other positive properties, they avoid instabilities at the poles. The introduction of unstructured grids introduces algorithmic and programming complexity. First, it is harder to devise second-order accurate schemes, although recent approaches from computational fluid dynamics, such as the Method of Transport, appear promising. Secondly, the implementation for parallel computers – a requirement due to the extreme computational requirements of these simulations – requires new utilities and techniques. The project goal is to develop a conservative dynamical core employing a non-orthogonal grid which is computationally competitive for decadal-scale climate simulations.

References: A paper on "Parallel Unstructured Grid Manipulations for Geophysical Flow" has been accepted for publication in the proceedings of the *PPAM'01* conference (Springer-Verlag).

Title: Numerical procedures for PDEs using the Feynman–Kac Formula

Researchers: Fabian Buchmann
Wesley P. Petersen

Institute/ Group: Seminar for Applied Mathematics

Description:

A significant limitation of finite element and finite difference schemes for PDEs is that when the spatial dimension is larger than two, simulation of any non–trivial problem may easily become an industrial scale endeavor. For elliptic and parabolic problems in high dimensional spaces, therefore, Monte–Carlo methods are very attractive. The basic idea is to simulate independent sample paths of stochastic differential equations (SDE) whose drift and diffusion coefficients are taken from the PDE. The solution of the PDE is given by expectations (averages) of functions of values of the sample paths. Non–linear and complex problems can in principle be treated too. We especially focus on boundary value problems in bounded domains in n–space.

References:

Title: Inverse flow modelling in river channels

Researchers: Sabine Sulzer
Wolfgang Kinzelbach
Peter Rutschmann

Institute/ Institute of Hydromechanics and Water Resources
Management ETH Hoenggerberg
Group: Group of W. Kinzelbach

Description:

The SNF–financed project aims to combine both new measurement technologies and computation in order to obtain improved discharge measurements for extreme floods. Hydrology today is very much interested in extreme flood events. In these situations the measurement of flow rates is often impossible as gauging stations are flooded. In the project a method is developed in which information on the surface shape and the surface velocities (e.g. visualized by coloured floats) is used in an inverse procedure to deduce the flow rate. The free parameters to be determined in the optimisation process are the flow rate and lateral and vertical shape parameters describing its distribution at the inflow. A 3D flow model on the basis of the Reynolds averaged Navier-Stokes equations is used which can handle the free surface and considers turbulence by means of a k-epsilon theory module.

Contacts:
Sabine Sulzer, IHW, ETH-Zürich, ETH-Zürich, Wolfgang Kinzelbach, IHW, ETH-Zürich, Peter Rutschmann, VAW

Publications:

S. Sulzer, Flood discharge estimation for complex river geometries by inverse numerical modelling, Dissertation ETH 2001

S. Sulzer, P. Rutschmann, W. Kinzelbach, 2001. Determination of flood discharge in rivers with an inverse numerical model. J. Hydraulic Engineering, in print

Title: Particle methods for the solution of transport equations and their application to nonlinear problems

Researchers: Stephanie Zimmermann
Petros Koumoutsakos
Wolfgang Kinzelbach

Institute/ Institute of Hydromechanics and Water Resources
Management ETH Hoenggerberg
Group: Group of W. Kinzelbach

Description:

The interest in particle methods is big due to the fact that accurate solutions without numerical dispersion and spurious oscillations can be obtained at competitive costs. Furthermore, with particles of particular properties, subscale physics can be explicitly injected into the method. Our modelling tool is a fast vortex code, originally developed by Prof. Petros Koumoutsakos (IFD, ETHZ), which has been adapted for the simulation of convection diffusion equations with an anisotropic, velocity dependent dispersion coefficient. The Lagrangian particle method deals with diffusive effects by approximating the Laplace operator of the convection diffusion transport equation with an integral operator. The integration uses particles and a subsequent appropriate redistribution of the strengths among the particles ("Particle Strengths Exchange Method"). The distorted particle field must be occasionally remeshed onto a new structured field in order to maintain stability and accuracy.
The goal of the work is to develop a particle code, which is capable to calculate the phenomena of density fingering with variable fluid density in porous media-This work is embedded in a joint ETH project between the Institute of Computational Science (Prof. Petros Koumoutsakos), the Laboratory for Emerging Technologies (Prof. Dimos Poulikakos), and the Institute of Hydromechanics and Water Resources Management (Prof. Wolfgang Kinzelbach). The aim of the joint effort is to develop a fast "billion particle code" which is modular and useful for a number of applications.

Contacts:
Stephanie Zimmermann, IHW, ETH Zürich, Petros Koumoutsakos, IFD, ETH Zürich, Wolfgang Kinzelbach, IHW, ETH Zürich

Publications:
Zimmermann et al., Simulation of Pollutant Transport Using a Particle Method, Journal of Computational Physics **173**, 322-347, 2001

Title: Bioclogging of porous media

Researchers: M. Thullner
J. Zeyer
W. Kinzelbach

Institute/ Institute of Hydromechanics and Water Resources Management ETH Hoenggerberg
Group: Group of W. Kinzelbach

Description:
The ability of bacterial biomass to change hydraulic properties of a saturated porous medium has been observed in laboratory studies. The occurrence of this phenomenon, bioclogging, in the field has been assumed, but is difficult to prove. Focussing on the possible influence of bioclogging on the applicability of bioremediation techniques, two contrary effects can be envisioned. Bioclogging may reduce the success of bioremediation because due to microbial activity contaminated parts of an aquifer can clog and rates of degradation can decrease in these parts. On the other hand, controlled clogging of an aquifer may be used to build up biobarriers, which could be used to increase the success of remediation. While this is not intended it may well be an interesting means to suppress heterogeneity and fingering which usually render remediation rather inefficient. For these reasons, it is necessary to investigate and understand the way bacteria or biomass related to bacterial growth (e.g. polysaccharides) can change the flow parameters of a given medium. Only if these processes are evaluated the occurrence of bioclogging in field scale applications can be controlled. The study has an experimental and a theoretical component. In the experimental part the clogging is visualized in a quasi-2D sandbox using image analysis techniques to visualize organisms and color tracers in the surrounding flow field. In the theoretical part of the project a fully coupled 3D reactive transport model with clogging is developed. Especially for modelling purposes, it is important to answer the question whether the clogging of a porous medium is caused by a homogeneous biofilm, which reduces the porosity significantly, or by colonies of bacteria which are distributed heterogeneously in the pore space with only a negligible volume. The present project uses pore network models (percolation models) to simulate the change of the hydraulic properties of pore networks due to microbial growth. With these models it is possible to study the ability of the biomass to reduce the hydraulic conductivity of the entire pore network for the different growth scenarios. The results are then upscaled for use in the continuous macroscopic model of reactive transport.

Contacts: M. Thullner, IHW und ITÖ, ETH Zürich, J. Zeyer, ITÖ, ETH Zürich, W. Kinzelbach, IHW, ETH Zürich

Publications: M. Thullner, Experimental and numerical investigations of bioclogging in porous media using two-dimensional flow fields, Dissertation ETH, 2001

M. Thullner et al., Modeling of a Microbial growth experiment with biocloggin in a two-dimensional flow field in saturated porous media, 2001, submitted to Water Resources Research

M. Thullner et al., 2001, Influence of microbial growth on hydraulic properties of pore networks, Transport in Porous Media, in print.

Title: Stochastic modelling of well catchments

Researchers: Hendricks-Franssen
F. Stauffer
Wolfgang Kinzelbach

Institute/ Institute of Hydromechanics and Water Resources
Management ETH Hoenggerberg
Group: Group of W. Kinzelbach

Description:

Wellhead protection zones of drinking water wells serve as measure against pollution. Capture zones of drinking water wells in Switzerland (Foothills of the Alps and Plateau region) are often characterized by a relatively high permeability of the aquifer and relatively large flow gradients, which result in large groundwater flow velocities. Moreover, the extent of these areas and their related flow field often show strong time dependence. The problem of modelling well catchments typically consists of incorporating sparse data in a highly heterogeneous subsurface environment. In this project a combination of direct and inverse deterministic and stochastic techniques (analytical methods and numerical Monte Carlo techniques) is developed, which takes into account measured data for conditioning. Data to be incorporated are hydrological and geophysical data (discharge measurements, head data, extent of formations), Further, tracer data can serve in a time-dependent calibration of the model including a consideration of the tracer travel times. The investigations should yield an improved methodology and procedure for an efficient modelling of capture zones, which is necessary for an assessment of risks drinking water wells are exposed to. Furthermore, the methods will be used to develop a strategy for reducing the uncertainty of the results.

Contacts:
Harrie-Jan Hendricks-Franssen, IHW, ETH Zürich, F. Stauffer, IHW, ETH Zürich, W. Kinzelbach, IHW, ETH Zürich

Publications:

Fritz Stauffer, Sabine Attinger, Stephanie Zimmermann, and Wolfgang Kinzelbach, Uncertainty estimation of well head protection zones: A Lagrangian approximation. Paper submitted to Int. Groundwater Symp. Berkeley, 2002.

Fritz Stauffer, Sabine Attinger, Stephanie Zimmermann, and Wolfgang Kinzelbach, Uncertainty estimation of well catchments in heterogeneous aquifers. Paper submitted to Water Resour. Res., 2001.

H.J.W.M. Hendricks Franssen, F. Stauffer and W. Kinzelbach, Impact of spatio-temporal variable recharge on the characterisation of well capture zones. Abstract submitted to Int. Conf. MODELCARE'2002, Prague.

Title: Reactive transport in heterogeneous porous media

Researchers: J. Dimitrova
S. Attinger

Institute/ Institute of Hydromechanics and Water Resources Management ETH Hoenggerberg
Group: Group of W. Kinzelbach

Description:

Many solutes transported by groundwater are not inert but undergo chemical reactions. Most commonly, one encounters adsorption resulting in an exchange of solute between the mobile fluid and immobile regions of the solid matrix. In the case of non-linear equilibrium adsorption the adsorbed concentration is a non-linear function of the dissolved concentration. This usually intensifies its influence on the transport behaviour compared to linear adsorption. At the same time the mathematical treatment becomes more difficult. Transport processes through heterogeneous porous media are usually investigated with stochastic models, which incorporate the heterogeneous structure of the medium. The stochastic theory is well established and linear transport phenomena have been studied using analytical and numerical methods. In the framework of this project we focus on transport processes with a non-linear Freundlich isotherm in a heterogeneous porous medium. Using methods of statistical physics such as perturbation theory and homogenisation theory we investigate the large-scale behaviour of the effective transport parameters. For strongly heterogeneous media, the semi-analytic approach fails and extensive Monte Carlo simulations are required to obtain ensemble properties of the medium. In the framework of a project of the Gesellschaft für Reaktorsicherheit, (Germany) a fast computation code is developed together with the Institute für Wissenschaftliches Rechnen in Heidelberg, the Institut of Mathematics of Bonn University and the Institut of Mathematics at the University of Freiburg. This code allows to compute ensembles on 3D heterogeneous media in a reasonable discretization. The results are of interest to nuclear waste repository planning.

Contacts:
J. Dimitrova, IHW, ETH-Zürich, S. Attinger, IHW, ETH-Zürich

Publications:

P. Bauer, S. Attinger, W. Kinzelbach, 2001. Transport of a decay chain in homogenous porous media: analytical solutions. J. Cont. Hydr., 49(2001)217-239
S. Attinger, J. Dimitrova and W. Kinzelbach, 2001, Nonlinear adsorbing transport behaviour in heterogeneous porous media: Asymptotic behaviour, submitted to Water Resour. Res.
J. Dimitrova, S. Attinger and W. Kinzelbach, 2001, Nonlinear adsorbing transport behaviour in heterogeneous porous media: Transient behavior, submitted to Water Resour. Res.

Title: Modelling of Density Driven Flows in Porous Media

Researchers: Wolfgang Kinzelbach

Institute/ Institute of Hydromechanics and Water Resources Management ETH Hoenggerberg
Group: Group of W. Kinzelbach

Description:

Density driven flow is of interest in situations of seawater intrusion or up coning of salt water from deep saline aquifers. The latter is the case in Brandenburg, Germany. In arid environments such as Botswana or Usbekistan freshwater lenses form around ephemeral rivers and represent the only year-long available drinking water resource, the surrounding groundwater being saline or brackish. In this situation the exploitation of the freshwater lens by pumping must be well planned in order to avoid the attraction of saline water into drinking water wells. When a salt water layer forms on top of the aquifer, a phenomenon observed under saltpans or swamp islands in the arid tropics, fingering phenomena develop and constitute an important mechanism of transporting salt water downward. We simulate density driven flow, which is quite demanding as far as discretization is concerned. Especially the instable fingering situation is very sensitive to numerical mixing. We start out to investigate the instability onset by network models in 2 and 3 D. We also apply a code on the basis of the method of characteristics and a code, which is developed in a ETH-project described above.

The work is embedded in the EU SALTRANS project involving the Weitzmann institute, Israel, the Politechnical University of Catalonia, Barcelona, the universities of Rennes and Edinburgh, and others. Further means are made available in an INTAS project together with Moscou University and colleagues from Usbekistan.

Publications:

K. Johannsen, W. Kinzelbach, S. Oswald, G. Wittum, 2001. Numerical simulation of density driven flow in porous media. Adv. in Wat. Resources, in print

S. Oswald, M.B. Scheidegger, W. Kinzelbach, 2001. A three-dimensional physical benchmark test for verification of variable-density flow models. Water Resources Research submitted

Title: Direct and Large-Eddy Simulation of compressible free shear flows, wall-bounded flows and shock-turbulence interaction

Researchers: Nikolaus A. Adams
Thierry Maeder
Steffen Stolz
Benjamin Rembold
Roland von Kaenel
Leonhard Kleiser

Institute/ Group: Institute of Fluid Dynamics
Prof. L. Kleiser

Description:

High Reynolds number turbulent flows are not amenable to Direct Numerical Simulation (DNS) due to their wide range of flow scales. In Large-Eddy Simulations (LES) one only resolves the large scales, while the interaction between large scales and non-resolved subgrid scales is modeled. For this purpose the Approximate Deconvolution Model (ADM) was developed. The interaction between resolved and non-resolved scales is taken into account by a relaxation term. LES using ADM have been shown to give excellent results for a range of physically complex flows including compressible isotropic turbulence, incompressible channel flow and supersonic compression ramp flow, at a fraction (a few percent) of the cost needed for a DNS of the same flow.
The reliable computation of transitional and turbulent free shear flows, in particular jets, at high Reynolds numbers is a necessary prerequisite for a numerical investigation of jet-mixing and jet-noise control. In order to achieve an affordable computational tool for parametric studies, LES using ADM is employed. To validate the jet flow LES, a DNS of a low-Mach number transitional jet exiting from a rectangular nozzle was performed. The turbulence statistics and flow structure were analyzed in detail. It was found that the LES with ADM is able to accurately predict transition and the resolved-scale flow structure.
After successful demonstration of the power of ADM in high-order research codes, this approach was also implemented in an industrial-type finite volume code. Test computations for a compressible turbulent channel flow have been performed successfully. A more challenging case will be the LES of turbulent shock-boundary-layer interaction.
The effects of Mach number and wall temperature on the turbulence structure of a supersonic turbulent flat-plate boundary layer have been investigated by means of an extended temporal direct numerical simulation (ETDNS) approach which allows for the simulation of spatially developing boundary layers using a temporal approach, thus considerably reducing the computational effort compared with a truly spatial simulation.

References: See separate list.

Title: Simulation of density currents and particle-laden flows

Researchers: Carlos Härtel
Frieder Necker
Eckart Meiburg*
Thorsten Bosse
Leonhard Kleiser

Institute/ Group: Institute of Fluid Dynamics
Prof. L. Kleiser
*Dept. of Mechanical and Environmental Engineering,
University of California, Santa Barbara, CA, USA

Description:

The first part of the project is concerned with the direct numerical simulation of the gravity-driven dispersion of a dense fluid in a lighter ambient fluid. Such flows are termed gravity currents or density currents. The simulations are based on the Boussinesq equations, where density variations are assumed to be small. The research addresses both lock-exchange flows and deeply submerged gravity currents. One focus of the project is on the analysis of a finger-like structure at the leading edge of the current which originates from a buoyancy-induced linear instability mechanism, the so-called lobe-and-cleft instability. Simulations of the later nonlinear stages of the frontal instability revealed that the fingers at the head may develop into either a stationary equilibrium solution or a time-dependent chaotic state.
The second problem we studied by numerical simulation is the dispersion of a suspension of small particles in a plane channel filled with clear fluid. The study considers dilute flows, i.e. flows with small particle concentrations, where the particle-fluid interaction is the dominant process while particle-particle interactions may be neglected. Moreover, the case of small particle Stokes numbers is considered, which allows us to use a Eulerian approach for the treatment of the particulate phase. High-resolution two- and three-dimensional simulations were performed to study issues such as the propagation speed of the suspension, the deposition of particles at the bottom wall, the mixing with ambient fluid, and the energy budget of the flow.
The third part of the project aims at an improved numerical modeling of turbulent particulate flows. The case of dilute two-way coupled flows is considered where the particles have a significant effect on the dynamics of the carrier fluid. The particulate phase is treated in a Lagrangian fashion by tracking each particle along its trajectory. A simplified one-dimensional test case has been employed to investigate different interpolation techniques, which significantly affect the overall accuracy of the simulation. In addition, the problem of turbulence modification by particles in a three-dimensional homogeneous isotropic setting is being addressed.

References: See separate list.

Title: Computational analysis of flow over a forward-facing step

Researchers: Dirk Wilhelm
Carlos Härtel
Leonhard Kleiser

Institute/ Group: Institute of Fluid Dynamics
Prof. L. Kleiser

Description:

Flow separation and recirculation caused by a sudden constriction in the flow geometry in the form of a forward-facing step play an important role in many practical applications. Knowledge of such flows is crucial e.g. for the design of heat transfer devices (such as used in cooling systems for electronic equipment) or combustion chambers.
Numerical simulations of the flow over a forward-facing step have been performed with the objectives of clarifying the scaling of the dimensions of the recirculating regions with the Reynolds number in the two-dimensional base flow, and of analysing the mechanisms behind the formation of intense three-dimensional vortices at the step that have been observed in various experiments.
For this purpose, a spectral-element code has been developed which combines very high accuracy with the flexibility of handling geometries such as channels with built-in steps or obstacles. An inherent instability related to certain formulations of the nonlinear term could be clarified. The singularity in the pressure and the velocity derivatives at the step corner is accounted for by a geometric mesh refinement strategy.
An investigation of the dependence of the length and height of the separated regions was performed for a wide range of Reynolds numbers Re. At low Re (creeping flow) these dimensions are nearly constant, while they increase algebraically at higher Re. Three-dimensional simulations have provided insight into the 2D - 3D transition, and in particular into the mechanisms responsible for the formation of the peculiar flow pattern observed at the step. Comparisons of the simulation results with experiments show good agreement of the flow topology in the step region and of the spanwise spacing of the characteristic streaks that form downstream of the step. It has been shown that the three-dimensionality is not induced by an absolute instability but is caused by oncoming disturbances to which the flow in the step region reacts most sensitively. A smooth transition from an almost 2D to a fully 3D state is observed if the inflow disturbance level is gradually increased.

References: See separate list.

Title: Numerical Schemes for Nonlinear Heat Conduction and their Application to Astrophysical Flows

Researchers: Simin Motamen*
Jürg Marti*
Rolf Walder**

Institute/ *Seminar für angewandte Mathematik
**Institut für Astronomie
Group: Gruppe von Prof. Marti, ETHZ, Switzerland

Description:

Nonlinear heat conduction plays an important role for high energy astrophysical flows. For ionized plasma the thermal diffusivity K depends on temperature ($K \propto T^{(5/2)}$). This high nonlinearity affects the dynamics of strong shocks and is an essential process in governing the emission of X-ray photons. The numerical method must be able to deal with stiff equations, have second order accuracy, and require reasonable computational time. We analyze the effect of nonlinear heat conduction in one dimension.

Our application, colliding winds in a particular binary star system, shows the appearance of isothermal shocks and steep heat fronts. Both properties are important physical aspects.

We use a fractional step method to solve the Euler equations, including cooling and thermal diffusion. This allows us to use an existing solver for the Euler equations plus cooling, and to investigate different numerical schemes for the diffusion part. The diffusion part must be solved by an implicit scheme as explicit time steps are far too small. We use the AMRCART code (Adaptive Mesh Refinement for Cartesian grid) (See http://www.astro.phys.ethz.ch/staff/walder/). We implemented different numerical schemes for the nonlinear diffusion part. The numerical scheme by Dai & Woodward and the L-stable TR-BDF2 scheme. The L-stable TR-BDF2 scheme allows us to use larger time steps and thus reduce computational time. Adaptive mesh refinement would help to have a better spatial solution in steep fronts and also reduce CPU time. Thus the implementation of an adaptive mesh refinement would be desirable.

References: S. M. Motamen and R. Walder and D. Folini, Heat conduction and colliding winds in Wolf-Rayet Phenomena in Massive Stars and Starburst Galaxies, Proceedings IAU Symposium No. 193, 1999, 378-379.

Title: Modeling and Simulation

Researchers: Kai Nagel

Institute/ Group: Institute for Scientific Computing
Group of Kai Nagel

Description:

In our work in **transportation**, we focus on large scale microscopic simulations. This means that all objects, such as travelers, vehicles, roads, intersections, traffic lights, etc., are individually resolved. Since we simulate large metropolitan regions with 10 million or more travelers, the computing burden is considerable. The computational challenges are approached by using parallel computers.
Transportation simulations do not only consist of the simulation of the traffic itself, but also of the modeling and simulation of the human decision-making which leads to traffic. In consequence, we also have modules for synthetic population generation (where do people live?), for activities generation (what do people do during a day and where?), and for modal choice and route planning (how do people get to their destinations?). Since these modules interact, it is necessary to iterate between them, meaning that the computing burden increases even further. This iteration can be seen both as a relaxation method similar to numerical analysis, and as a simulation of human learning.
Future work will include the following aspects: microscopic simulation of all of Switzerland; improvements of computational performance; plug-and-play system for the integration of the different modules.
We also do modeling and simulation of **other socio-economic systems**. Recently, we have worked on simple models for dynamic market simulations. In these models, we have economic agents which produce, trade, and consume; and they set prices and decide where to buy and how much. Our work has concentrated on stability conditions for adaptive simulations, which includes the question in how far the steady state of an adaptive simulation is related to standard economic equilibrium theory.

Title: Mathematical modelling of human neck muscles for trauma research

Researchers: Beat Müller
Kai-Uwe Schmitt
Peter Niederer

Institute/ Group: Institute of Biomedical Engineering
Fachgruppe Biomechanik und Medizinische Optik

Description:

Soft tissue neck injuries sustained in low speed rear-end collisions are observed with increasing frequency. To analyse the dynamics of the human cervical spine under representative impact conditions, a comprehensive Finite Element (FE) model of a neck has been developed. The geometry of the model was derived from Magnetic Resonance measurements and it includes both the relevant solid structures of the neck (bony structures, ligaments, and muscles) as well as a fluid compartment representing a typical blood vessel.

An important aspect of the neck dynamics is related to the musculature which exhibits active mechanical properties. To analyse the influence of muscle activity on the dynamic response of the head-neck-upper torso complex, elements based on a Hill-type muscle definition were introduced in the model. Hence, the muscle force is described within the framework of an active contraction process and as such a function of time, deformation and deformation rate. Input parameters for the mathematical description of the muscle behavior were taken from results obtained in volunteer tests using EMG measurements.

The results of the simulation of the kinematics of the cervical spine agreed well the experimental data.

Reference: K-.U. Schmitt, „A contribution to the trauma-biomechanics of the cervical spine", VDI-Verlag, ISBN 3-18-321117-3

Title: Simulation of Global Climate and Climate Change with General Circulation Models

Researchers: Martin Wild
Andreas Roesch
Atsumu Ohmura

Institute/ Group: Institute for Atmospheric and Climate Sciences ETH
Global Climate Modeling Group

Description:

In a joint project with the Max-Planck-Institute for Meteorology (MPI), Hamburg, simulations of the global climate with the general circulation model ECHAM are performed at the Swiss center for scientific computing, CSCS, Manno. Simulations have been conducted with unprecedented high horizontal resolution at global scales (1.1°), a resolution previously restricted to numerical weather prediction models with short integration periods. The emphasis is on simulations for present-day conditions and climate change scenarios with increased levels of CO_2 concentration. The analysis of present climate simulations allows an estimate of the model accuracy and identifies weaknesses in the model parameterizations as guideline for further model improvement. The focus is on the radiation budget, on surface hydrology and snow characteristics, and on the boundary layer structure.
High resolution climate change experiments with doubled CO_2 concentration are performed to study possible changes in the mass balance of the polar ice sheets and associated sea-level rise, and changes in the earth's heat budget and surface hydrology. Regional changes with focus on the European and Alpine area are a further subject of analysis.

Selected references:

Ohmura, A., Wild, M., and Bengtsson, L. 1996: A possible change in mass balance of greenland and antarctic ice sheets in the coming century. *J. Climate*, **8**, 2124-2135.

Wild, M., Ohmura, A., and Cubasch, U., 1997: GCM simulated surface energy fluxes in climate change experiments. *J. Climate*, **10**, 3093-3110.

Wild, M., Ohmura, A., Gilgen, H., Roeckner, E., Giorgetta, M., and Morcrette, J.J., 1998: The disposition of radiative energy in the global climate system: GCM simulated versus observational estimates. *Climate Dynamics*, **14**, 853-869.

Intergovernmental Panel on Climate Change (IPCC) 2001: Climate Change: The scientific basis. IPCC third assessment report. M. Wild contributing author Chapter 8 (Model evaluation), Chapter 10 (Regional Climate Simulation - Evaluation and Projections), Chapter 11 (sea level change), Cambridge university Press.

Title: A new versatile structure search system

Researchers: Pius Portmann
Engelbert Zass
Ernö Pretsch

Institute/ Group: Laboratory of Organic Chemistry
Group of Prof. E. Pretsch
In cooperation with
Prof. M.E. Munk, Arizona State University
Pius Portmann, Upstream Solutions, Zürich

Description:

The prototype of a structure search system has been developed. It uses a very versatile query with features presently not available in any of the publicly accessible structure retrieval systems. The new structure search system can be adapted to any database having structures in a standard format (e.g., SD file). The results can be exported or used as input for further searches.

References:

E. Pretsch, P. Portmann, M.E. Munk, and E. Zass
A database search system using a versatile combination of structural and property information. Proceedings of the International Chemical Information Conference & Exhibition, Nîmes, France, 21-24 October 2001, in press.

Title: Automatic structure elucidation

Researchers: Patrick Fontana
Martin Badertscher
Pius Portmann
Ernö Pretsch

Institute/ Group: Laboratory of Organic Chemistry
Group of Prof. E. Pretsch
In cooperation with
Prof. M.E. Munk, Arizona State University
Renate Bürgin Schaller and Pius Portmann, Upstream Solutions, Zürich

Description:

A program has been developed that automatically extracts structural information from infrared, ^{1}H and ^{13}C NMR spectra. The resulting substructures that must be present or absent and other structural constraints can be edited by the user or directly processed by the structure generator, Assemble 2.1. Tests with over 100 sets of spectra have shown a high reliability in that not a single incorrect interpretation has occurred. The automatic spectra interpretation has allowed the number of possible isomers defined by the molecular formula alone to be reduced to 1.5% on an average. After ranking the resulting structures based on their ^{1}H and ^{13}C NMR chemical shifts and multiplicities, the correct structure in each case has been found as the best or within the few best solutions.

References:

M. Badertscher, A. Korytko, K.P. Schulz, M. Madison, M.E. Munk, P. Portmann, M. Junghans, P. Fontana, and E. Pretsch
Assemble 2.0: A structure generator
Chemom. Intell. Lab. Syst. **51** (2000) 73-79.

M. Badertscher, K. Bischofberger, M.E. Munk, and E. Pretsch
A novel formalism to characterize the degree of unsaturation of organic molecules
J. Chem. Inf. Comput. Sci. **41** (2001), 889-893.

Automatic spectra interpretation, structure generation and ranking
P. Fontana and E. Pretsch
J. Chem. Inf. Comput. Sci., submitted.

Title: Diode laser jet spectra and analysis of the ν_1 and ν_4 fundamentals of CCl_3F

Researchers: M. Snels**
G. D'Amico**
L. Piccarreta**
H. Hollenstein*
M. Quack*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Istituto per Materiali Speciali, CNR, Potenza

Description:

High-resolution infrared spectra have been measured for mixtures of CCl_3F in Ne, expanded in a supersonic planar jet. We present the first analysis for the ν_4 fundamental and a complete analysis for the ν_1 band. Accurate spectroscopic constants have been obtained for both the ν_1 fundamental of the most abundant isotopic species, $C^{35}Cl_3F$, $C^{35}Cl_2{}^{37}ClF$, and $C^{35}Cl^{37}Cl_2F$. With respect to an earlier work [2], the observation of Q branches of the three most abundant isotopomers allowed for an unambiguous determination of the ν_1 band origins. The ν_4 fundamental has not been the subject of a high-resolution analysis up to now. The observation of high-resolution spectra of the central part of the band permitted the determination of band origin, rotational constants, and Coriolis constant for the symmetric-top species, $C^{35}Cl_3F$. Extensive numerical calculations are carried out in the simulations of the spectra.

References:

[1] Diode laser jet spectra and analysis of the ν_1 and ν_4 fundamentals of CCl_3F
M. Snels, G. D'Amico, L. Piccarreta, H. Hollenstein and M. Quack
J. Mol. Spectrosc. **205**, 102–109 (2001)
[2] M. Snels, A. Beil, H. Hollenstein, M. Quack, U. Schmitt and F. d'Amato, J. Chem. Phys. **103**, 8846-8853 (1995)

Title: Parity violation in fluorooxirane

Researchers: R. Berger**
M. Quack*
J. Stohner*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Institut für Chemie, TU Berlin

Description:

In contrast to what has been accepted, electroweak quantum chemistry predicts the heats of formation, the structures, the microwave and infrared spectra of enantiomers of chiral molecules tobe different. The *R* enantiomer of fluorooxirane is calculated to be more stable than the *S* enantiomer by the minute amount of 2×10^{-12} $Jmol^{-1}$, and the relative IR frequency shifts are $\leq 10^{-18}$. Nevertheless, this recently synthesized compound may prove useful for fundamental experimental tests and calculations of parity violation in chiral molecules because of its particularly simple rovibrational spectrum and its rigid cyclic structure composed of light atoms.

References:

[1] R. Berger, M. Quack and J. Stohner, Angew. Chem. Intl. Ed. (Engl.) **40**, 1667–1670 (2001)
[2] H. Hollenstein, D. Luckhaus, J. Pochert, M. Quack and G. Seyfang, Angew. Chem. Intl. Ed. (Engl.) **36**, 140-143 (1997)

Title: Some simple mechanisms of multiphoton excitation in many level systems

Researchers: E. Donley
R. Marquardt
M. Quack
J. Stohner
I. Thanopulos
E. U. Wallenborn

Institute/Group: Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

Results are reported on coherent monochromatic multiphoton excitation in many-level systems, which are representative for some of the basic mechanisms for atomic and molecular multiphoton processes. Numerical solutions are discussed that use the Floquet and quasiresonant approximations in the framework of the URIMIR program package. The excitation schemes include direct three-photon excitation, two-photon excitation with diagonal coupling, Göppert-Mayer-type two-photon processes, multiphoton excitation with off-resonant intermediates, and practically irreversible coherent excitation into dense spectral structures. Several interesting phenomena are observed, such as nonlinear line shifts and broadenings of multiphoton resonances of relevance for multiphoton spectroscopy and almost constant intermediate population inversions, potentially useful for laser design. The accurate numerical results are compared with approximate solutions from perturbation theory, and with simple analytical solutions from Rabi-type formulae.

References:

[1] E. Donley, R. Marquardt, M. Quack, J. Stohner, I. Thanopulos and E. U. Wallenborn, Mol. Phys. **99**, 1275–1287 (2001)
[2] M. Quack in "Encyclopedia of Computational Chemistry", Vol. 3, p. 1775-1791, P. von Ragué Schleyer, N. Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III and P.R. Schreiner eds., John Wiley and Sons, 1998

Title: Gas Phase Kinetics, Encyclopedia of Chemical Physics and Physical Chemistry, Chapter A.3.4

Researchers: D. Luckhaus
M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

Experimental and theoretical including computational work on gas phase kinetics is reviewed.

References:

D. Luckhaus and M. Quack
Encyclopedia of Chemical Physics and Physical Chemistry, Chapter A.3.4, IOP publishing, Bristol in press (2001)

Title: Energy Redistribution in Reacting Systems

Researchers: R. Marquardt
M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

Experimental and theoretical including computational work on energy redistribution is reviewed.

References:

R. Marquardt and M. Quack
Encyclopedia of Chemical Physics and Physical Chemistry, Chapter A.3.13, IOP publishing, Bristol, in press, (2001)

Title: Gas Phase Kinetics Studies

Researchers: D. Luckhaus
M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

Experimental and theoretical including computational gas phase kinetics studies are reviewed.

References:

D. Luckhaus and M. Quack, Encyclopedia of Chemical Physics and Physical Chemistry, Chapter B.2.5, IOP publishing, Bristol, in press (2001)

Title: Mode selective Stereomutation and Parity violation in disulphane isotopomers H_2S_2, D_2S_2, T_2S_2

Researchers: M. Gottselig
D. Luckhaus
M. Quack
J. Stohner
M. Willeke

Institute/Group: Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

We report quantitative calculations of stereomutation tunneling in the disulfane isotopomers H_2S_2, D_2S_2, and T_2S_2, which are chiral in their equilibrium geometry. The quasi-adiabatic channel, quasi-harmonic reaction path Hamiltonian approach used here treats stereomutation including all internal degrees of freedom. The torsional motion is handled as an anharmonic reaction coordinate in detail, whereas all the remaining degrees of freedom are taken into account approximately. We predict how stereomutation is catalyzed or inhibited by excitation of the various vibrational modes. The agreement of our theoretical results with spectroscopic data from the literature on H_2S_2 and D_2S_2 is excellent. We furthermore predict the influence of parity violation on stereomutation as characterized approximately by the ratio ($\Delta E_{pv}/\Delta E_{\pm}$) of the (local or vibrationally averaged) parity violating potential ΔE_{pv} and the tunneling splittings $\Delta E_{\pm}$ in the symmetrical case. This ratio is exceedingly small for the reference molecules H_2O_2 and D_2O_2, and still very small ($2 \cdot 10^{-6}$ cm^{-1}) for H_2S_2, which, thus, all exhibit essentially parity conservation in the dynamics. However, for D_2S_2 it is ca. 0.002, and for T_2S_2 it is ca. 1, which seems to be the first case where such intermediate mixing through parity violation is quantitatively predicted for spectroscopically accessible molecules. The consequences for the spectroscopic detection of molecular parity violation are discussed briefly also in relation to other molecules.

References:

[1] Mode selective Stereomutation and Parity violation in disulphane isotopomers H_2S_2, D_2S_2, T_2S_2
M. Gottselig, D. Luckhaus, M. Quack, J. Stohner, M. Willeke
Helv. Chim. Acta **84**, 1846–1861 (2001)
[2] M. Quack, Angewandte Chemie (Intl.Ed.) **28**, 571-586 (1989)
[3] M. Quack, Nova Acta Leopoldina **81**, Neue Folge (No. 314) 137-173 (1999)

Title: Analytical three-body interaction potentials and hydrogen bond dynamics of hydrogen fluoride aggregates $(HF)_n$, $n \geq 3$

Researchers: M. Quack*
J. Stohner*
M. Suhm**

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Institute of Physical Chemistry, University of Göttingen

Description:

Oligomeric aggregates of hydrogen fluoride are important prototype molecules for a detailed understanding of the structure, energetics, spectroscopy and dynamics of hydrogen bonding. The pairwise additive description of these oligomers is known to be inadequate. We have sampled the three-body potential for HF at 3000 $(HF)_3$ configurations selected by various classical and quantum sampling techniques, including dynamic sampling based on Voronoi step representation. The counterpoise-corrected Møller-Plesset second-order three-body energies using a double zeta gaussian basis set with polarization functions (DZP+MP2) at these configurations are fitted by analytical 12-dimensional potentials. Cooperative effects are found to be sizeable and predominantly stabilizing in hydrogen fluoride ring aggregates. Test calculations with larger basis sets and for larger HF aggregates show that in combination with available high quality pair potentials, the analytical three-body terms give an excellent description of the $(HF)_3$ surface in the hydrogen bonding region and a good approximation for clusters up to at least the hexamer. Multidimensional vibrational quantum Monte Carlo calculations indicate that degenerate HF stretch excitation in $(HF)_3$ (3712 cm^{-1}) is in close coincidence with $(HF)_3 \rightarrow 3$ HF dissociation channels at low HF angular momentum, whereas degenerate DF stretch excitation in $(DF)_3$ (2725 cm^{-1}) falls slightly below any $(DF)_3 \rightarrow (DF)_2$ + DF dissociation channels. The $(HF)_3$ potential surface, its stationary points, possible interconversion tunneling pathways, zero point energies, adiabatic channels, unusual isotope effects, fully centrifugal rotational states and the harmonic infrared spectrum are discussed in detail and compared to ab initio calculations and experiment.

References:

[1] M. Quack, J. Stohner and M. Suhm, J. Mol. Structure in press (2001)
[2] M. Quack and M.A. Suhm, in "Conceptual Perspectives in Quantum Chemistry", p. 415-463, E.S. Kryachko and J.L. Calais eds., Kluwer, Dordrecht 1997
[3] M. Quack and M.A. Suhm, in "Advances in Molecular Vibrations and Collision Dynamics, Vol. III, Molecular Clusters", p. 205-248, Z. Bacic & J. Bowman eds., JAI press, Stamford, Conn. and London, England 1998 (ISBN: 1-55938-790-4)

Title: High resolution analysis of the complex symmetric stretching chromophore absorption in CF_3I

Researchers: Y. He*
H. Hollenstein*
M. Quack*
E. Richard*
M. Snels**
H. Bürger***

Institute/Group: * Group for Molecular Kinetics and Spectroscopy, Physical Chemistry, ETH Zürich
** Istituto per Materiali Speciali, CNR, Potenza
*** Anorganische Chemie, Bergische Universität, Wuppertal

Description:

Very high resolution spectra of CF_3I have been measured by slit jet diode laser and FTIR techniques and are analyzed theoretically. Extensive numerical calculations are carried out in the simulations of the spectra.

References:

[1] Y. He, H. Hollenstein, M. Quack, E. Richard, M. Snels and H. Bürger
J. Chem. Phys. in press (2001)
[2] H. Hollenstein, M. Quack and E. Richard, Chem. Phys. Lett. **222**, 176-184 (1994)
[3] M. Quack, Annual Rev.Phys. Chem. **41**, 839-874 (1990)

Title: Molecules in Motion

Researchers: M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy,
Physical Chemistry, ETH Zürich

Description:

The group for molecular kinetics and spectroscopy at ETH Zürich investigates the fundamental physical-chemical primary processes of chemical reactions. We have developed a conceptually new approach to derive these primary processes of intramolecular kinetics on time scales leading into the femtosecond and subfemtosecond domain on the basis of infrared spectroscopy with high frequency resolution but without short-time resolution. Selected applications include intramolecular wavepacket dynamics of chemical functional groups of isolated, individual molecules and IR-laser chemistry of molecules under infrared multiphoton excitation, hydrogen bond tunneling dynamics in hydrogen fluoride clusters $(HF)_2$ and the tunneling stereomutation of prototypical chiral molecules. One of the greatest current challenges is the elucidation of the influence of the parity violating weak interaction mediated by the *Z*-Boson of high energy physics on the dynamics of chiral molecules.
Experimental and theoretical work including computational work is reviewed.

References:

[1] M. Quack, Chimia in press (2001)
[2] M. Quack, chapter 27 in: "Femtosecond Chemistry", J. Manz and L. Woeste eds., Proc. Berlin Conf. Femtosecond Chemistry, Berlin (March 1993), Verlag Chemie, Weinheim (1994), p. 781-818

Title: Parity violation dominates the Dynamics of Chirality in Dichlorodisulfane

Researchers: R. Berger**
M. Gottselig*
M. Quack*
M. Willeke*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Institut für Chemie, TU Berlin

Description:

According to the traditional point of view on the structure and dynamics of chiral molecules, parity violation would be too small to be of any real importance. Enantiomers would thus exist as symmetry related structures, which are *de facto* stable because of very long tunneling times. We present here with ClSSCl the first example of a chiral molecule, where electroweak and tunneling dynamics calculations demonstrate that the *de lege* asymmetry arising from the parity-violating energy difference ΔE_{pv} between the two enantiomers (about $1.5 \cdot 10^{-11}$ J mol^{-1}/N$_A$ with time for parity violation $t_{pv} \simeq 30$ s) dominates by far over the tunneling splitting $\Delta E_{\pm} \ll 10^{-70}$ J mol^{-1}/N$_A$ in the symmetrical case, with tunneling time $t_{\pm} \gg 10^{60}$ s. These results are of fundamental interest for our concept on molecular chirality as well as for potential experiments on parity violation in molecules.

References:

[1] R. Berger, M. Gottselig, M. Quack and M. Willeke, Angew. Chem. in press (2001)
[2] M. Quack, Nova Acta Leopoldina **81**, Neue Folge (No. 314) 137-173 (1999)
[3] M. Quack, Angewandte Chemie (Intl.Ed.) **28**, 571-586 (1989)

Title: Molecular chirality and the fundamental symmetries of physics: Influence of parity violation on rovibrational frequencies and thermodynamic properties

Researchers: M. Quack
J. Stohner

Institute/Group: Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

We introduce the topic of fundamental symmetries of physics in relation to molecular chirality by a brief review of the development and current status of the theory for parity violation in chiral molecules. We then discuss in some detail CHBrClF (bromochlorofluoromethane) as a test case, to which the work of André Collet has contributed importantly. For this molecule and its isotopomers we report here the first detailed theoretical calculations of the influence of parity violation on statistical thermodynamic properties.

High quality *ab initio* calculations (RPA, random phase approximation and CASSCF, complete-active-space self-consistent-field) are performed to determine the small energy difference between R- and S-enantiomers of H and D isotopomers of bromochlorofluoromethane (CHBrClF, CDBrClF), and fluorooxirane $^{1}H_3C_2OF$) introduced by the parity violating weak interaction. Together with vibrational and rotational frequency shifts caused by parity violation these are used to determine the statistical thermodynamic quantities from the corresponding partition functions within the separable harmonic and in part also anharmonic adiabatic approximation. Temperature dependent equilibrium constants for the stereomutation are calculated and discussed in relation to biochemical homochirality.

References:

M. Quack and J. Stohner, Chirality, in press (2001)

Title: Spectroscopy and dynamics of the isolated sp^2 CH chromophore in trideuteroacetaldehyde CD_3CHO as derived from extrapolated SDCI ab initio calculations

Researchers: T.K. Ha
M. Quack
J. Stohner

Institute/Group: Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

Ab initio CI potential energy (PES) and dipole moment (DMS) surfaces have been calculated with singles and doubles excitation configuration interaction (SDCI) for the two-dimensional isolated sp^2 CH chromophore subspace of trideuteroacetaldehyde CD_3CHO. Different extrapolation schemes to full-CI have been applied after the extrapolation to full-SDCI. Vibrational band centers and absolute intensities are determined variationally on six extrapolated surfaces. The band centers are analyzed within the effective Hamiltonian model for isolated CH chromophores and the effective spectroscopic parameters are compared for the different extrapolation schemes. Time-dependent population evolution for vibrational quantum motion with a pure CH stretching state being initially populated is calculated for some of the extrapolated surfaces within the effective Hamiltonian model.

References:

A manuscript has been submitted.

Title: Anchoring the water dimer potential energy surface with explicitly correlated computations and focal point analyses

Researchers: G.S. Tschumper*
M.L. Leiniger**
B.C. Hoffmann**
E.F. Valeev**
H.F. Schaefer III**
M. Quack*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Center for Computational Quantum Chemistry,
University of Georgia, Athens

Description:

Ab initio calculations of very high level on the title compound are carried out.

References:

G.S. Tschumper, M.L. Leiniger, B.C. Hoffmann, E.F. Valeev, H.F. Schaefer III and M. Quack
J. Chem. Phys. in press (2001)

Title: High-resolution FTIR and cw-diode laser cavity ring-down spectroscopy of the $\nu_2 + 2\nu_3$ band of methane near 7510 cm^{-1} in slit jet expansions and at room temperature

Researchers: M. Hippler
M. Quack

Institute/Group: Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich

Description:

The $\nu_2+2\nu_3$ combination band of $^{12}CH_4$ near 7510 cm^{-1} was studied with the recently introduced technique of cavity ring-down spectroscopy employing a cw-diode laser in a pulsed supersonic slit jet expansion and with Doppler-limited Fourier-transform infrared spectroscopy at room temperature. $\nu_2+2\nu_3$ is the strongest absorption band in the high-wavenumber region of the $N = 2.5$ icosad of methane. First assignments of the combination band are provided. The vibrational origin of $\nu_2+2\nu_3$ at 7510.3378 ± 0.0010 cm^{-1}, the integrated band strength $G = (1.3 \pm 0.2)\times10^{-4}$ pm^2 and the vibrational transition moment $|\langle\mu_v\rangle| = (1.0 \pm 0.1)\times10^{-3}$ D have been determined. The values represent benchmarks to test effective vibrational Hamiltonians and *ab initio* calculations for methane. Although an isolated band analysis was possible at low J-values, the influence of strong perturbations becomes evident at higher rotational excitation. The F_1-component of $\nu_2+2\nu_3$ interacting by a strong Coriolis resonance with the IR-active F_2-component appears to be a dominant perturber.

Extensive numerical calculations are carried out in the simulations of the spectra.

References:

M. Hippler and M. Quack, a manuscript has been submitted

Title: Nonlinear intensity dependence in the infrared multiphoton excitation and dissociation of methanol preexcited to different energies

Researchers: O.V. Boyarkin**
T. R. Rizzo**
D.S. Rueda**
M. Quack*
G. Seyfang*

Institute/Group: * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Laboratory of Physical Chemistry, EPF Lausanne

Description:

We report quantitative dissociation yields for the reaction $CH_3OH(v_{OH}) \xrightarrow{nh\nu} CH3 + OH$ induced by infrared multiphoton excitation of methanol preexcited to various levels of the OH stretching vibration (v_{OH} = 0, 1, 3, 5) by detecting OH using laser induced fluorescence. It is demonstrated that for low levels of preexcitation (v_{OH} = 0, 1, 3) there is a substantial nonlinear intensity dependence, as a higher yield is found for self mode-locked CO_2 laser pulses (with higher peak intensity) as compared to single mode pulses of the same laser fluence, but lower peak intensity. In contrast, at high levels of preexcitation (v_{OH} = 5) this nonlinear intensity dependence is absent. Quantitative model calculations are carried out using a case B/case C master equation approach that takes nonlinear intensity dependence into account. The calculations are consistent with the experimental results and confirm the prediction that an important part of the selectivity of the CO_2 laser excitation step in IRLAPS (Infrared laser assisted photofragment spectroscopy) of CH_3OH is due to this nonlinear intensity dependence. We discuss further consequences of these experimental observations and theoretical predictions, which are also extended to IR multiphoton excitation of C_2H_5OH. Infrared (C–O) chromophore band strengths are reported for CH_3OH and C_2H_5OH.

References:

[1] O.V. Boyarkin, T. R. Rizzo, D.S. Rueda, M. Quack and G. Seyfang, J. Chem. Phys, (submitted)
[2] M. Quack in "Encyclopedia of Computational Chemistry", Vol. 3, p. 1775-1791, P. von Ragué Schleyer, N. Allinger, T. Clark, J. Gasteiger, P.A. Kollman, H.F. Schaefer III and P.R. Schreiner eds., John Wiley and Sons, 1998

Title: Numerical investigation of Strongly correlated systems

Researchers: A. Läuchli, C. Honerkanp, Th. Siller, M. Troyer, T.M. Rice [*]
S.R. White [**]
M. Salmhofer [***]
D. Poilblanc [****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] University of California at Irvine, USA
[***] Theoretische Physik, Universität Leipzig, Germany
[****] Université Toulouse, France

Description:

The physics of strongly correlated electrons is one of the most active research fields in condensed matter physics. Next to technologically relevant developments such as high-temperature superconductors and colossal magnetoresistance materials, the field raises many important and difficult questions to basic research such as new exotic states of matter and the breakdown paths of the more conventional metallic or ordered states. We analyzes the latter issue by means of extensive numerical renormalization group calculations for two-dimensional electron systems. Furthermore novel correlation phenomena like the binding of holes or magnetic excitations with impurity sites are investigated using modern numerical techniques such as density matrix renormalization group and exact diagonalization.

References:

- C. Honerkamp, M. Salmhofer, N. Furukawa, and T.M. Rice, Phys. Rev. B **63**, 035109 (2001)
- C. Honerkamp, Euro. Phys. J. B 21, 81 (2001)
- Thomas Siller, M. Troyer, T.M. Rice and S.R. White, Phys. Rev. B **63**, 195106 (2001).
- J. Riera and D. Poilblanc , Phys. Rev. B **63**, 241102 (2001)
- P. Maurel, M.-B. Lepetit and D. Poilblanc , Eur. Phys. J. B (2001), in press.
- Kenji Tsutsui, Didier Poilblanc and Sylvain Capponi, Phys. Rev. B (2001), in press.
- Samuel Wehrli, Didier Poilblanc and T.M. Rice, Eur. Phys. J. B (2001) in press
- Carsten Honerkamp, Manfred Salmhofer, to be published in Phys. Rev. B.
- David Lidsky and Matthias Troyer, Preprint, submitted to Phys. Rev. B
- A. Läuchli, D. Poilblanc, T.M. Rice and S.R. White, submitted to Phys. Rev. Lett.
- K. Völker and S. Chakravarty, submitted to Phys. Rev. B
- Carsten Honerkamp and Manfred Salmhofer, submitted to Phys. Rev. Lett.
- Carsten Honerkamp and Manfred Sigrist, submitted to Journal of Physics C

Title: The Role of π–π Stacking Interactions in Organometallic Compounds. Combined Quantum Mechanics/Molecular Mechanics Studies

Researchers: Alessandra Magistrato*
Paul S. Pregosin**
Alberto Albinati***
Ursula Rothlisberger*

Institute/ Group: *Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie
** Laboratory of Inorganic Chemistry
*** Chemical Pharmacy, University of Milan, I-20131, Milan, Italy

Description:

Density functional (DFT) studies, and hybrid QM/MM-DFT calculations demonstrate the importance of π–π stacking interactions in determining the structural features of two exemplary d^8 palladium complexes, PdBr(p-NCC_6H_4)({S}-MeO-Biphep) **1** and PdBr(C_6F_5)({S}-MeO-Biphep) **2**. In spite of the superficial similarity of the two compounds, the former shows marked distortions from square planar geometry, while the latter exhibits an almost ideal structure. Attractive π–π stacking interactions between two pairs of P-phenyl rings and the arene backbone of the MeO-Biphep are the main origin of the distortion in complex **1**. The planar structure of complex **2** is preferred as a consequence of an additional stacking interaction between one P-phenyl ring and the pentafluoro-phenyl σ-ligand. The artificial introduction of an analogous stacking interaction in complex **1** re-establishes an ideal square planar geometry, thus demonstrating that switching on/off specific π–π interactions distinctly alters the coordination geometry. These results reveal a previously unrecognised role for π–π stacking interactions in the stabilisation of structural features in transition metal compounds. This suggests π–π stacking interactions as a potential new design principle in tailoring coordination compounds.

References: Organometallics **20** (2001) 4178-4184

Title: First-Principles Simulations of C-S Bond Cleavage in Rhenium Thioether Complexes

Researchers: Alessandra Magistrato*
Thomas Fässler**
Ursula Rothlisberger*

Institute/ Group: *Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie
** Eduard Zintl Insitute, D-64289 Darmstadt, Germany

Description:

We present first-principles molecular dynamics studies of the reductive C-S bond cleavage reaction in hexathioether complexes of the form $[Re(9S3)_2]^{m+}$ (with 9S3 = 1,4,7 trithiacyclononane and m = 1,2). Our calculations show that electron transfer and bond dissociation take place as two distinct consecutive reaction steps. For the reduced complex, C-S bond fission and subsequent release of ethene can be observed directly at only slightly elevated temperatures. Car-Parrinello molecular dynamics of the reactive process demonstrate that for the dissociation to occur two carbon sulfur bonds have to be broken quasi simultaneously. For the oxidized form on the other hand, no release of ethene takes place at the same temperature within the limited time scale of our simulations. The activation energies of the dissociation process calculated at the gradient-corrected density functional (BP) level are 16 kcal/mol and 8 kcal/mol for the oxidized and the reduced form, respectively. A detailed analysis of the electronic structure in the transition states confirms the presence of a strong π-back donation from rhenium d-orbitals into antibonding σ^*-orbitals of the C-S bonds that is responsible for the pronounced weakening of the carbon-sulfur bond upon reduction.

References: accepted in J. Phys. Chem. A

Title: Enantioselective Palladium Catalyzed Hydrosilylation of Styrene: I. Detailed Reaction Mechanism from First-Principles and Hybrid QM/MM Molecular Dynamics Simulations

Researchers: Alessandra Magistrato*
Tom K. Woo**
Antonio Togni***
Ursula Rothlisberger*

Institute/ Group: * Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie
** University of Western Ontario, N6A 5B7, London, Ontario, Canada
*** Laboratory of Inorganic Chemistry

Description:

The mechanism of the enantioselective hydrosilylation of styrene catalyzed by Pd^0 species generated in situ from dichloro{1-{(*R*)-1-[(*S*)-2(diphenylphosphino-κ*P*)ferrocenyl]ethyl}-3-trimethylphenyl-5-1*H*-pyrazole-κ*N*}palladium, **1**, has been investigated in detail through ab initio molecular dynamics and hybrid ab initio molecular dynamics/molecular mechanics (QM/MM) calculations. Different QM/MM models have been adopted in order to probe the specific steric and electronic contributions of different substituents.
The catalytic cycle is initiated by the formation of a weakly bound π-complex (DE~ -4.8 kcal/mol) under simultaneous detachment of the pyrazole ligand. In agreement with a Chalk-Harrod mechanism, this is followed by the migratory insertion of the hydride, which leads to a η^3-coordination mode of the benzylic fragment. The significant stabilization of the allylic intermediate (ΔE~ -14 kcal/mol) is responsible for the high regioselectivity of the reaction (as well as for its enantioselectivity). The rate-determining step with an activation barrier of 16 kcal/mol is the migration of the silyl ligand to the α-carbon of the substrate with concomitant closure of the ligand chelate ring. This step leads to the formation of an intermediate in which the phenyl moiety of the product remains coordinated in an η^2-mode to the palladium. The addition of trichlorosilane leads to product formation and hence to the regeneration of the catalyst. A unimolecular reaction pathway on the other hand, in which the transfer of the silyl ligand to the benzylic fragment is concerted with the addition of a molecule of $HSiCl_3$ to the catalyst, is disfavoured by an activation barrier of ~ 30 kcal/mol.

References: submitted to J. Am. Chem. Soc.

Title: Enantioselective Palladium Catalyzed Hydrosilylation of Styrene: II. Influence of Electronic and Steric Effects in the Enantioselectivity. Catayst Design via First-Principles and Hybrid QM/MM Molecular Dynamics Simulations

Researchers: Alessandra Magistrato*
Antonio Togni**
Ursula Rothlisberger*

Institute/ Group: * Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie
** Laboratory of Inorganic Chemistry

Description:

The extent and the sense of chiral induction of the palladium-catalyzed hydrosilylation of styrene are affected by the electronic properties of both the substrate and the ligand. The factors determining the enantioselectivity of the reaction have been rationalized by performing mixed QM/MM Car-Parrinello molecular dynamics simulations with styrene and 4-(di-methylamino)styrene as substrates. Our results demonstrate that the formation of an η^3-benzylic intermediate plays a crucial role in determining the stereoselectivity of the reaction. The relative thermodynamic stabilities (ΔE~1-2 kcal/mol) of the *endo* and *exo* η^3 forms of the benzylic intermediates, precursors of the *R* and *S* enantiomeric products, are inverted as a function of the electron releasing or withdrawing nature of the *para*-substituent of the substrate. A study of the charge distribution of the coordinated and the free benzyls confirms a strong dependence of the enantioselectivity on the electronic nature of the substrate. In addition, a structural analysis of the *endo* and *exo* η^3-benzylic intermediates shows that, in the presence of substrates bearing large *para*-substituents, steric effects may play an important role for the inversion of enantioselectivity. Based on these results, a computational design of the catalyst has been performed aiming at increasing the observed enantiomeric excess (ee). The designed catalyst (with an additional methyl group on the mesityl substituent) increases the relative thermodynamic stability of the *endo* and *exo* allylic forms to 3.2 kcal/mol. This energy difference should induce an ee of 99% for the *R* form.

References: submitted to J. Am. Chem. Soc.

Title: Electrostatic Potential Derived Charges from Quantum Mechanics/Molecular Mechanics Calculations

Researchers: Alessandro Laio
Joost VandeVondele
Ursula Rothlisberger

Institute/ Group: Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie

Description:

A scheme is proposed for calculating electrostatic potential (ESP) derived charges from mixed Quantum Mechanics/ Molecular Mechanics (QM/MM) molecular dynamics simulations. These charges are fitted to the electrostatic field due to the quantum charge density evaluated on the MM atoms close to the QM system. The charges are restrained to the Hirshfeld value by a quadratic penalty function. In this way, the ESP charges can be obtained as a function of time along a finite temperature molecular dynamics trajectory with essentially no computational overload with respect to a standard QM/MM calculation. The ESP charges estimated by this procedure reproduce the field due to the charge density polarized by the environment and can be used as a reliable indicator of the chemical state of the system.

References: submitted to J. Phys. Chem. B

Title: Estimating equilibrium properties from non-Hamiltonian dynamics

Researchers: Joost VandeVondele
Ursula Rothlisberger

Institute/ Group: Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie

Description:

We derive an expression that enables the accurate estimation of equilibrium properties using non-Hamiltonian dynamics. The major advantage of our scheme is that a time average over a single non-Hamiltonian trajectory can be employed instead of an ensemble average. Hence, it can directly be used in standard molecular dynamics simulations. The connection between non-Hamiltonian dynamics and equilibrium properties is established by assigning to the individual frames of the trajectory a weight that is based on the fluctuations of the phase space compression factor. Additionally, a simple scheme that takes into account only fluctuation of a given maximum duration is introduced to reduce the statistical error. By systematically extending the duration of the allowed fluctuations, increasingly accurate results can be obtained.
Non-Hamiltonian dynamics schemes that are capable to enhance sampling efficiency are applied to two model systems in order to demonstrate the practical performance of our approach for the calculation of equilibrium free energy differences and probability density profiles.

References: J. Chem. Phys. **115** (2001) 7859-7864

Title: Cis-Trans Isomerization in Triply-Bonded Ditungsten Complexes: A Multitude of Possible Pathways

Researchers: Joost VandeVondele
Alessandra Magistrato
Ursula Röthlisberger

Institute / Group: Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie

Description:

We have investigated different possible mechanisms for the cis-trans isomerization in triply-bonded ditungsten complexes with stoichiometry $W_2Cl_4(NHEt)_2(PMe_3)_2$ using static density functional calculations as well as Car-Parrinello simulations. Our studies reveal an unexpected richness of possible reaction pathways that include both unimolecular and bimolecular mechanisms. Among the possible routes that have been identified are processes involving successive dissociation/reassociation of phosphine ligands, intramolecular chloride hopping, intertungsten phosphine exchange as well as numerous combinations of these basic reaction types. All pathways involve maximal activation barriers of less than 35 kcal/mol and include phosphine concentration dependent and independent routes. The energetically most favorable phosphine-dependent pathway is based on the dissociation/reassociation of phosphine ligands. This path is characterized by a maximal dissociation barrier of 18 kcal/mol. The fastest alternative unimolecular route (with a maximal activation barrier of 24 kcal/mol) is based on a direct exchange of phosphine between the two metallic coordination centers. All the identified pathways, with the exception of a previously proposed internal flip mechanism that can be ruled out on energetic grounds, are competitive and may contribute in various combinations to the overall reaction rate. The identified isomerization mechanisms are fully consistent with the experimentally observed 3-state-kinetics and the dependence of the overall reaction rate on the excess concentration of phosphine which is demonstrated with a simplified kinetic model of the process.

References: Inorg. Chem. (ASAP article)

Title: Canonical Adiabatic Free Energy Sampling (CAFES): A Novel method for the Exploration of Free Energy Surfaces

Researchers: Joost VandeVondele
Ursula Rothlisberger*

Institute/ Group: Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie

Description:

We present a novel method, canonical adiabatic free energy sampling (CAFES), that allows for the efficient exploration of the free energy surface of a subsystem (S) embedded in an environment (E) using molecular dynamics simulations. The dynamics of S is decoupled from the environment by introducing fictitious masses that ensure that S evolves slowly and adiabatically on the potential of mean force generated by E. In addition, the decoupling enables the use of different temperatures for the two parts of the system without introducing an irreversible heat flow. Using a higher temperature for the subsystem, a high efficiency for the sampling of rare events on the physical free energy surface is obtained.
The performance of this approach is demonstrated with a conformational analysis of a Gly-Ala dipeptide in aqueous solution. Rare conformational transitions, which naturally occur on a millisecond time scale, are observed within a few nanoseconds of a classical molecular dynamics simulation. The same method has also been applied in a hybrid Car-Parrinello/classical molecular dynamics investigation of the proton-catalyzed conversion of 2-bromoethanol to dibromoethane in water. Using CAFES, the anchimeric assistance of the bromine atom and the occurrence of a bromonium ion intermediate, a process which involves a barrier of ca. 23 kcal/mol, is observed spontaneously on the subnanosecond time scale.

References: J. Phys. Chem. B (accepted)

Title: Reaction Mechanism of Caspases: Insights from Mixed QM/MM Car-Parrinello Simulations

Researchers: Maria Lore Sulpizi*
Alessandro Laio**
Joost VandeVondele**
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Institute/ *[1]SISSA, International School for Advanced Studies, via Beirut 2-4, 34013 Trieste, Italy and INFM, Istituto Nazionale di Fisica della Materia, Italy
** Laboratory of Inorganic Chemistry
Group: Gruppe für Rechnergestützte Anorganische Chemie

Description:

Caspase cysteine proteases are fundamental targets for pharmaceutical intervention in a variety of diseases, which cause disregulated apopotosis. Here, we present a QM/MM Car-Parrinello study of key steps of the enzymatic reaction for a representative member of this family, caspase-3. The hydrolysis of the acyl-enzyme complex is studied at the density functional (BLYP) level of theory while the protein frame and solvent is treated using the GROMOS96 force field. These calculations show that the attack of the hydrolytic water molecule implies an activation free energy of ca. ΔF_A ~ 20 kcal/mol and leads to a gem-diol intermediate that can readily (ΔF_A ~ 5 kcal/mol) evolve to the enzyme products. These findings help elucidate the striking difference in catalytic activity between the caspase family and the cysteine protease papain.

References: submitted to J. Biol. Chem.

Title: Flexibility-Assisted Catalysis: Molecular Mechanisms of Compensatory Mutations in HIV-1 PR

Researchers: Stefano Piana*
P. Carloni**
Ursula Rothlisberger*

Institute/ Group: *Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie
** [1]SISSA, International School for Advanced Studies, via Beirut 2-4, 34013 Trieste, Italy and INFM, Istituto Nazionale di Fisica della Materia, Italy

Description:

The emergence of drug-resistant variants is a serious side effect associated with AIDS therapies based on inhibition of HIV-1 protease (HIV-1 PR). In these variants, compensatory mutations, usually located far from the active site, are able to affect the enzymatic activity via molecular mechanisms that have not been clearly established yet.
Here, we perform multi-nanosecond molecular dynamics simulations on the wild-type (WT) of HIV-1 PR and one of its most frequently occurring compensatory mutations, M46I, complexed with the substrate and an enzymatic intermediate. The quality of the calculations is established by comparison with the available NMR data. The molecular dynamics simulations indicate that the protein fluctuations in the mutated enzyme differ from those in the WT. These differences in the dynamic properties of the substrate adduct can be directly related to variations in the enzymatic activity (Piana, S; Parrinello, M and Carloni, P *J. Mol. Biol.* 2001 *submitted*) and therefore offer an explanation of the observed changes in catalytic rate between WT and mutated enzyme. We anticipate that this "flexibility-assisted" mechanism might be effective in the vast majority of compensatory mutations, which do not change the electrostatic properties of the enzyme.

References: submitted to Proteins

Title: Hybrid QM/MM Car-Parrinello Simulations

Researchers: Joost VandeVondele
Alessandro Laio
Ursula Rothlisberger

Institute/ Group: *Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie

Description:

First-principles molecular dynamics (Car-Parrinello) simulations based on density functional theory have become a valuable tool in the investigation of physical, chemical and biological systems. Here, we describe an extension of the Car-Parrinello method into a mixed quantum mechanical/molecular mechanical (QM/MM) scheme in which (i) the electrostatic coupling with the classical environment is based on a fully Hamiltonian approach; (ii) the occurrence of electron-spill out from the QM system onto neighboring classical point charges is impeded by the use of a suitable modification of the Coulomb interactions at short range;(ii) boundary atoms involved in chemical bonds between QM and MM part of the system are treated with empirical monovalent pseudopotentials; and (iii) the exclusion rules of standard (bio)molecular force fields are incorporated in a consistent manner.
Our approach enables efficient and robust hybrid Car-Parrinello simulations of extended systems in which the chemically relevant part is treated at the quantum mechanical level while the effects of the surroundings are taken explicitly into account through the embedding in the classical environment.

References: to appear in J. Phys. Cond. Mat.

Title: A Hamiltonian Electrostatic Coupling Scheme for Hybrid Car-Parrinello Molecular Dynamics Simulations

Researchers: Alessandro Laio
Joost VandeVondele
Ursula Rothlisberger

Institute/ Group: Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie

Description:

We present a fully Hamiltonian and computationally efficient scheme to include the electrostatic effects due to the classical environment in a Car-Parrinello mixed Quantum Mechanics / Molecular Mechanics (QM/MM) method. The polarization due to the MM atoms close to the quantum system is described by a Coulombic potential modified at short range. We show that the functional form of this potential has to be chosen carefully in order to obtain the correct interaction properties and to prevent an unphysical escape of the electronic density to the MM atoms (the so-called spill-out effect). The interaction between the QM system and the more distant MM atoms is included by a Hamiltonian term explicitly coupling the multipole moments of the quantum charge distribution with the classical point charges. Our approach remedies some of the well-known deficiencies of current electrostatic coupling schemes in QM / MM methods, allowing molecular dynamics simulations of mixed systems within a fully consistent and energy conserving approach.

References: submitted to J. Chem. Phys.

Title: Chiral Pd(II)-Bis(trichlorosilyl) Complexes. Synthesis, Structure, and Combined QM/MM Computational Studies

Researchers: Tom K. Woo*
Giorgio Pioda**
Ursula Rothlisberger*
Antonio Togni**

Institute/ Group: * Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie
** Laboratory of Inorganic Chemistry

Description:

The $PdCl_2$ complexes **1-3** (**1**, dichloro{1-{(R)-1-[(S)-2-(diphenylphosphino-κP)ferrocenyl]-ethyl}-3,5-dimethyl-1H-pyrazole-κN}palladium; **2**, dichloro{1-{(R)-1-[(S)-2-(diphenyl phosphino -κP)ferrocenyl]-ethyl}-3-phenyl-5-methyl-1H-pyrazole-κN}palladium; **3**, dichloro{1-{(R)-1-[(S)-2(diphenylphosphino-κP)ferrocenyl]-ethyl}-3-(2,4,6-trimethylphenyl)-1H-pyrazole-κN} palladium), previously used as catalyst precursors in the asymmetric hydrosilylation of olefins, were found to react with an excess of $HSiCl_3$ in CH_2Cl_2 to afford the corresponding bis(trichlorosilyl) derivatives **4-6**, respectively. Two of the new complexes (**5** and **6**) were characterized by X-ray crystallography and revealed unusual structural properties. A severe deviation from the ideal square-planar geometry was observed, as well as extremely elongated Pd-P bonds (Pd-P = 2.4559(16) Å for **5** and 2.504(2) Å for **6**). The nature of the uncommon structural features observed in the bis(trichlorosilyl) derivatives has been explored with density functional theory calculations and the combined quantum mechanics/ molecular mechanics (QM/MM) method. Using the combined QM/MM approach a systematic series of model systems have been constructed in which the steric and electronic influences of substituent groups were selectively removed or altered. The technique has allowed the exact nature of the geometric distortions to be pinpointed.

References: Organometallics **19** (2000) 2144-2152

Title: Three and Four Center trans Effects in Triply-bonded Ditungsten Complexes: An Ab initio Molecular Dynamics Study of Compounds with Stoichiometry $W_2Cl_4(NHEt)_2(PMe_3)_2$

Researchers: Alessandra Magistrato
Joost VandeVondele
Ursula Rothlisberger

Institute/ Group: Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie

Description:

We have performed ab initio molecular dynamics simulations based on density functional theory to characterize the structural, electronic, and dynamic properties of the three major isomeric forms of the title compound. In agreement with experimental results, calculations with two different parameterizations of the exchange-correlation functional (BLYP and BP) both indicate the cis-C_2 form as the most stable isomer. The relative energies of the different forms are, however, small (≈ 1-2 kcal/mol), and the three compounds show overall very similar ground state properties. Larger differences exist in their finite temperature behavior, which is dominated by the facile dissociation of one or both phosphine ligands. The calculated activation energies for phosphine dissociation differ clearly for the trans and the cis isomers and vary in the order trans << cis-C_2 < cis-C_i. Analysis of the electronic structure of the transition states shows that the difference in activation energy between cis and trans isomers can be rationalized in terms of a classic trans effect caused by a molecular orbital spanning the three atomic centers N-W-P. The subtle difference between the two cis isomers, on the other hand, is likely due to an analogous four-center trans effect N-W-W-P which is mediated via metal-metal orbitals and involves ligands on both tungsten atoms.

References: Inorg. Chem.**39** (2000) 5553-5560

Title: Electronically and Sterically Induced Structural Distortions in Square Planar d^8 Complexes

Researchers: Alessandra Magistrato*
Massimo Merlin**
Paul S. Pregosin**
Alberto Albinati***
Ursula Rothlisberger*

Institute/ Group: * Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie
** Laboratory of Inorganic Chemistry
*** Chemical Pharmacy, University of Milan, I-20131, Milan, Italy

Description:

The solid-state structure of the cationic MeO-Bihep Rh(I) compound, [Rh(S-MeO-Bihep)($POMe_3$)$_2$]BF_4, **3**, has been determined by X-ray diffraction. The four P-donors deviate markedly from square planar geometry, with the phosphite ligands P2 and P2', ca. +/-0.61 (7) Å, respectively, from the P1-Rh-P1' plane. This distortion resembles that found for PdBr(p-NCC_6H_4)(S-MeO-Bihep), **1**. Density functional calculations on a series of systematically varied models of **1** reveal three major components to be responsible for the observed distortion from square planar geometry: (i) attractive aromatic π–π interactions; (ii) electronic stabilization of coplanar aromatic rings in pseudo-trans position and (iii) P-phenyl- and MeO-Bihep phenyl intra-ligand repulsive steric interactions. Additional DFT studies on the p-tolyl Binap analog of **1**, PdBr(p-NCC_6H_4)(R-p-Tol-Binap), **2**, explain the source of the extremely long Pd-P2 bond distance, 2.437 (1) Å, in **2**. In spite of the structural similarity between **1** and **2**, the calculations rationalize the observation of a pronounced distortion from a square planar geometry in the former that is essentially absent in the latter.

References: Organometallics **19** (2000) 3591-3596

Title: Efficient multidimensional free energy calculations for ab initio molecular dynamics using classical bias potentials

Researchers: Joost VandeVondele
Ursula Rothlisberger

Institute/ Group: * Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie

Description:

We present a method for calculating multidimensional free energy surfaces within the limited time scale of a first-principles molecular dynamics scheme. The sampling efficiency is enhanced using selected terms of a classical force field as a bias potential. This simple procedure yields a very substantial increase in sampling accuracy while retaining the high quality of the underlying ab initio potential surface and can thus be used for a parameter free calculation of free energy surfaces. The success of the method is demonstrated by the applications to two gas phase molecules, ethane and peroxynitrous acid, as test case systems. A statistical analysis of the results shows that the entire free energy landscape is well converged within a 40 picosecond simulation at 500K, even for a system with barriers as high as 15 kcal/mol.

References: J. Chem. Phys. **113** (2000) 4863-4868

Title: Ditantalum Hydride Complexes with Bridging (2,6-$^{i}Pr_2C_6H_3$)NSiHPh Silanimine Ligands Resulting from $PhSiH_3$-Imido Ligand Coupling. A Combined Spectroscopic and Theoretical Investigation.

Researchers: Urs Burckhardt**
Gary L. Casty**
T. Don Tilley**
Tom K. Woo*
Ursula Rothlisberger*

Institute/ Group: * Laboratory of Inorganic Chemistry
Gruppe für Rechnergestützte Anorganische Chemie
** Department of Chemistry, University of California at Berkeley, Berkeley,USA

Description:

In this contribution, we report the preparation and characterization of two novel dinuclear tantalum hydride complexes featuring bridging silyl amido ligands. The two compounds, a diamagnetic main product and a related paramagnetic intermediate, form on treatment of $Cp^{*}Ta(=Nar)[Si(SiMe_3)_3]H$ (Cp^{*} = $\eta 5$-C_5Me_5; Ar = 2,6-$^{i}Pr_2C_6H_3$) with phenyl silane. For the diamagnetic complex $Ta_2Cp_2^{*}(NAr\text{-}SiHPh)H_2$, the single crystal X-ray analysis resolves to a molecular structure possessing nearly exact two-fold symmetry, while NMR spectroscopy indicates that the two molecular moieties are different. In order to elucidate the structural and bonding properties of the compound, a theoretical study based on density functional theory and ab initio molecular dynamics was carried out. Calculations of the whole 140 atom system, outline a molecular structure with one bridging and one terminal hydride ligand, and suggest a non-classical bonding scheme for the $(Ta\text{-}Si\text{-}N)_2$ ring. The paramagnetic compound, $Ta_2Cp_2^{*}(NAr\text{-}SiHPh)H_2$ exhibits similar structural features; in this case, the presence of two asymmetrically bound hydrides is confirmed by X-ray analysis and calculation.

References: Organometallics **19** (2000) 3830-3841

Title: Implementation of a gFEM for Homogenization Problems

Researchers: A. W. Rüegg, A.-M. Matache, Ch. Schwab

Institute/
Group: Seminar for Applied Mathematics

Description:

Many problems in engineering and the sciences involve media with (patch-wise) periodic microstructure, for example strong, yet lightweight lattice block materials. Such composite materials are constructed by replicating periodically a unit-cell of length ε. The microscopic details strongly influence the macroscopic behavior and have to be resolved by direct numerical simulation. Limited however by computing resources, many practical problems are still out of reach by using direct methods.

Generalized FEM summarized in [1] use a-priori knowledge about the solution to construct problem adapted shape functions. In [2] the standard Finite Element spaces based on piecewise polynomial shape functions on a macroscopic triangulation of the computational domain are augmented with problem dependent, non-polynomial micro shape functions that are periodic and oscillating on the length scale ε. The size of the macro elements is typically much larger than ε. Under the assumption of scale separation, i.e., the spatial variation of the solution is concentrated at the macro and micro length scales, these spaces lead to exponential rates of convergence for analytic input data. It should be remarked that the gFEM does not require scale resolution since the micro shape functions reflect the correct oscillatory behavior of the exact solution. In regions where the scales are not separated standard FE spaces should be employed in order to resolve all the solution scales. Our approach is to use the gFE spaces in regions of two-scale regularity and to employ standard FE spaces elsewhere.

This method is implemented in C++ for two-dimensional problems on anisotropic refined meshes with constrained nodes.

This Resarch is supported by the Swiss National Science Foundation, project 2100-058754.99/1: "Hierarchic FE-Models for periodic lattice and honycomb materials".

References:

[1] C.A. Duarte, I. Babuška and J.T. Oden, *Generalized Finite Element Methods for Three-Dimensional Structural Mechanics Problems*, Computers and Structures, **77** (2000), 215–232.

[2] A.M. Matache, I. Babuška and Ch. Schwab, *Generalized p-FEM in Homogenization*, Numerische Mathematik, **86** Issue 2 (2000), 319–375.

Title: Loss calculations of eddy currents in complex 3-d geometries

Researchers: Gregor Schmidlin[1,2]
Christoph Schwab[1]

[1] Seminar for Applied Mathematics
[2] supported under the TMR network
(BBW 97.0404)

Description:

In this project we compute the electromagnetic field in complex 3-d geometries. Cooperation with the industry (ABB CRC Germany) is very important since the industry supplies us with the used infrastructure (CAD systems, net generators).

The loss within a transformer is determined by the eddy currents in the magnetic core. The calculation of these currents requires the solution of the Maxwell equations which describe the electrical and magnetic field. We neglect the capacitance current (Eddy current approximation) since in our problem only relatively small frequencies occur. It is possible to reduce the system to four boundary integral equations, one equation for the potential outside of the conductor and the remaining three for the components of the surface current. Computed the potential and the surface current we calculate the electromagnetic fields.

The four boundary integral equations cannot be solved accurately. Therefore the solution is approximated with the help of the boundary element method. A fine lattice is put over the surface and the integral equation system is collocated in the n nodes of the grid. With this we get $4n$ linear equations for the four unknowns per node.

This system is solved iteratively. In our problem the material parameters as used in practice lead to a badly conditioned set of equations, such that the iterative solvers cannot solve it accurately. At the ETHZ we developed a preconditioner for this set of equations which reduces the iteration number of the solver and makes it possible to treat large problems.

The models computed with this new preconditioner possess thousands of nodes. Since the matrix of the system is fully populated enormous memory and computing time is required. Doing the computations in parallel it is possible to solve such problems on large computers.

Reference: An article was published in *Int. J. Numer. Meth. Engng*

Title: The hydration-free energy of CO_2 with quantum mechanical interaction energies from classical simulations at high pressures

Researchers: Oleg M. Suleimenov
Terry M. Seward

Institute/ Group: Institut für Mineralogie und Petrographie
Gruppe Geochemie
ETH-Zentrum

Description:

A free energy perturbation technique is employed in which configurations from a classical simulation with empirical CO_2-H_2O interactions are used to calculate the hydration-free energy of CO_2 with quantum mechanically derived solute-solvent interactions. A flexible CO_2 model and the fluctuating charge model for water was used in the classical simulations. The quantum mechanical solute-solvent interaction energies were calculated using MP2/mg-cc-pVTZ level of theory. Computational costs were reduced by using a cluster approximation in which ab initio pair interaction energies are calculated between the solute and up to 80 solvent molecules while multi-body interactions are calculated with small (up to 12 solvent molecules) clusters.

Title: Iodide ion hydration in high temperature water solvent

Researchers: Terry M. Seward
Oleg M. Suleimenov

Institute/ Group: Institut für Mineralogie und Petrographie
Gruppe Geochemie
ETH-Zentrum

Description:

The hydration of ions in high temperature aqueous electrolyte solutions plays a fundamental role in determining the nature of stable isotope fractionation (e.g. $^{18}O/^{16}O$ and D/H) in hydrothermal fluids which occur throughout the Earth's crust. In order to better understand these processes, we have been studying the structural aspects of iodide ion solvation in a high temperature liquid water using X-ray absorption and uv spectroscopy together with Car-Parinello ab initio molecular dynamics simulations. Iodide ion charge-transfer-to-solvent transitions in the ultraviolet indicate that the first shell hydration environment expands (in contrast to cation hydration) with increasing temperature from 25 to 350°C and this is confirmed by X-ray absorption fine structure (EXAFS) measurements which demonstrate that first shell iodide-oxygen(water) distances change from 3.55 to 3.63Å over the temperature range from 25 to 350°C. The ab initio MD computed iodide-oxygen(water) distance (i.e. first maximum in g(r)) is 3.54 Å at 25°C and in good agreement with that derived from X-ray absorption spectroscopy. The computation of iodide ion-first shell water distances at high temperatures is currently underway.

Title: Electronic Structure of Strongly Correlated Materials

Researchers: T.M. Rice, M. Sigrist [*]
V.I. Anisimov [**]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Inst.of Metal Physics, Russian Academy of Sciences, Yekaterinburg

Description:

Modifications of standard density functional theory are needed to calculate the electronic structure in the presence of strong correlations among the electrons. One method known as LDA+U, allows the treatment of broken symmetries in spin and orbital degrees of freedom. A second method combines the local density approximation with the dynamical mean field theory to describe systems without a broken symmetry. These methods are applied to materials of high current interest.

References:

- F. Mila, R. Shiina, F.C. Zhang, A. Joshi, M. Ma, V.I. Anisimov and T.M. Rice, Phys Rev. Lett. **85**, 1714 (2000).
- V.I. Anisimov, I.A. Nekrasov, D. Ekondkov, T.M. Rice and M. Sigrist, submitted to Eur. J. Phys. B

Title: Simple and accurate computations of solvatochromic shifts in $\pi \rightarrow \pi^*$ transitions of aromatic chromophores

Researchers: Hendrik Heinz
Epameinondas Leontidis
Ulrich W. Suter

Institute/Group: Department of Materials, Institute of Polymers,
and University of Cyprus, Nicosia, Department of Chemistry

Description:

A new approach is introduced for calculating the spectral shifts of the most bathochromic $\pi \rightarrow \pi^*$ transition of an aromatic chromophore in apolar environments. As an example, perylene in solid and liquid n-alkane matrices was chosen, and all shifts were calculated relative to one well-defined solid-inclusion system. It was shown that a simple two-level treatment of the solute using Hückel theory yields spectral shifts in excellent agreement with experimental results for the most prominent inclusion sites of perylene in solid n-alkane surroundings, and for the dilute solutions in liquid n-alkanes. The idea is general enough to be applied to any aromatic chromophore in a nonpolar solvent matrix. In contrast to earlier treatments, this approach is based on geometry- and environment-dependent polarizabilities, employs a r^{-4} dependence for the dispersion energy, and is conceptually very simple and computationally very efficient.

References:

H. Heinz, E. Leontidis, U. W. Suter, *J. Am. Chem. Soc.* (2001) ASAP

Title: Numerical Simulation of the effective thermoelastic properties of short fiber composites

Researchers: Hans Rudolf Lusti
Peter J. Hine
Andrei A. Gusev

Institute/Group: Department of Materials, Institute of Polymers

Description:

Direct finite-element calculations were conducted to predict the elastic and thermoelastic properties of short fiber reinforced composites. We studied various morphologies with perfectly aligned as well as with misaligned or randomly in-plane oriented fibers. Measured data on the orientation distribution of fibers were used to bias the Monte-Carlo runs. Computer models comprising 100 fibers were tessellated into three-dimensional, morphology-adaptive, periodic finite-element meshes. We considered several different real orientational distributions, typical of both conventionally and shear controlled injection molded short glass fiber polypropylene composites. In all cases, numerically predicted and measured elastic constants were in excellent agreement. Based on this successful validation, one can readily employ our finite-element based numerical methodology for simultaneous computer aided materials and structural design of advanced components made up of short-fiber-reinforced composites.

References: A manuscript is in preparation

Title: Finite element analysis of the elastic and dielectric properties of composite materials with core-shell inclusions

Researches: Ilia A. Karmilov
Andrei A. Gusev

Institute/Group: Department of Materials, Institute of Polymers

Description:

In this work we have used a finite element based approach for predicting the overall elastic and dielectric properties of shell-egg-particle reinforced polymers. Multiscale tetrahedra-based meshes were employed for reproducing the morphology. The particles were approximated by core-shell spheres and spheroids with the walls of different thickness. For the particles, typical titanium dioxide properties were assumed in calculations. We investigated the dependence of macroscopic properties on the inclusion volume fraction, thickness of the titanium dioxide walls, and aspect ratio of the spheroids. It appears that the core-shell-particle reinforced polymers exhibit a unique portfolio of technological properties that can be indispensable in various demanding weight-saving applications.

References: A manuscript is in preparation.

Title: Influence of the topology and the polydispersity on the Young's modulus of a polymer network

Researchers: Chantal Oberson
Ulrich W. Suter

Institute/Group: Department of Materials, Institute of Polymers

Description:

As it is still unclear, which theoretical model should be used to predict the deformation of a polymer network, we study a simplified model of a network of harmonic phantom springs, adding more and more defects or taking more and more complex topologies. The written algorithm makes it possible to generate a large variety of networks, and to obtain the corresponding shear modulus by a Polak-Ribière energy minimization. The cubic network, for example, has a very interesting behavior, tending either to the phantom or to the affine model, depending on the importance of the topology or polydispersity modifications.

References: Manuscript in preparation

Title: Elastic behavior of sphere-reinforced polymers: does microstructure matter?

Researchers: Andrei A. Gusev
Chantal Oberson

Institute/Group: Department of Materials, Institute of Polymers

Description:

The goal of this work is to understand the microstructure effects on the linear elastic behavior of sphere-filled polymers. Assuming different geometric arrangements and matrix properties typical of solid, rubber, and melt-like polymers, we predict the effective elastic constants of silica-sphere-filled polymers numerically. Full scale, accurate in principle, finite-element calculations are employed. Apart from solving an interesting problem in its own right, we also provide reliable numerical predictions indispensable to calibrate the elastic responses of empirical models that are commonly employed in practice to explain large-strain and dynamic properties of filled polymers.

References: Manuscript in preparation

Title: Normal and defective perylene substitution sites in alkane crystals

Researchers: Epameinondas Leontidis
Hendrik Heinz
Krystyna Palewska
Ernst-Udo Wallenborn
Ulrich W. Suter

Institute/Group: Department of Materials, Institute of Polymers,
and University of Cyprus, Nicosia, Department of Chemistry

Description:

We examine experimentally and computationally the nature of substitution of perylene in polycrystalline solid alkane matrices (Shpol'skii systems). The technique of low temperature excitation-emission matrix spectroscopy is used to determine all substitution sites in alkane matrices from hexane to decane. A theoretical method from the group of Jortner [Shalev et al., J. Chem. Phys. **95**, 3147 (1991)], which was extended and applied by us to this problem in the past [Wallenborn et al., J. Chem. Phys. **112**, 1995 (2000)], allows one to separate the perylene sites in all alkanes into normal and defective sites. Normal sites are obtained by direct substitution of two alkane molecules by a perylene molecule, while defective sites are derived from normal sites by eliminating one of the four nearest neighbors of perylene in the lattice planes parallel to the chromophore. We discuss the strengths and limitations of the present theoretical treatment, which can serve as a valuable supplement and guide to line-narrowing and single- molecule spectroscopic investigations of impurity centers in low-temperature solids.

References:

(1) E. Leontidis, H. Heinz, K. Palewska, E.-U. Wallenborn, U. W. Suter *J. Chem. Phys.* 114, 3224 (2001).
(2) E.-U. Wallenborn, E. Leontidis, K. Palewska, U. W. Suter, U. Wild *J. Chem. Phys.* 112, 1995 (2000).

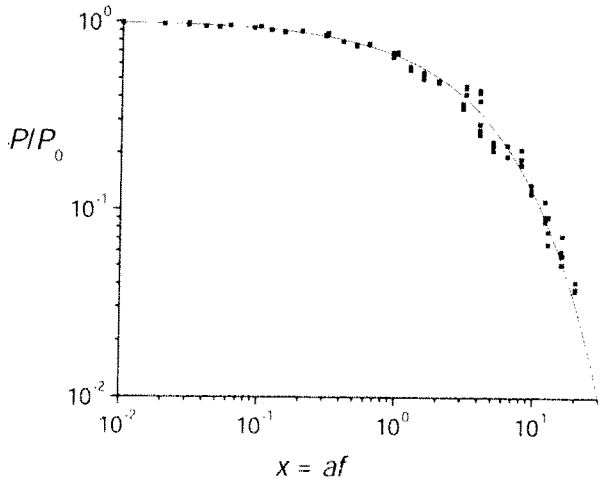
Title: Computer-aided design of nanocomposites for barrier applications

Researchers: Hans Rudolf Lusti
Andrei A. Gusev

Institute/Group: Department of Materials, Institute of Polymers

Description:

Sheets of layered minerals like mica or clay are impermeable for molecular species. By putting just a few percent of exfoliated high-aspect-ratio atomic-thickness sheets of a layered mineral into a polymer, one can significantly improve barrier properties but still retain the flexibility and optical clarity of the pure polymer. It is a problem is to understand the permeability levels that can be achieved with a particular nanocomposite. For the first time to our best knowledge, we have conducted direct finite-element permeability calculations with multi-inclusion computer models. We studied three-dimensional periodic computer models comprised of a random dispersion of perfectly aligned impermeable round platelets in an isotropic matrix. Based on unstructured morphology-adaptive meshes, we solved Laplace's equation for the local chemical potential m with position-dependent local permeability coefficient $P(\mathbf{r})$ taken to be 0 inside the platelets and P_0 everywhere in the matrix.
The overall, effective permeability coefficients were calculated based on a linear-response relation between the overall flux and the external chemical potential gradient applied. We studied the overall permeability coefficient P relating the z-components of overall flux and chemical potential gradient. It is exactly this permeability coefficient P that is of interest in most barrier applications including advanced coatings, food packaging, and beverage bottling. We have conducted numerical calculations assuming various platelet aspect ratios between 1 and 400 and volume fractions up to 5 vol%. The results are shown in the figure. One can see that the permeability reduction is governed by the product $x = a \cdot f$, where a is the platelet aspect ratio and f the volume fraction. Moreover, for the practical design, one can readily use the stretched exponential form $P/P_0 = \exp(x/x_0)^{\beta}$ with $\beta = 0.71$ and $x_0 = 3.47$.



References: A.A. Gusev, H.R. Lusti, *Advanced Materials (2001, in print)*

Title: Phase Diagrams of 2D Bosonic Systems

Researchers: G. Schmid, S. Todo, M. Troyer [*]
G.G. Batrouni, K. Bernardett, F. Hebert [**]
A. Dorneich, W. Hanke [***]
R.T. Scalettar [****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Université de Nice, France
[***] Universität Würzburg, Germany
[****] University of California, Davis

Description:

The behavior of bosons in two dimensions is of major current interest for several reasons. Such systems describe, for example, Helium adsorbed on surfaces. They can also be mapped (approximately) to models for Josephson junction arrays, which can be manufactured and studied experimentally. In addition, a Hamiltonian describing a system of hardcore bosons, can be mapped exactly onto models of spin-1/2 Heisenberg quantum antiferromagnets. Such quantum spin models are of great theoretical and experimental interest: There are several recently discovered materials, exhibiting a variety of interesting properties such as magnetization plateaus, which are very well described by these Hamiltonians. In addition, such bosonic models can be used as effective models for fermionic systems where the bosonic Cooper pairs are well formed. In several extensive simulations we could determine the ground state and finite temperature phase diagram of the bosonic hardcore Hubbard model. Previously conjectured supersolid phases turned out to be phase separation instead. Unusual reentrant behavior and ordering upon *increasing* the temperature have been found.

References:

- F. Hebert, G. G. Batrouni, R. T. Scalettar, G. Schmid, Matthias Troyer, and A. Dorneich, preprint, submitted to Phys. Rev. B
- A. Dorneich, W. Hanke, E. Arrigoni, M. Troyer, S.C. Zhang, preprint, submitted to Phys. Rev. Lett.
- A. Dorneich and Matthias Troyer, preprint, submitted to Phys. Rev. E
- K. Bernardet, G.G. Batrouni, J.-L. Meunier, Guido Schmid and Matthias Troyer, preprint submitted to Phys. Rev. B
- Guido Schmid, Synge Todo, Matthias Troyer and A. Dorneich, preprint submitted to Phys. Rev. Lett.

Title: Quantitative modeling of quantum magnets

Researchers: A. Läuchli, M. Troyer [*]
D.C. Johnston [**]
A. Honecker [***]
F. Mila [****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Ames Laboratories, Ames, Iowa
[***] Universität Braunschweig, Germany
[****] Université de Lausanne

Description:

Unusual behavior is observed in materials where quantum effects are strong. These materials typically consist of low-dimensional structures, such as weakly coupled chains or planes. The most prominent examples are the high temperature superconductors, which consist of doped copper oxide layers. While we are still far from a complete understanding of these doped systems, we could make rapid progress on the undoped parent compounds, which are quantum magnets. Modern quantum Monte Carlo algorithms allow quantitative comparisons between models and experimental measurements on these quantum magnets. These comparisons allow the determination of microscopic coupling constants and the explanation of unusual magnetic properties of low-dimensional quantum magnets, such as copper and vanadium oxide materials.

References:

- D.C. Johnston, Matthias Troyer, S. Miyahara, D. Lidsky, K. Ueda, M. Azuma, Z. Hiroi, M. Takano, M. Isobe, Y. Ueda, M.A. Korotin, V.I. Anisimov, A.V. Mahajan, and L.L. Miller, Preprint, submitted to Phys. Rev. B
- R. Melzi, P. Carretta, A. Lascialfari, M. Mambrini, Matthias Troyer, P. Millet and F. Mila, Phys. Rev. Lett. **85**, 1318 (2000)
- David Johnston, R.K.. Kremer, M. Troyer, X. Wang, A. Klümper, S. L. Bud'ko, A. F. Panchula, and P. C. ,Phys. Rev. B **61**, 9558 (2000).
- A. Honecker and A. Läuchli, Phys. Rev. B **63**, 174407 (2001)

Title: Quantum criticality

Researchers: M. Troyer [*]
M. Vojta [**]
S. Sachdev [***]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] Universität Augsburg, Germany
[***] Yale University, USA

Description:

In low dimensional systems, such as layered materials quantum fluctuations are especially strong. They can lead to a destruction of an ordered ground state, just as thermal fluctuations can destroy order at finite temperatures. In the vicinity of a quantum critical point (a continuous phase transition in the ground state of a quantum system at zero temperatures) universal quantum critical behavior can be observed. This is similar to classical critical behavior observed near classical phase transitions at finite temperatures. Universal here means that the behavior does not depend on details of the system, material, lattice structure, but only on the symmetries of the phases and on the dimensionality. Simulations on simple models can thus provide results valid for a large class of materials. In the determination of universal classical critical behavior (characterized by universal critical exponents and amplitude ratios) numerical simulations were essential. The biggest challenge for these simulations is that the relevant length scales diverge at the phase transition, requiring extremely large lattices for accurate and reliable results. Recent breakthroughs in algorithmic developments for quantum systems now allow similar calculations to be performed near quantum critical points.

References:

- Subir Sachdev, M. Troyer and M. Vojta. Phys. Rev. Lett. **86,** 2617 (2001)
- Jae-Kwon Kim and M. Troyer, Preprint, to be published in Phys. Rev. B

Title: Quantum Monte Carlo Study of Randomness-Driven Quantum Phase Transitions in Two-Dimensional Antiferromagnets

Researchers: Synge Todo[*]
Chitoshi Yasuda, Munehisa Matsumoto, Hajime Takayama [**]
Shigeru Koikegami[***]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] ISSP, University of Tokyo, Japan
[***] AIST Tsukuba, Tsukuba, Japan

Description:

We investigate effects of randomness, such as site dilution and bond randomness, on the ground state of two-dimensional Heisenberg antiferromagnets and also the nature of randomness-driven quantum phase transitions by means of the quantum Monte Carlo method.

References:

- Chitoshi Yasuda, Synge Todo, Munehisa Matsumoto, and Hajime Takayama, Phys. Rev. B. **64**, 092405 (2001).
- Chitoshi Yasuda, Synge Todo, Kenji Harada, Naoki Kawashima, Seiji Miyashita, and Hajime Takayama, Phys. Rev. B **64**, R140415 (2001).
- Synge Todo and Kiyoshi Kato, Phys. Rev. Lett. **87**, 047203 (2001).
- Synge Todo, Munehisa Matsumoto, Chitoshi Yasuda, and Hajime Takayama, Preprint, to be published in Phys. Rev. B.
- Shigeru Koikegami, Synge Todo, and Hajime Takayama, Preprint submitted to J. Phys. Soc. Jpn.
- Munehisa Matsumoto, Chitoshi Yasuda, Synge Todo, and Hajime Takayama, Preprint submitted to Phys. Rev. B.

Title: Multiparticle ring exchange in the Wigner glass

Researchers: K. Völker [*]
S. Chakravarty [**]
M. Salmhofer [***]
D. Poilblanc [****]

Institute/Group: [*] Theoretische Physik, ETH Zürich
[**] University of California at Los Angeles, USA

Description:

The two-dimensional electron gas (2DEG) occurs in a variety of systems, such as semiconductor heterostructures, the Copper-Oxide layers of high-temperature superconductors, or on liquid-Helium surfaces. Potential applications are in nanotechnology and spintronics. From a theoretical point of view, it provides an opportunity to study the rich and often novel physics arising from strong electron interactions. One example is the unexpected metal-insulator transition (MIT) in two dimensions. At very low densities, and zero temperature, the 2DEG is expected to freeze into a crystalline state, the so-called Wigner crystal (or a Wigner glass in the presence of disorder), which is an insulator. Under certain conditions (in very clean systems) the Wigner glass can melt into a metal. The nature of this metallic state is at present not understood. An important part of the problem is to determine the magnetic properties of the 2DEG close to the MIT. From a numerical point of view, the determination of magnetic interactions involves the minimization of the action functional, which is represented as a function of about 1000 variables. Minimization is performed by a variable metricalgorithm (Broyden-Fletcher-Goldfarb-Shanno, BFGS).

References:

- K. Völker and S. Chakravarty, preprint submitted to Phys. Rev. B

Title: Supersonic turbulence in shock bounded slabs

Researchers: Rolf Walder*
Doris Folini**

Institute/ Group: *Institut für Astronomie
Gruppe für Rechnergestützte Astrophysik
**Observatoire de Strasbourg
Université Louis Pasteur, Strasbourg, France

Description:

Colliding hypersonic flows co-determine the dynamics of galaxy formation, star-forming molecular clouds, accretion into black-holes, supernova remnants, and atmospheres of hot stars. We investigate the character of the excited turbulence by means of 2D plane-parallel shock-bounded slabs.

Shock bounded slabs are unstable for a wide range of flow-parameters typically found in various astrophysical objects. It is demonstrated that the instabilities saturate in supersonic turbulence. The density fluctuates by several orders of magnitude. Its probability distribution function (pdf) is Gaussian on a log-scale. Compared to the stationary value, the mean density of the slab is strongly reduced. A few volume-percent of the slab, however, consist of overcompressed knots. The mean Machnumber in the slab is only mildy supersonic even for colliding high Machnumber flows. Peak Machnumbers, however, can be much higher. The velocity is isotropized on the scale of the shell but is strongly anisotropic on smaller scales. Video-animations of the turbulent shell are a valuable tool to analyze the turbulence.

References: R. Walder and D. Folini Astrophysics and Space Science **274/1-2** (2000), 343-352, video-animations at http://www.astro.phys/staff/walder/

Title: Alfvén-wave support and filamentation of molecular clouds

Researchers: Doris Folini**
Rolf Walder*
Jean Heyvaerts**

Institute/ Group: *Institut für Astronomie
Gruppe für Rechnergestützte Astrophysik
**Observatoire de Strasbourg
Université Louis Pasteur, Strasbourg, France

Description:

We investigate for the first time by means of 1D, plane parallel, isothermal MHD simulations to what degree Alfvén-waves originating at a central symmetry plane can contribute to the support of a self-gravitating molecular cloud. We find that reasonably strong Alfvén-waves delay the contraction of an accreting molecular cloud significantly. In addition, the Alfvén-waves cause the cloud to become strongly inhomogeneous with regard to density, velocity, and magnetic field. The thin, high density sheets we observe first form due to a parametric instability of the Alfvén-wave, but the evolution soon becomes highly non-linear. Magnetic energy can be trapped between two sheets through reflection of MHD-waves at sheet boundaries. There, wave energy can also be transferred to compressible modes, resulting in partial loss of this energy through radiation processes. We currently study a wide variety of physical scenarios, which is only possible in 1D as the numerical simulations require a sufficiently high spatial resolution and order of integration in order to observe the fragmentation of the cloud into sheets.

References: Results have been presented at a workshop and a manuscript has been submitted to *Astronomy and Astrophysics*

Title: The A-Maze Code package

Researchers: Rolf Walder*
Doris Folini**

Institute/ Group: *Institut für Astronomie
Gruppe für Rechnergestützte Astrophysik
**Observatoire de Strasbourg
Université Louis Pasteur, Strasbourg, France

Description:

Our numerical simulation package A-MAZE comprises adaptive mesh codes to compute 3D magnetic, compressible, and reactive flows, 3D NLTE radiative transfer under optically thick and optically thin conditions, and scripts for data-management and visualization. Currently, we are working on the implementation of non-linear diffusion and self-gravity. The codes are publically available at the given reference.

References: The A-MAZE code package, http://www.astro.phys/staff/walder/

Title: NMR structure calculation using torsion angle dynamics with the program DYANA

Researchers: Peter Güntert
Torsten Herrmann
Francisco López García
Thomas Szyperski
Aizhuo Liu
César Fernández
Lars Ellgaard
Daniel Braun
Roland Riek
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:

The program DYANA (DYnamics Algorithm for Nmr Applications) for efficient calculation of three-dimensional protein and nucleic acid structures on the basis of conformational constraints collected by nuclear magnetic resonance (NMR) experiments performs simulated annealing by molecular dynamics in torsion angle space and uses a fast recursive algorithm to integrate the equations of motions. In 2000/2001 the program DYANA was used in our group for the NMR structure calculation of four proteins as well as in our project on the structure of prion proteins (see next project description).

References:

F. López García, T. Szyperski, J. H. Dyer, T. Choinowski, U. Seedorf, H. Hauser and K. Wüthrich
J. Mol. Biol. **295** (2000) 595–603

A. Liu, P. Luginbühl, O. Zerbe, C. Ortenzi, P, Luporini and K. Wüthrich
J. Biomol. NMR **19** (2001) 75–78

C. Fernandéz, K. Adeishvili and K. Wüthrich
Proc. Natl. Acad. Sci. USA **98** (2001) 2358–2363

L. Ellgaard, R. Riek, T. Herrmann, P. Güntert, D. Braun, A. Helenius and K. Wüthrich
Proc. Natl. Acad. Sci. USA **98** (2001) 3133–3138

Title: Structure determination of prion proteins

Researchers: Luigi Calzolai
Martin Billeter
Peter Güntert
Aizhuo Liu
Francisco López García
Thorsten Lührs
Dominikus Lysek
Roland Riek
Christine von Schroetter
Gerhard Wider
Ralph Zahn
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:

Prion proteins are associated with transmissible spongiform encephalopathies (TSE), a group of invariably fatal diseases characterized by loss of motor control, dementia, and paralysis wasting. Human TSEs include Creutzfeldt-Jakob disease, fatal familial insomnia, the Gerstmann-Sträussler-Scheinker syndrome and kuru, and there is bovine spongiform encephalopathy in cattle ("mad cow disease"), and scrapie in sheep. The "protein-only" hypothesis proposes that TSEs are by the conversion of the ubiquitous cellular form of the prion protein into an aggregated "scrapie form". According to this model, the prion protein would at the same time be the target and the infectious agent in TSEs. Our project aims at elucidating the molecular basis of TSEs and the origin of the species barrier their transmission by determination of the three dimensional structures of the human and bovine prion proteins, as well as by structure determinations of three variants of the human prion protein.

References:

R. Zahn, A. Z. Liu, T. Lührs, R. Riek, C. von Schroetter, F. López García, M. Billeter, L. Calzolai, G. Wider and K. Wüthrich
Proc. Natl. Acad. Sci. USA **97** (2000) 145–150

F. López García, R. Zahn, R. Riek and K. Wüthrich
Proc. Natl. Acad. Sci. USA **97** (2000) 8334–8339

L. Calzolai, D. A. Lysek, P. Güntert, C. von Schroetter, R. Riek, R. Zahn and K. Wüthrich
Proc. Natl. Acad. Sci. USA **97** (2000) 8340–8345

M. Billeter and K. Wüthrich
Arch. Virol. (Suppl.) **16** (2000) 251–263

Title: Sequence-specific NMR assignment of proteins by global fragment mapping with the program MAPPER

Researchers: Peter Güntert
Michael Salzmann
Daniel Braun
Kurt Wüthrich

Institute: Institut für Molekularbiologie und Biophysik

Description:

A new program, MAPPER, for semiautomatic sequence-specific NMR assignment in proteins is introduced. The program uses an input of short fragments of sequentially neighboring residues, which have been assembled based on sequential NMR connectivities and for which either the $^{13}C^{\alpha}$ and $^{13}C^{\beta}$ chemical shifts or data on the amino acid type from other sources are known. MAPPER then performs an exhaustive search for self-consistent simultaneous mappings of all these fragments onto the protein sequence. Compared to using only the individual mappings of the spectroscopically connected fragments, the global mapping adds a powerful new constraint, which results in resolving many otherwise intractable ambiguities. In an initial application, virtually complete sequence-specific assignments were obtained for a 110 kDa homooctameric protein, 7,8-dihydroneopterin aldolase from *Staphylococcus aureus*.

References: P. Güntert, M. Salzmann, D. Braun and K. Wüthrich
Sequence-specific NMR assignment of proteins by global fragment mapping with the program MAPPER
J. Biomol. NMR **18** (2000) 129–137

Title: Point-centered domain decomposition for parallel molecular dynamics simulation

Researchers: Reto Koradi
Martin Billeter
Peter Güntert

Institute: Institut für Molekularbiologie und Biophysik

Description:

A new algorithm for molecular dynamics simulations of biological macromolecules on parallel computers, point-centered domain decomposition, is introduced. The molecular system is divided into clusters that are assigned to individual processors. Each cluster is characterized by a center point and comprises all atoms that are closer to its center point than to the center point of any other cluster. The point-centered domain decomposition algorithm is implemented in the new program OPALp using a standard message passing library, so that it runs on both shared memory and massively parallel distributed memory computers. Benchmarks show that the program makes efficient use of up to 100 and more processors for realistic systems of a protein in water comprising 10,000 to 20,000 atoms.

References: R. Koradi, M. Billeter and P. Güntert
Point-centered domain decomposition for parallel molecular dynamics simulation
Comp. Phys. Comm. 124 (2000) 139–147

6
High-Performance Hardware

6.1 Competence Center for Computational Chemistry

The following resources are available:

- a cluster of 7 more than 8-year old IBM RS6000 workstations to be replaced in the year 2002;
- two Compaq AlphaServers with 6 and 8 EV6/525 processors;
- two IBM SP machines, one with 64 processors and one with 32 processors.

The research activities of the Competence Center for Computational Chemistry C^4, its members and the operation of the C^4 hardware are described in the C^4 Annual Report 2000/2001, which is published in November 2001.

6.2 HPCN Technology at CSCS Manno

In the frame of its national service mission, CSCS provides its academic, governmental and industrial user community with High Performance Computing and Networking resources and support competencies. The CSCS HPCN technology division staff offers expertise and support in the following fields of enabling technologies for computational sciences and engineering:
- high performnace systems and networks
- applications support and performance optimization
- benchmarking and software engineering
- data mining and visualization.

Computing Resources

Parallel Vector Processing: NEC/Cray SX-5

The SX-5 system consists of a single node with 10 CPUs (8 Gigaflops each) and 64 Gbytes of shared main memory (expandable up to 16 CPUs and 128 GB memory max.) having a peak performance of 80 gigaflops and allowing both the shared-mamory and MPI-based parallel programming model.

Hardware/OS Specification:
10 VP (vector processors) (8 GFLOPS each)
64 GB (giga bytes) main memory
600 GB disk
SUPER-UX R11.1 operating system

Compilers and libraries:
ANSI C: Compiler
FORTRAN-90: Compiler
C++: Compiler
HPF: Compiler
Psuite: Program development environment
MathKeisan: Highly tuned and well-tested collection of Math libraries
ASL: Scientific library for the SX Series
NAG: NAG FORTRAN Library (Mark 19)
NetCDF: Network Common Data Form
FISHPACK: Subroutines for solving separable partial differential equations in various coordinate systems.
Zufall: Random Numbers Generator

Computational Chemistry:
ADF: Density functional
Gamess-US: Package for Hartree-Fock and semiempirical methods
Gaussian: Hartree-Fock, CI and DFT methods
MolPro: Multiconfiguration SCF and CI, MCSCF, DFT

CFD/Structure analysis:
STAR-CD
FLUENT
CFX

HP N-Class Cluster

The symmetric multiprocessing (SMP) HP-based compute serving environment is composed by 4 N-Class systems based on 360MHz PA-8500 64 bit processors. Three N400 server systems are configured with 8 CPUs and one with 6 CPUs, 2 GB main memory and 100 GB local temporary disk space each. The system runs under HP-UX 11.0 and therefore allows the access to a wide applications portfolio, especially in the field of engineering and computational chemistry. The N-Class cluster integration, job scheduling and load balancing is done via Load Sharing Facility (LSF).

Compilers and libraries:
HP ANSI C: Compiler
HP FORTRAN-90: Compiler
HP FORTRAN-77: Compiler
HP C++: Compiler
Maple: Symbolic Calculus
Mathematica: Integrated technical computing system
Matlab: Language for technical computing
MLIB: Scientific library
VECLIB: Scientific library
LAPACK: Scientific library

Computational chemistry:
ADF: Density functional
Gamess-US: Package for Hartree-Fock and semiempirical methods
Gaussian: Hartree-Fock, CI and DFT methods
MolPro: Multiconfiguration SCF and CI, MCSCF, DFT
Meldf-x: Single-/multi-reference CI
Molcas: Multiconfiguration SCF and CI, MCSCF, CASSCF
Prddo/M: Approximative Hartree-Fock for very large molecules
Turbomole: Program Package for ab initio Electronic Structure Calculations

CFD/Structure analysis:
STAR-CD
FLUENT
CFX

List of current projects (reviewed by the CSCS Research Committee)

Quantum Simulation of Materials
Prof. A. Baldereschi (Inst. for Numerical Research in the Physics of Materials (IRRMA), EPFL)

Location of Conical Intersections at the Multi-State CASPT2 Level
Prof. T. Bally (Inst. fr Physikalische Chemie, Uni-Fribourg)

Structures and Rearrangements of Organic Radical Cations
Prof. T. Bally (Inst. fr Physikalische Chemie, Uni-Fribourg)

Global and Regional Climate Modeling
Prof. M. Beniston (Inst. of Geography, Uni-Fribourg)

Enantioselective Hydrogenation of Activated Carbonyl Compounds over Chirally Modified Pt
Prof. Buergi (Lab. fr Technische Chemie, ETHZ)

Protein Folding and Misfolding
Prof. A. Caflish (Dept. of Biochemistry, Uni-Zurich)

The Modeling of Incommensurate Structures by MD Techniques
Prof. G. Chapuis (Inst. de Cristallographie, Uni-Lausanne)

Computation of Stellarator Coils, Equilibrium and Stability
Dr. W. A. Cooper (CRPP-Centre de Recherches en Physique des Plasmas, EPFL)

Computational Chemistry of Inorganic Compounds and Materials
Prof. C. Daul (Inst. de Chimie Inorganique et Analytique, Uni-Fribourg)

Non-hydrostatic Modeling of Gravity Wave Propagation into the Stratosphere
Prof. H. Davies (Inst. fr Atmosphre und Klima, ETHZ)

DNS of Condensation of Steam/Air Mixtures in Two-Phase Sheared Flows
Dr. Fulgosi (Inst. for Energy Technology, ETHZ)

Formation and Evolution of the Milky Way
Prof. G. Ortwin (Inst. of Astronomy, Uni-Basel)

Structure and Dynamics of Proteins in Solution
Dr. P. Gntert (Inst. fr Molekularbiologie und Biophysik, ETHZ)

Chiral Symmetric Dirac Operator in Lattice QCD
Prof. P. Hasenfratz (Inst. of Theoretical Physics, Uni-Bern)

Ab initio Molecular Dynamics in Electronically Excited States
Prof. J. Hutter, Inst. of Organic Chemistry, Uni-Zurich)

Transition Metal Catalyzed Reactions and CPMD
Prof. J. Hutter, Inst. of Organic Chemistry, Uni-Zrich)

Numerical Simulation of Transitional, Turbulent and Multiphase Flows
Prof. L. Kleiser (Inst. fr Fluiddynamik, ETHZ)

Active Flow Control for Drag Minimization with Machine Learning Algorithms
Prof. P. Koumoutsakos (Inst. for Computational Sciences, ETHZ)

Large Scale Numerical Simulations using Particle Methods
Prof. P. Koumoutsakos (Inst. for Computational Sciences, ETHZ)

Proton Transfer in Microsolvent Clusters: Theory and Dynamics
Prof. S. Leutwyler (Dep. fr Chemie und Biochemie, Uni-Bern)

Compressible Navier Stokes Simulations
Dr. P. Leiland (Inst. de machines hydrauliques et de mchanique des fluides, EPFL)

Performance Analysis of a Simulation Software Package
Dr. P. Leiland (Inst. de machines hydrauliques et de mchanique des fluides, EPFL)

Computational Quantum Chemistry of Large Molecules
Dr. H. P. Lthi (Lab. fr Physikalische Chemie, ETHZ)

Quantum Chemical Investigations of Cyclization Reactions Involving Cationic Spacies
Dr. J. Mareda (Dpartement de Chimie Organique, Uni-Genve)

Computational Solid State Physics
Prof. P.F. Meier (Physik-Institut, Uni-Zrich)

Global Climate Change: Modeling Atmosphere/Ocean Variability
Prof. A. Ohmura (Inst. of Geography, ETHZ)

Disordered Network-forming Materials
Prof. A. Pasquarello (Inst. for Numerical Research in the Physics of Materials (IRRMA), EPFL)

Palladium Phosphinoxazolin Olefin and Allyl Complexes
Prof. D. Plattner (Lab. fuer Organische Chemie, ETHZ)

Structural and Electronic Properties of Solids and Surfaces
Dr. M. Posternak (Inst. de physique applique, EPFL)

Quantum Mechanical Simulation of Molecules and Molecular Clusters
Prof. M. Quack (Lab. fr Physikalische Chemie, ETHZ)

QM/MM - Car Parrinello Study of the Catalytic Mechanism of DNA Repair Enzimes
Prof. U. Rothlisberger (Inst. of Inorganig Chemistry, ETHZ)

Rational Design of Biomimetics Via Mixed Quantum/Classical Car Parrinello Simulations
Prof. U. Rothlisberger (Inst. of Inorganig Chemistry, ETHZ)

Ab initio Hybrid Simulations of Electron Transfer Reaction
Prof. U. Rothlisberger (Inst. of Inorganig Chemistry, ETHZ)

First Principles Characterization and Design of Radiopharmaceuticals
Prof. U. Rothlisberger (Inst. of Inorganig Chemistry, ETHZ)

Modeling Alpine Heavy Precipitation with a High-performance Non-hydrostatic Model
Prof. C. Schr (Institut fr Atmosphrenphysik, ETHZ)

Variability of the Sun and Global Climate
Dr. Schmutz (Inst. fr Schnee- und Lawinenforschung, Davos)

Quantum Chemical Calculations on the Stereoselective Selenenylation Reactions of Alkenes
M. Spichty (Inst. fur Organische Chemie, Uni-Basel)

Modeling of Nanostructured Materials
Dr. H. Van Swygenhoven (Paul Scherrer Institute, Villigen)

New Organic Chemistry with Sulfur Dioxide
Prof. J. A. Sordo (Departamento de Quimca Fsica y Analtica, Uni. de Oviedo) and Prof. P. Vogel (Inst. de Chimie Organique, Uni-Lausanne)

Computational Quantum Chemistry of Increasing Complex Systems
Prof. J. Weber (Dp. de chimie physique, Uni-Genve)

6.3 The Beowulf Cluster "Asgard"

Beowulf clusters are massively parallel supercomputers built from commodity components, standard PCs running Linux and Ethernet networks. They profit from the low cost of the building blocks and offer the best price/performance ratio for many applications that are not limited by network bandwidth or latency. Most applications in physics are perfectly parallelizable and run with optimal speedup on a cluster – no fast network is needed except for access to the file server. These applications include embarrassingly parallel applications such as parameter studies, where a single program has to be run thousands of times with different input parameters. Other methods that are well suited to a cluster are Monte Carlo simulations, where independent samples can be created on different CPUs with minimal communication needs. Since the majority of applications in physics are of these types, the cluster provides an ideal platform, complementary to the traditional supercomputers at ETH.

An increased importance of numerical simulations in all field of physics and the special needs of the physics department for massive amounts of CPU time, but only moderate network demands motivated the procurement of a Beowulf-cluster type machine in 1999. These efforts were initiated by M. Troyer and E. Heeb at the Department of Physics and were later joined by the Department of Mathematics and the Institute of Polymer Science (Prof. H.C. Öttinger).

The first stage, 192 dual-CPU PCs running Linux, connected by a two-stage network built from 100Mbit and Gigabit Ethernet switches was installed on December 22nd, 1999, and production codes were running on the whole cluster from the first day. The acceptance tests were successfully passed in March 2000. Since then the cluster has been fully operational and open to users from all departments of ETH. From the start the cluster was intended to open, 20% of the CPU time reserved for users from outside the two core departments, an in summer 2000 an upgrade with additional 96 machines was installed, funded by Prof. Hans Christian Öttinger at the Institute for Polymers. The Asgard cluster is open to further groups that wish to participate.

This upgrade to a a total of 502 CPUs (including front end machines) made the "Asgard" Beowulf cluster the largest of its kind in Europe, when it was officially inaugurated and presented to the public at a press conference in June 2000. Media coverage included all major Swiss German newspapers, as well as TV reports by Tele 24 and by SFDRS (in "10 vor 10"). Additional public relations efforts included presentations at the Supercomputer 2000 conference in Mannheim, and the HiPer 2000 conference in Barcelona, where the cluster was compared to traditional supercomputers. Other activities related to the Asgard cluster included two "Beowulf days", in December 2000 and June 2001, where users got the opportunity to meet, present their results and exchange experiences.

The users were very satisfied with the performance of the machine, which was to be expected for the majority of CPU-intense but not network-demanding applications. Surprisingly, besides these perfectly parallelizing applications the network bandwidth and latency turned out to be good enough not only for the development and testing of nontrivial parallel applications, but also for

many production runs of problems such as beam dynamics, relativistic stellar plasmas and strongly correlated quantum systems.

As regards the operating mode, the cluster us split into two main queues, one for parallel jobs with up to 256 CPUs, and one for a large number of serial applications. In addition, processes with low memory demands are run as low-priority background jobs, using up the remaining idle time. We can thus achieve near-optimal usage of more than 95% - a very high number compared to traditional supercomputers.

For further details about the hardware, software, operating mode, account applications and user projects we refer to the Asgard web page at http://www.asgard.ethz.ch.

Asgard research projects

Since not all of the projects on Asgard are included in this annual report we list the main user projects here. For details we refer to the description of these projects on the Asgard web page at http://www.asgard.ethz.ch.

Theoretical Physics

- Soliton's Dissipation Through Emission Of Radiation
  by G. Interlandi,W. Aschbacher, J.Fröhlich and M.Troyer
- *Vortex Collisions: Crossing or Recombination?*
  by M.Bou-Diab andG.Blatter
- *Quantum Phase Transitions in the 2D Hardcore Bosonic Hubbard Model*
  by G. Schmid and M.Troyer
- *Quantum critical behavior in antiferromagnets and superconductors*
  by M. Troyer
- *Quantitative modeling of strongly correlated materials*
  by M. Troyer
- *High Temperature Series Expansion for Quantum Lattice Models*
  by M. Körner and M. Troyer
- *N-Patch Renormalization Group Study of the Two-Dimensional t-t' Hubbard Model*
  by C. Honerkamp, M. Salmhofer and T.M. Rice
- *Multiparticle Exchange Processes in the Two-Dimensional Wigner Glass*
  by K. Völker
- *Exact Diagonalization Studies of Strongly Correlated Electron Systems*
  by A. Läuchli, M. Troyer and T.M. Rice
- *Simulation of the vortex texture in a superconductor*
  by F. Mohamed, G. Blatter and M. Troyer
- *Topologically protected quantum bits*
  by D. Ivanov, M. Troyer and G. Blatter

Particle Physics

- *Monte Carlo Simulation of the L3+C Experiment at CERN*
  by Renzo Ramelli and Pierre Le Coultre
- *Monte Carlo Simulations of the AMS Detector*
  by Adrian Biland
- *Backtracing of Cosmic Ray Particles*
  by Adrian Biland
- *Simulation of Csmic Ray Showers*
  by Haitao Liu
- *Magnetic Shielding for Synchrotron Radiation Detector (SRD)*
  by Hans Anderhub
- *Atlas Event Filter Studies*

Astrophysics

- *Kinetic Simulation of Solar Plasmas*
  by Peter Messmer and Arnold O. Benz
- *Dynamics of Free-floating Planets in Stellar Clusters*
  by Kester Smith

Mathematics

- *Parallelization of Low-Communication Processes*
  by Jörg Waldvogel and Peter Leikauf
- *Solving of Boundary Integral Equations*
  by Gregor Schmidlin and C. Schwab
- *Numerical procedures for PDEs using the Feynman-Kac Formula by*
  Wesley P. Petersen and Rolf Jeltsch
- *Multi-dimensional FFT algorithms on Asgard*
  by W. Petersen
- *Accuracy comparison of N-body codes*
  by Luzi Schucan, and M. Troyer
- *Parallel Smoothing for Multigrid via Sparse Approximate Inverses*
  by Oliver Bröker and Marcus J. Grote
- *A new Field Solver for Space Charge dominated Beams*
  by Andreas Adelmann, Stefan Adam, Rolf Jeltsch and Ralph Eichler

Polymer Science
by the group of Hans Christian Öttinger

- *Rheology and Thermodynamics (GENERIC)*
- *New Models in Polymer Kinetic Theory*
- *Dynamic Models Describing the Glass Transition*
- *Crystallization in Polymer Melts under Elongational Flow*
- *Nonequilibrium dynamics computer simulation of polymer fluids*

Computer Science

- *Development and Application of Biologically Inspired Optimization Algorithms*
  by Sibylle Müller and Petros Koumoutsakos
- *Traffic simulations*
  by Kai Nagel and Res Voellmy
- *Macro-economic modeling, computational economics and statistics*
  by E.J. Kontoghiorges and P. Arbenz

6.4 Information Technology Services

The following resources are available:

- Cray SV1 Cluster consisting of
  - 1 Cray SV1-B/16-8 (Athos): 16 Vector CPUs (300 MHz), 8 MB Memory
  - 1 Cray SV1-B/8-4 (Porthos): 8 Vector CPUs (300MHz), 4 GB Memory
  - 320 Gigabyte Disk, shared through Gigaring among the cluster
  - Unicos Operating System

  The clusters major usage is highly vectorized, moderately (up to 8 processors) parallel code in the fields of climate modeling, theoretical physics and astronomy.

  The following compilers, libraries and applications are installed on the cluster:

  ANSI II C: Compiler
  C++: Compiler
  FORTRAN-90: Compiler
  MPGS: graphical library and viewer
  GROMOS: biomolecular simulation
  UniChem 5.0 (Cadpac, DGauss, MNDO): chemistry
  MOPAC, DISCO, ACES2: chemistry
  AMBER 5: chemistry
  Gaussian-94 (for educational purposes only): chemistry
  PAM: finite elements
  CFX-F3D: fluid dynamics
  NAG Mk 19, IMSL 10: numerical libraries
  Maple 4.3: symbolic calculus
  ranq, zufall: random number libraries
  mfft: multitasked fast forier transforms
  egm: graphical library
- Hewlett Packard Superdome (Stardust): 48 PA8600 CPUs (550 MHz), 48 GB Memory, 360 GB Disk, HP/UX Operating System

  It is used for parallel code taking advantage of the shared memory programming model offered by the cc-numa architecture of this system. Many standard applications (finite element modeling, mathematics, simulations, etc.) are in this category.

  The systems major usage is in the fields of thermodynamics, fluiddynamics, virtual production (FEM) and theoretical physics.

  The following software is available on the Superdome:

  HP Fortran: Compiler and associated products
  HP Fortran 90: Compiler and associated products
  HP C/ansi: C Developer's Bundle for HP-UX 11.00
  HP C++: Compiler
  KAI Guide C++: Open MP
  Abaqus 5.8: General-purpose finite element analysis
  ACSL: Advanced continuous simulation language
  Ampl 9.5.13: Modeling language for Mathematical Programming
  ANSYS 5.5: Finite element analysis

AVS: Advanced visual system
CPLEX 65: Linear optimization solver
CFX Tascflow: CFD analysis and design tool
Diana 7.2: Finite element analysis
Gaussian 98: semi empirical and ab initio molecular orbital (MO) calculations.
MARC/MENTAT K7.3: Nonlinear finite element program
Matlab 11.1: Language for technical computing
Molcas 5: Quantum chemistry software
NAG F95: Fortran library
IMSL: Fortran Numerical Libraries
Para Phoenics 32: CFD
Patran 9.0: Finite element (Modeling, Analysis, Results evaluation)
Tecplot 8.0: Tool for visualizing a wide range of technical data
PV-Wave: Signal Processing Toolkit

7
Outlook

This report shows that ETH has become highly active in CSE. Hence, the question should be asked, how things should proceed. There are two major tracks, research and education. The fact that CSE is declared a "Strategische Erfolgsposition (SEP)", an area of strategic importance for the ETH, guarantees that the leaders of the ETH will stimulate strenghtening and broadening of the field of CSE and Computing in the departments of ETH.

Concerning the curriculum, a proposal has been made to modify the existing program so that a student can obtain a Bachelor degree after the first six semesters. The ETH diploma will be equivalent to a Master degree in CSE. The lectures will be given in English and the new program in English will start in the autumn of 2002. It will be advertised world wide so that good students will be attracted from abroad.

Early this year the president of ETH, Prof. Olaf Kübler, created a task force to formulate proposals for the future. In October 2001, this task force produced a report with two key proposals, one concerning research and one concerning education. For the interdisciplinary research an ETH wide Center of Computational Science and Engineering (CCoSE) should be formed. Members are recruited from a variety of departments which have an interest in this field. On the educational side, the picture is less clear because the task force proposes one or two curricula in CSE.

On the positive side, I would like to mention that we see currently large efforts by ETH to hire computationally oriented colleagues in many different areas, such as astrophysics, physics, mathematics, bioinformatics, to mention just a few. On the negative side, we note that in recent years ETH has lagged behind world trends. We can only hope that a major step forward will be made soon.

Overall, we have a very optimistic look in the future and I am already eager to see the next annual report to find out about new exciting research happening at ETH.

Zürich, October 20, 2001
Rolf Jeltsch

8
Publications* in 2000/2001

*only CSE-related articles
in refereed journals

Group of G. Blatter

M. Bou-Diab, H. Nordborg and G. Blatter
Vortex collisions: crossing or recombination?
Phys. Rev. Lett. **86**, 5132 (2001).

L. Ioffe, M.V. Feigel'man, A. Ioselevich, D. Ivanov, M. Troyer and G. Blatter
Topologically protected quantum bits from Josephson junction arrays
Preprint, submitted to Nature

F. Mohamed, Matthias Troyer, Gianni Blatter and I. Luk'yanchuk
Interaction of vortices in superconductors with κ close to $1/\sqrt{2}$
Preprint, submitted to Phys. Rev. B

Group of K. Boulouchos

C. E. Frouzakis, A. Tomboulides, J. Lee, K. Boulouchos,
From diffusion to premixed flames in an H_2/air opposed-jet burner: the role of edge flames, *Combust. Flame*, submitted, (2001).

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Proper Orthogonal Decomposition of Direct Numerical Simulation data: data reduction and observer construction, *Proc. Combust. Inst.*, **28**, pp. 75-81, (2000).

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Numerical Study of Opposed-jet H_2/air Diffusion Flame - Vortex Interactions, *Combust. Sci. Techn.*, **158**, pp. 365-388, (2000).

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Application of Resonant Holographic Interferometry to OH Concentration Measurements in a two-dimensional CO-Flow H2/Air Diffusion Flame and Comparison with Direct Numerical Simulations, *Flow Turb. Combust.*, **64**, p. 183-196, (2000).

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Simulation and Analysis of Laminar Flow Reactors, *Combust. Sci. Techn.*, **159**, pp. 199-211, (2000).

Group of H. C. Davies

Fehlmann, R., C. Quadri und H. C. Davies, 2000. An Alpine rainstorm: Sensitivity to the mesoscale upper-level structure. *Wea. Forecasting,* **15,** 4-28.

Rossa, A. M., H. Wernli und H. C. Davies, 2000. Growth and decay of an extra-tropical cyclone's PV-tower. *Meteorol. Atmos. Phys.*, **73,** 139-156.

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Wernli, H., S. Dirren, M. A. Liniger und M. Zillig, 2001. Dynamical aspects of the life-cycle of the winter storm 'Lothar' (24-26 December 1999). *Quart. J. Roy. Meteor. Soc.*, in press.

Group of W. Fichtner

A. Scholze, A. Schenk, W. Fichtner
Single-Electron Device Simulation
IEEE Transactions on Electron Devices **47** (2000) 1811-1818

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Efficient Monte Carlo Device Modeling
IEEE Transactions on Electron Devices **47** (2000) 1891-1897

J. Krause, N. Strecker, W. Fichtner
Boundary-Sensitive Mesh Generation using an Offsetting Technique
International Journal for Numerical Methods in Engineering (2000) 51–59

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A Multidimensional Laser Simulator for Edge-Emitters Including Quantum Carrier Capture
IEEE Transactions on Electron Devices **47** (2000) 1926-1934

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Review of FDTD Time-Stepping Schemes for the Efficient Simulation of Electric Conductive Media
Microwave and Optical Technology Letters **25** (2000) 16-21

Group of J. Fröhlich

W.H. Aschbacher, J. Fröhlich, G.M. Graf, K. Schnee, and Matthias Troyer
Symmetry Breaking Regime in the Nonlinear Hartree Equation
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D. Seebach, J.V. Schreiber, S. Abele, X. Daura and W.F. van Gunsteren
Structure and Conformation of β-Oligopeptide Derivatives with Simple Proteinogenic Side-Chains: Circular Dichroism and Molecular Dynamics Investigations
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β-Hairpin Stability and Folding: Molecular Dynamics Studies of the First β-hairpin of Tendamistat
J. Mol. Biol. **296** (2000) 255-268

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Computer Simulation of Proton Transfers of Small Acids in Water
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