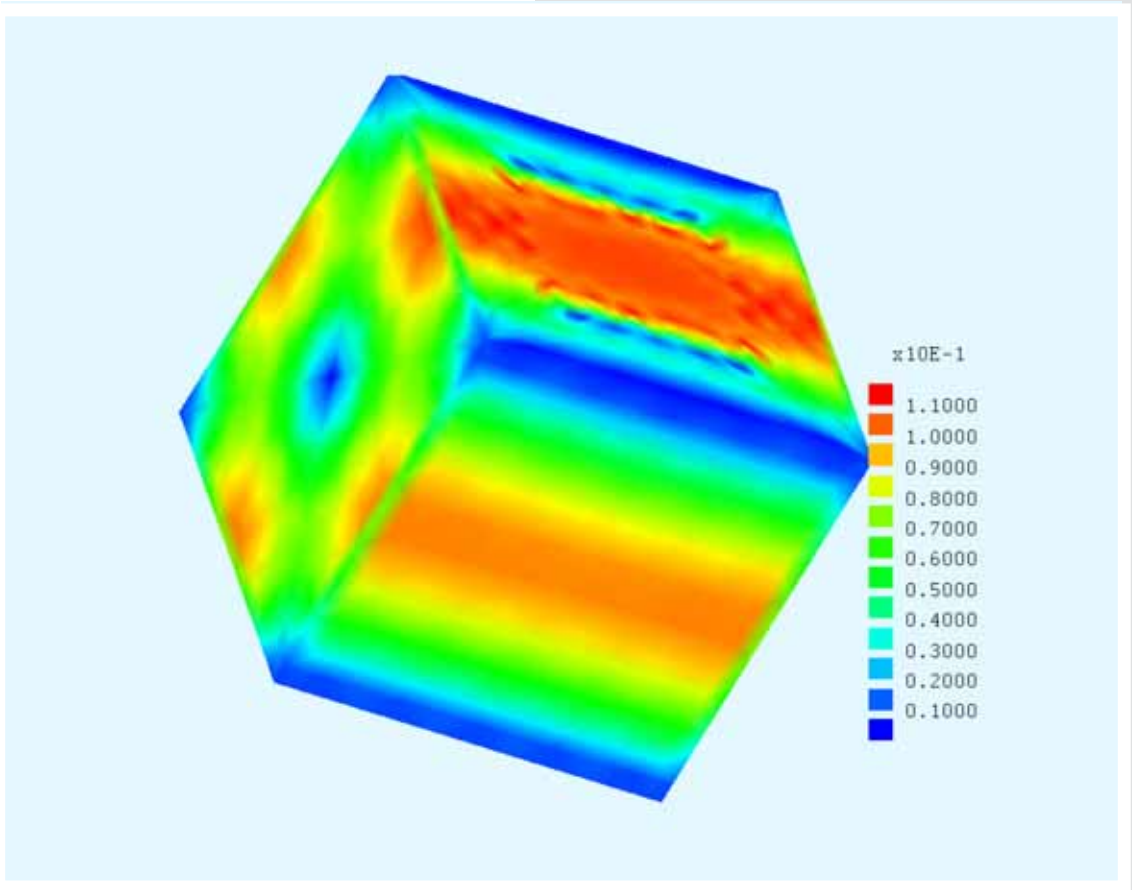
# CSE

Computational Science and Engineering

## Annual Report
## 2003 / 2004




ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

# CSE

Computational Science and Engineering

# Annual Report
# 2003 / 2004

## July 2003 to July 2004

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*Cover:*
Modulus of tangential magnetic field for electromagnetic wave scattering at a partially coated cube
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# Groups that have contributed to this report:

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# 1

# Introduction

This is already the fourth Annual Report of Computational Science and Engineering (CSE) at ETH. Moving with time it is the first one of which no paper copy will be produced. Most people will find it more convenient to have it accessible on the web or browsing through the CD. The success of the previous reports makes it important that it is more accessible than a paper version ever could be. More and more persons are interested in research and education in CSE, students and colleagues, visitors and people form other universities. They all want to know what is going on at ETH in this exciting field. This new edition documents the changes that happened in the last year and gives a glimpse of the developments immediately ahead of us.

Last fall the first students started with the newly established Bachelor program. Contrary to our old diploma program these students entered the curriculum in CSE ("Rechnergestützte Wissenschaften") right after two semesters of studies in one of those programs which are closely related to CSE. With this the program leading to the Bachelor and afterwards to the Master in CSE could be designed in a more optimal way for the needs of our students. In addition, we have created more courses which are directly tailored to students in CSE. For example in the course in numerical methods more weight could be placed on the understanding of algorithms and the use of software rather than on mathematical proofs of theorems. In a year these students will be the first ones to graduate as Bachelors in CSE.

The last group of students of the diploma studies in CSE enrolled last fall. Due to this the overall number of students enrolled in any of our programs almost doubled. The Master program in CSE will be started next fall and hopefully many of the newly graduated Bachelors will enroll.

On the research side we have seen again new professors being hired who use computing as one of their important tools to do science and/or engineering. As the field CSE has grown and broadened, it was in a sense only natural to phase out, as planned, the initial support by the "Strategische Erfolgs-Position", SEP, in Computational Science and Engineering.

Work has started for the organization of ICIAM 2007 which will be held in Zürich. ICIAM stands for International Congress on Industrial and Applied Mathematics and a large portion of the congress will cover CSE.

At this point we thank the Schulleitung for supporting CSE in research and education. We also thank all those at ETH who have contributed to this report.

Zürich, October 22, 2004
Rolf Jeltsch, Studiendelegierter und Mitglied des Ausschusses Rechnergestützte Wissenschaften

# 2

# Education

The new Bachelor Curriculum in CSE has started in October 2003 with 13 students in their second year of studies at ETH Zürich. The students had done their first year's studies in another curriculum at ETH in the following fields: Mathematics 2 students, Computer Science 5, Physics 4, Mechanical Engineering 1, Chemistry 1.
The first year's examinations are counted for 60 ECTS (credit points). In the subsequent two years of the Bachelor studies in CSE the students have to gather 120 ECTS in: mandatory Basic Courses (second year; the basics in Mathematics, Science and Engineering, Computer Science), Core Courses (third year; computational mathematical methods, advanced knowledge in Computer Science), Fields of Specialization (third year; more profound knowledge in one application area), Elective Courses (third year; emphasis on computational aspects), Bachelor Thesis (after third year; application oriented, computational). The overall requirement for getting the degree of a Bachelor of Science ETH in CSE is 180 ECTS in three years of studies.

The Bachelor diploma in CSE will allow students to continue their studies in a Master curriculum, in particular, in the Master Curriculum in CSE at the ETH Zürich which is in preparation and is planned to get started in October 2005. The Master studies will take one and a half years including the five months of the Master thesis and will lead to the degree of a Master of Science ETH in CSE.

The two and a half years Diploma curriculum in CSE existing since October 1997 has started for the last turn in October 2003 with 17 students. They had taken their basic two years studies in the following fields at ETH: Mathematics 5, Computer Science 2, Physics 2, Mechanical Engineering 3, Electrical Engineering 3; and outside ETH in Computer Science at SUPSI Lugano 1, Computational Science at TU Chemnitz 1.

The presentation of the CSE Bachelor/Master curriculum for ETH students of the second semester of May 26, 2004 was attended by around 50 persons. It is hoped that a fair number of them will start with the CSE Bachelor studies this fall.

In the past academic year 8 students have successfully finished their CSE studies and have received a CSE diploma with very good scores. They chose the following fields of specialization: Chemistry, Robotics, Physics of the Atmosphere and Theoretical Physics. In the following list we give the name of the students, the title of the diploma thesis and, in parentheses, the name and the department/institute of the adviser.

*Diploma Theses*

| | |
|---|---|
| A. Burri | Implementation of a nonlinear multiphase fluid flow simulator using a fully upwind Galerkin method within the CSP Multiphysics Toolkit<br>(C. A. Heinrich, Geology / R. Jeltsch, Applied Mathematics) |
| A. Jost | Computational power of event-based recurrent networks<br>(R. J. Douglas, Neuroinformatics) |
| M Köpfli | Global optimization of clusters using evolutionary algorithms<br>(P. Koumoutsakos, Computer Science) |
| S. Müller | Hydrostatic balance and gravity/acoustic modes in nonhydrostatic atmospheric models<br>(C. Schär, Atmospheric and Climate Science) |
| M. Rütti | Random number test suite for the C++ standard<br>(M. Troyer, Theoretical Physics) |
| G. Stark | Implementation of a computational framework for level set representations<br>(M. Troyer, Theoretical Physics) |
| G. Widmer | Auxiliary space methods for edge elements<br>(R. Hiptmair, Applied Mathematics) |
| C. Winkelmann | A discontinuous Galerkin scheme for elastic waves in nearly incompressible materials<br>(R. Hiptmair, Applied Mathematics) |

The total number of CSE students enrolled in the past academic year was 41. Listed below are the term papers written by the CSE students in the past two semesters.

*Term Papers*

| | |
|---|---|
| T. Aka | Numerische Modellreduktion für komplexe Eigenwertprobleme<br>(R. Hiptmair, Applied Mathematics) |
| T. Aka | Berechnung der Persistenz eines chemischen Stoffes<br>(W. Gander, Computer Science) |
| U. Battaglia | Multicast XML messages for distributed mobility simulations<br>(K. Nagel, Computer Science) |
| U. Battaglia | FE-Formulierung der nichthydrostatischen Gleichungen in terrainfolgenden Koordinaten<br>(C. Schär, Atmospheric and Climate Science) |
| L. Blaser | Simulation eines Hummelstaates<br>(Prof. Nagel, Computer Science) |

| | |
|---|---|
| A. Dobler | Spezielle Riemann-Löser für die Gleichungen der idealen Magnetohydrodynamik<br>(R. Jeltsch, Applied Mathematics) |
| M. Guidon | Transient simulation of eddy currents in Ferromagnetics<br>(R. Hiptmair, Applied Mathematics) |
| M. Jörg | Hardware-accelerated normal fairing<br>(M. Gross, Computer Science) |
| T. Kühne | Karmakar's algorithm for linear programming<br>(G. Gonnet, Computer Science) |
| T. Oesch | Quantenchemische Rechnungen zur sauer katalysierten Amidhydrolyse<br>(Dirk Bakowies. Physical Chemistry) |
| I. Oppermann | High speed data streaming for distributed mobility simulations<br>(K. Nagel, Computer Science) |
| I. Oppermann | Image processing and particle tracking for biological applications<br>(P. Koumotsakos, Computer Science) |
| P. Rousselot | Implementierung eines Lagrangeschen Berechnungsverfahrens für die Partikeldynamik in kompressibler Strömung<br>(L. Kleiser, Fluid Dynamics) |
| R. Veprek | On computational FE modelling of indentation experiments on hard coatings<br>(M. Farshad, EMPA Dübendorf) |
| C. Winkelmann | A finite volume nonhydrostatic atmospheric model for the simulation of mountain waves |
| M. Wittberger | 3D simulations of protein bunches in the Injector II Cyclotron<br>(R. Jeltsch, Applied Mathematics) |
| S. Wunderlich | Implementation of a Semi-Lagrangean scheme in the meteorological model Meso-NH<br>(C. Schär, Atmospheric and Climate Science) |

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 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, August 26, 2004
Kaspar Nipp, Mitglied des Ausschusses Rechnergestützte Wissenschaften

*For detailed information on the CSE curricula at ETH Zürich see:*
http://www.cse.ethz.ch

# 3

# 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 WS03/04

| | |
|---|---|
| 6. 11. 03 | J. Bernasconi, ABB-Forschungszentrum, Baden-Dättwil<br>Modellierung und Simulation von Elektrizitäts- und CO2-Märkten |
| 13. 11. 03 | C4 workshop, ETH Hönggerberg<br>Six 20 minutes talks from different chemistry groups,<br>followed by an apéro |
| 20. 11. 03 | H. Nordborg, ABB-Forschungszentrum, Baden-Dättwil<br>Lichtbogensimulationen in realen Schaltergeometrien<br>&&& Apéro vor der Aula (Begrüssung der Neueintretenden) |
| 27. 11. 03 | A.-M. Matache, Seminar für Angewandte Mathematik<br>Wavelet-Galerkin Pricing of Options beyond Black-Scholes |
| 11. 12. 03 | A. Quarteroni, Mathematics and Bernoulli Institute, EPFL<br>1) Modelling and Simulation of the Cardiovascular System<br>2) Numerical Simulation for the America's Cup |
| 18. 12. 03 | S. Merino, Wealth Management Research, UBS AG, Zürich<br>Numerical Techniques for Determining and Allocating<br>Portfolio Credit Risk |
| 22. 1. 04 | H. Blatter, W. Sawyer, Atmospheric and Climate Science (IAC)<br>Numerics in Glacier Modelling |
| 29. 1. 04 | T. Wintergerste, Fluid Technology, Sulzer Innotec, Winterthur<br>Numerische Simulation als Werkzeug im industriellen<br>Entwicklungsprozess - DeNOx-Anlage & Pulverherstellung |

## Case Studies Seminar SS04

| | |
|---|---|
| 15. 4. 04 | A. Candel, Theoretische Physik<br>Simulation of Electron Source for Next-Generation<br>X-ray Free Electron Laser |
| 29. 4. 04 | Thomas Schrefl, TU Wien<br>Simulation of the Write and Read Process in Magnetic Recording |
| 6. 5. 04 | J. Rappaz, Institut d'analyse et de calcul scientifique, EPFL<br>1) Numerical Simulation of the Motion of a Glacier<br>2) Analysis and Computation of Dendritic Growth in Binary Alloys |
| 13. 5. 04 | A. de Vries, Physikalische Chemie<br>Molecular Models of the Structure and Dynamics of<br>Phospholipid Aggregates in Water |
| 3. 6. 04 | T. Bosse, Fluiddynamik<br>Numerische Simulation von partikelbeladenen Strömungen |
| 10. 6. 04 | S. Geiger, Isotopengeologie<br>Realistische Simulationen von Fliessprozessen<br>in den Geowissenschaften |
| 17. 6. 04 | M. Rotach, Meteo Schweiz<br>Methoden der Luftschadstoffmodellierung |

# 4

# Computational Highlight

# Coupled Galerkin Boundary Element Methods in Electromagnetic Scattering

Z. Andjelic* B.Cranganu-Cretu* R. Hiptmair †

August 11, 2004

**Abstract**

Boundary integral equation methods play a key role in computational electromagnetics. Here we discuss a special variant designed for the simulation of electromagnetic scattering at a non-smooth partly PEC coated dielectric object.

## 1 Introduction

This report arose from a collaboration between engineers of ABB Corporate Research in Baden-Dättwil and mathematicians from the Seminar for Applied Mathematics (SAM) of ETH Zürich. It is a summary of [9]. It demonstrates that it takes advanced tools from numerical mathematics in order to meet the need of industrial simulation. Often these advanced methods are not yet available as parts of commercial simulation software so that they have to be adapted and implemented by specialists in industrial research departments.

## 2 The Problem Setting

A time-harmonic plane electromagnetic wave, described by the complex amplitudes of the accompanying electric and magnetic fields $\mathbf{e}_i, \mathbf{h}_i$, impinges on a linear dielectric object that is partly coated by a thin metallic layer, which acts as a perfect mirror for electromagnetic waves ("PEC boundary"): imagine a swimming pool with thin aluminum walls and a radar beam aimed at it.

A more serious application are issues of electromagnetic interference concerning measuring devices inside transformers filled with some fluid. There, one is interested in the strength of the electromagnetic fields at certain points in the fluid domain, which may correspond to the positions of sensors.

The propagation of electromagnetic inside the object (domain $\Omega^-$) and in the surrounding air region (domain $\Omega^+$) is governed by the (scaled) electric wave equation

$$\mathbf{curl}\,\mathbf{curl}\,\mathbf{e} - \kappa_\pm^2 \mathbf{e} = 0 \quad \text{in } \Omega^+/\Omega^- \text{ , respectively.} \tag{1}$$

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Here, $\kappa_- = \omega\sqrt{\epsilon_s\mu_s}$, $\kappa_+ = \omega\sqrt{\epsilon_0\mu_0}$ are the so-called wave numbers, depending on the dielectric constants $\epsilon_s, \epsilon_0$ and magnetic permeabilities $\mu_s, \mu_0$ prevailing in $\Omega^-$ and $\Omega^+$, respectively. Moreover, $\omega > 0$ denotes the angular frequency of the waves.

Please note, that in (1) $\mathbf{e}$ will stand for the total electric field inside $\Omega^-$, while in $\Omega^+$ it designates the scattered field, that is, the total field minus the incident field $\mathbf{e}_i$.

The boundary $\Gamma$ of $\Omega^-$ can be decomposed into a PEC part $\Gamma_0$ and a coupling boundary $\Gamma_a$ (aperture). On $\Gamma_0$ homogeneous Dirichlet boundary conditions are imposed on the total electric field

$$\gamma_{\mathbf{t}}^- \mathbf{e} = 0 \quad \text{and} \quad \gamma_{\mathbf{t}}^+ \mathbf{e} = 0 \,, \tag{2}$$

whereas we set *transmission conditions* for tangential components on $\Gamma_a$:

$$\gamma_{\mathbf{t}}^+ \mathbf{e} - \gamma_{\mathbf{t}}^- \mathbf{e} = -\gamma_{\mathbf{t}}^+ \mathbf{e}_i \quad , \quad \frac{\kappa_+}{\mu_0}\gamma_N^+ \mathbf{e} - \frac{\kappa_-}{\mu_s}\gamma_N^- \mathbf{e} = -\gamma_{\mathbf{t}}^+ \mathbf{h}_i \quad \text{on } \Gamma_a \,. \tag{3}$$

Here, $\gamma_{\mathbf{t}}$ stands for the rotated tangential component of a field onto a boundary, and $\gamma_N \mathbf{u} := \mathbf{curl}\, \mathbf{u} \times \mathbf{n}$ , with $\mathbf{n}$ denoting the unit normal on the boundary. Both, $\gamma_{\mathbf{t}}$ and $\gamma_N$ are the *trace operators* belonging to the electric wave equation (1).

The problem (1)-(3) is posed on all of $\mathbb{R}^3$ and we have to enforce the *Silver-Müller radiation conditions* for the scattered field at $\infty$

$$\lim_{|\mathbf{x}|\to\infty} \mathbf{curl}\, \mathbf{e} \times \mathbf{x} - i\omega\mu_0 |\mathbf{x}| \mathbf{e} = 0 \quad \text{uniformly} \,. \tag{4}$$

This ensures that the scattered wave carries energy away from the scatterer.

# 3 Boundary Integral Equations

In principle, (1) can be discretized by means of finite elements, see [12, Sect. 5]. However, this entails an artificial truncation of the unbounded air region $\Omega^+$, the definition of an appropriate absorbing boundary condition on the artificial boundary [11], and the meshing of $\Omega^-$ and the remaining part of $\Omega^+$. Moreover, the meshes need to be sufficiently fine to suppress numerical dispersion [2, 1].

Let us assume that the material coefficients $\epsilon, \mu$ and $\epsilon_0, \mu_0$ are constant in $\Omega^-$ and $\Omega^+$, respectively. Then $\mathbf{e}$ enjoys a simple *boundary integral representation* through its Dirichlet and Neumann boundary values [7, Sect. 4]

$$\mathbf{e}(\mathbf{x}) = -\mathbf{\Psi}_{DL}^{\kappa}([\gamma_{\mathbf{t}}\mathbf{e}]_\Gamma)(\mathbf{x}) - \mathbf{\Psi}_{SL}^{\kappa}([\gamma_N \mathbf{e}]_\Gamma) \,, \quad \mathbf{x} \in \Omega^- \cup \Omega^+ \,, \tag{5}$$

where $[\cdot]_\Gamma$ is the jump of a trace across $\Gamma$, and

$$\mathbf{\Psi}_{SL}^{\kappa}(\boldsymbol{\mu})(\mathbf{x}) := \int_\Gamma \kappa \frac{e^{i\kappa|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}\, \boldsymbol{\mu}(\mathbf{y}) + \frac{1}{\kappa}\, \mathbf{grad}_{\mathbf{x}} \left\{ \frac{e^{i\kappa|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|} \right\} (\mathrm{div}_\Gamma \boldsymbol{\mu})(\mathbf{y})\, \mathrm{d}S(\mathbf{y}) \,,$$

$$\mathbf{\Psi}_{DL}^{\kappa}(\boldsymbol{\mu})(\mathbf{x}) := \mathbf{curl}_{\mathbf{x}} \int_\Gamma \frac{e^{i\kappa|\mathbf{x}-\mathbf{y}|}}{4\pi|\mathbf{x}-\mathbf{y}|}\, \boldsymbol{\mu}(\mathbf{y})\, \mathrm{d}S(\mathbf{y}) \,,$$

are the so-called single and double layer potentials for the vector wave equation (1).

From (5) we obtain boundary integral equations in a canonical fashion: the trace operators $\gamma_{\mathbf{t}}^{\pm}$ and $\gamma_N^{\pm}$ are applied to (5) and, introducing the *boundary integral operators*

$$\mathbf{S}_\kappa := \{\gamma_{\mathbf{t}}\mathbf{\Psi}_{SL}^\kappa\}_\Gamma = \{\gamma_N\mathbf{\Psi}_{DL}^\kappa\}_\Gamma \quad , \quad \mathbf{C}_\kappa := \{\gamma_{\mathbf{t}}\mathbf{\Psi}_{DL}^\kappa\}_\Gamma = \{\gamma_N\mathbf{\Psi}_{SL}^\kappa\}_\Gamma \ ,$$

(where $\{\cdot\}_\Gamma$ is the average $\{\gamma\}_\Gamma := \frac{1}{2}(\gamma^+ - \gamma^-)$ for some trace $\gamma$ onto $\Gamma$) we arrive at the *boundary integral equations*

$$\gamma_{\mathbf{t}}^-\mathbf{u} = \tfrac{1}{2}\gamma_{\mathbf{t}}^-\mathbf{u} + \mathbf{C}_\kappa(\gamma_{\mathbf{t}}^-\mathbf{u}) + \mathbf{S}_\kappa(\gamma_N^-\mathbf{u}) \, , \qquad \gamma_{\mathbf{t}}^+\mathbf{u} = \tfrac{1}{2}\gamma_{\mathbf{t}}^+\mathbf{u} - \mathbf{C}_\kappa(\gamma_{\mathbf{t}}^+\mathbf{u}) - \mathbf{S}_\kappa(\gamma_N^+\mathbf{u}) \ , \quad (6)$$

$$\gamma_N^-\mathbf{u} = \mathbf{S}_\kappa(\gamma_{\mathbf{t}}^-\mathbf{u}) + \tfrac{1}{2}\gamma_N^-\mathbf{u} + \mathbf{C}_\kappa(\gamma_N^-\mathbf{u}), \qquad \gamma_N^+\mathbf{u} = -\mathbf{S}_\kappa(\gamma_{\mathbf{t}}^+\mathbf{u}) + \tfrac{1}{2}\gamma_N^+\mathbf{u} - \mathbf{C}_\kappa(\gamma_N^+\mathbf{u}). \quad (7)$$

They provide a means to determine unknown traces on $\Gamma$ without ever solving a problem in the volume. Only the two-dimensional surface $\Gamma$ has to be meshed for the sake of discretization. Moreover, we no longer need to worry about the unbounded domain $\Omega^+$. These attractive features account for the huge popularity of numerical methods based on boundary integral equations in computational electromagnetism.

We must not gloss over limitations and drawbacks. Firstly, we have to deal with non-local integral operators, which require a careful discretization. The non-local character means that we will end up with fully populated matrices that require much more storage than their sparse finite element counterparts, though their size may be significantly smaller. It takes elaborate matrix compression techniques to handle this, see Sect. 7.

Secondly, the boundary integral approach is restricted to homogeneous and linear media occupying $\Omega^-$ and $\Omega^+$. If, for instance, $\epsilon$ displays spatial variation inside $\Omega^-$, an analogue of (5) is no longer available. In this case, a classical spatial discretization is the only option remaining. Fortunately, coupling with a boundary integral method for $\Omega^+$ is possible [13].

# 4 Coupled Problem

Next, the boundary conditions (2) and transmission conditions (3) have to be combined with the boundary integral equations (6)-(7). This is fairly technical. To begin with, we introduce the scaled traces

$$(\boldsymbol{\zeta}^+, \boldsymbol{\lambda}^+) = (\gamma_{\mathbf{t}}^+\mathbf{e}, \tfrac{\kappa_+}{\mu_0}\gamma_N^+\mathbf{e}) \quad , \quad (\boldsymbol{\zeta}^-, \boldsymbol{\lambda}^-) = (\gamma_{\mathbf{t}}^-\mathbf{e}, \tfrac{\kappa_-}{\mu_s}\gamma_N^-\mathbf{e}) \ .$$

With these notations we have $\boldsymbol{\zeta}^- = 0$, $\boldsymbol{\zeta}^+ = -\gamma_{\mathbf{t}}^+\mathbf{e}_i$ on $\Gamma_0$ and the transmission conditions on $\Gamma_a$ read

$$\boldsymbol{\zeta}^- = \boldsymbol{\zeta}^+ + \gamma_{\mathbf{t}}^+\mathbf{e}_i \quad , \quad \boldsymbol{\lambda}^- = \boldsymbol{\lambda}^+ + \gamma_{\mathbf{t}}^+\mathbf{h}_i \ . \quad (8)$$

Recall that $\mathbf{e}$ is the scattered field in $\Omega^+$ and the total field in $\Omega^-$! From (6)-(7) we conclude

$$\begin{pmatrix} -\frac{1}{2}\,\mathrm{Id} + \mathbf{C}_{\kappa_-} & \frac{\mu_s}{\kappa_-}\mathbf{S}_{\kappa_-} \\ \frac{\kappa_-}{\mu_s}\mathbf{S}_{\kappa_-} & -\frac{1}{2}\,\mathrm{Id} + \mathbf{C}_{\kappa_-} \end{pmatrix} \begin{pmatrix} \boldsymbol{\zeta}^- \\ \boldsymbol{\lambda}^- \end{pmatrix} = 0 \ , \quad (9)$$

$$\begin{pmatrix} -\frac{1}{2}\,\mathrm{Id} - \mathbf{C}_{\kappa_+} & -\frac{\mu_0}{\kappa_+}\mathbf{S}_{\kappa_+} \\ -\frac{\kappa_+}{\mu_0}\mathbf{S}_{\kappa_+} & -\frac{1}{2}\,\mathrm{Id} - \mathbf{C}_{\kappa_+} \end{pmatrix} \begin{pmatrix} \boldsymbol{\zeta}^+ \\ \boldsymbol{\lambda}^+ \end{pmatrix} = 0 \ . \quad (10)$$

A few formal manipulations then lead to the final linear equations

$$\begin{pmatrix} \frac{\kappa_-}{\mu_s}\mathbf{S}_{\kappa_-} + \frac{\kappa_+}{\mu_0}\mathbf{S}_{\kappa_+} & \frac{1}{2}\,\mathrm{Id} + \mathbf{C}_{\kappa_-} & \frac{1}{2}\,\mathrm{Id} - \mathbf{C}_{\kappa_+} \\ -\frac{1}{2}\,\mathrm{Id} + \mathbf{C}_{\kappa_-} & \frac{\mu_s}{\kappa_-}\mathbf{S}_{\kappa_-} & 0 \\ \frac{1}{2}\,\mathrm{Id} + \mathbf{C}_{\kappa_+} & 0 & \frac{\mu_0}{\kappa_+}\mathbf{S}_{\kappa_+} \end{pmatrix} \begin{pmatrix} \boldsymbol{\zeta} \\ \boldsymbol{\lambda}^- \\ \boldsymbol{\lambda}^+ \end{pmatrix} = \begin{pmatrix} \gamma_{\mathbf{t}}^+ \mathbf{h}_i + \frac{\kappa_+}{\mu_0}\mathbf{S}_{\kappa_+}(\gamma_{\mathbf{t}}^+ \mathbf{e}_i) \\ 0 \\ (\frac{1}{2}\,\mathrm{Id} + \mathbf{C}_{\kappa_+})(\gamma_{\mathbf{t}}^+ \mathbf{e}_i) \end{pmatrix} \tag{11}$$

The next step is to derive a variational formulation. As is typical for linear problems, this will be posed on a suitable Hilbert space of functions, more precisely, a Sobolev space matching tangential traces $\gamma_{\mathbf{t}}$ and $\gamma_N$ for the vector wave equation, see [7, Sect. 2] for details. Crudely speaking, it will be a space $\mathcal{X}$ of tangential vectorfields on $\Gamma$ that have a meaningful surface divergence.

We note that, thanks to (2), the unknown $\boldsymbol{\zeta}$ is supported on $\Gamma_a$, whereas $\boldsymbol{\lambda}^-$ and $\boldsymbol{\lambda}^+$ live on all of $\Gamma$. Correspondingly, the first equation of (11) holds on $\Gamma_a$ and the others are posed on $\Gamma$. These considerations provide a clue on how to convert (11) into weak form: the first equation has to be tested against tangential vectorfields supported on $\Gamma_a$, whereas for equations #2 and #3 general tangential vectorfields on $\Gamma$ are admitted as test functions.

# 5 Galerkin Discretization

The gist of the Galerkin boundary element approach is to replace the function space $\mathcal{X}$ by a finite dimensional subspace that possesses locally supported basis functions and plug that into the variational equation.

We depart from a surface triangulation composed of flat triangles. This is sufficient, because we aim at a low order scheme, anyway. Piecewise polynomial boundary element spaces for $\mathrm{div}_\Gamma$-compliant tangential vectorfields are available in the form of so-called Raviart-Thomas surface elements [15]. The local shape functions are depicted in Fig. 1.

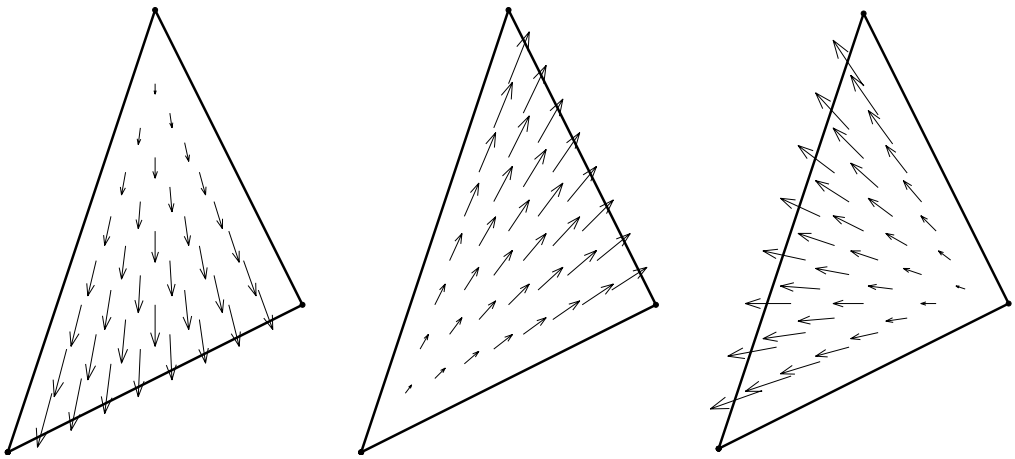

Figure 1: Local shape functions of boundary element space.

The boundary element functions are uniquely characterized by prescribing their normal fluxes through edges. It is obvious from Fig. 1 that the resulting piecewise linear tangential vectorfields on the surface triangulation will feature “normal continuity”, a

necessity, if $\mathrm{div}_\Gamma$ is to be well defined. Also, from a physical point of view, this requirement makes sense, because the unknowns in (11) can be read as (conservative) "surface currents".

The resulting scheme will be first order convergent as the meshwidth of the boundary triangulation tends to zero.

# 6 Computations

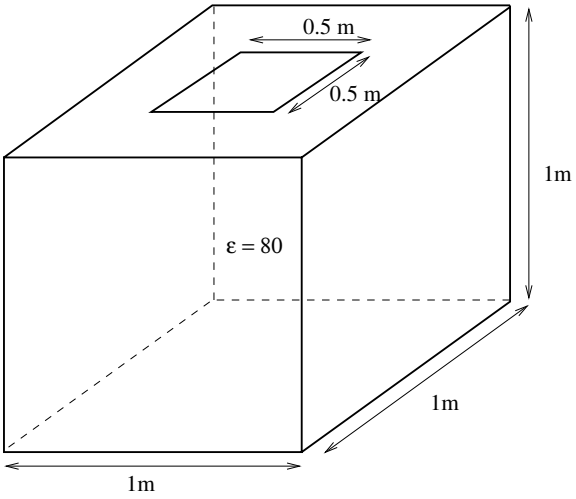


Figure 2: Sketch of the geometry for the metallic container filled with sea water.

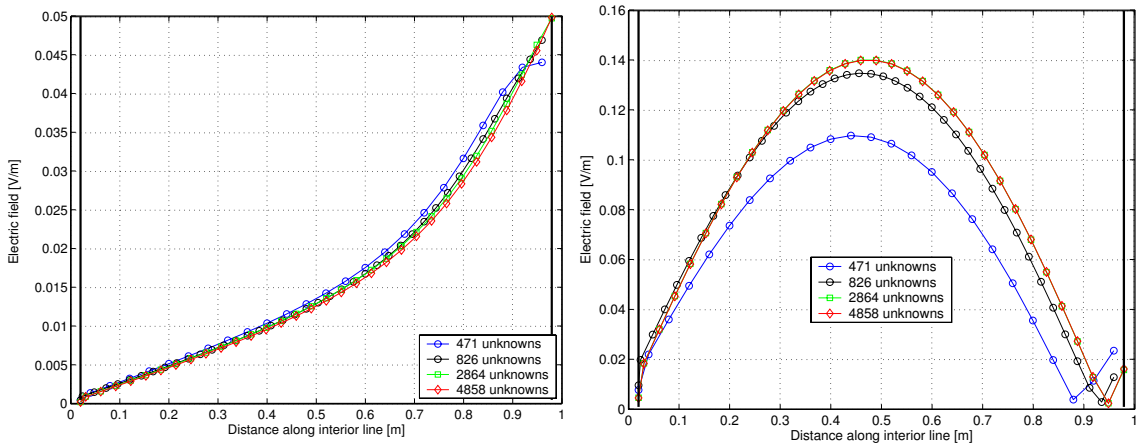


Figure 3: Influence of mesh refinement on accuracy of solution for a metallic container filled with sea water. Left: wave number $\kappa = 3\mathrm{m}^{-1}$, right: wave number $\kappa = 4.5\mathrm{m}^{-1}$

The interaction of a plane wave propagating in positive $\vec{e}_z$-direction with a metallic container filled with sea water, that is $\epsilon_s = 80\epsilon_0$, was computed. There is an opening on the top, see Fig. 2.

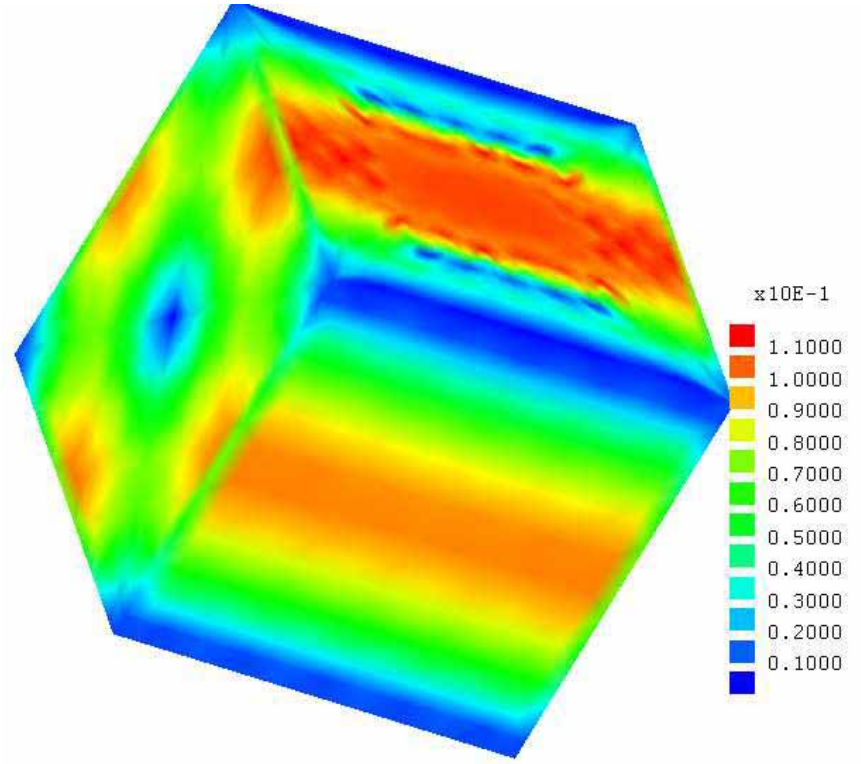


Figure 4: Modulus of inner tangential magnetic field [A/m]. Wave number $\kappa = 4.5\text{m}^{-1}$.

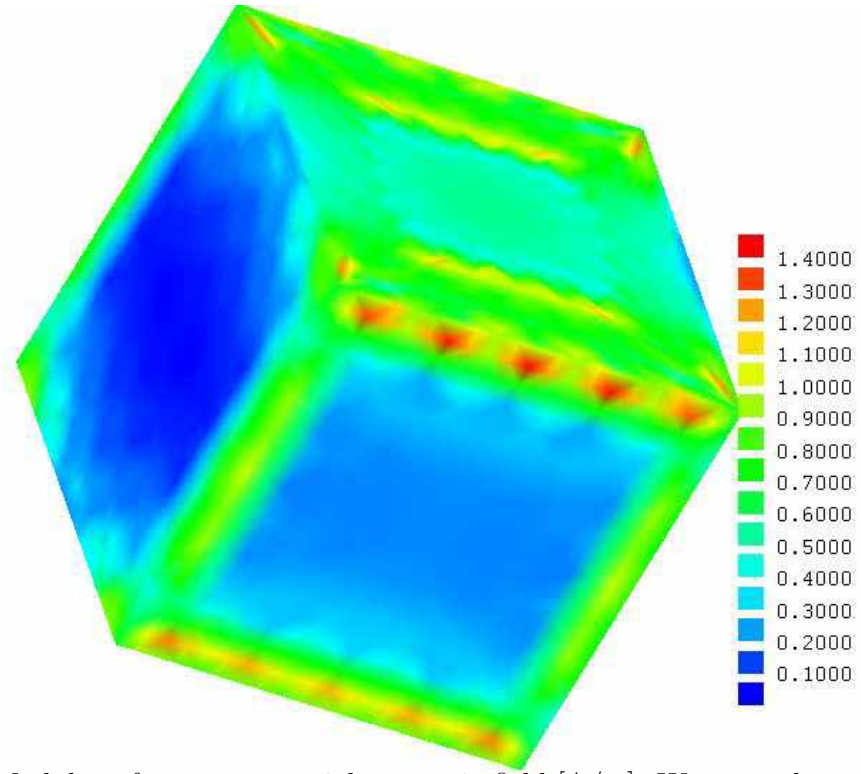


Figure 5: Modulus of outer tangential magnetic field [A/m]. Wave number $\kappa = 4.5\text{m}^{-1}$.

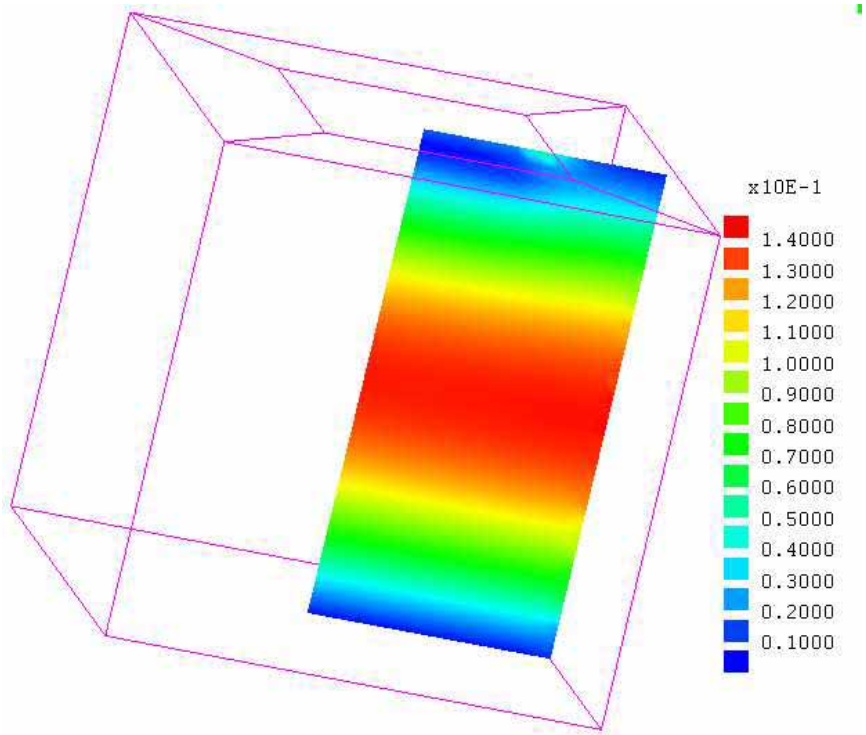


Figure 6: Modulus of transmitted electric field [V/m]. Wave number $\kappa = 4.5\text{m}^{-1}$.

A convergence study on four meshes ranging from very coarse (471 unknowns) to fine (4858 unknowns) is reported in Fig. 3 ($\kappa = 1\text{m}^{-1}$). Obviously, away from any resonance frequencies, the solution on the coarse meshes is satisfactory already, whereas on a resonance frequency fine meshes yield significantly better results.

Plots of the electromagnetic field on the surface of the cube are presented in Figs. 4-5. Field singularities at edges are conspicuous. A section of the transmitted field is shown in Fig. 6 for a wave number $\kappa = 4.5\text{m}^{-1}$.

For all the computations the dense matrices arising from the Galerkin discretization were computed approximately, using elaborate quadrature rules, see [18, Ch. 5]. The resulting linear system of equations were solved iteratively by means of the GMRES Krylov subspace algorithms [17].

# 7 Outlook

The reported computations are still preliminary, because the use of dense matrices will become unacceptably expensive when more complicated geometries are encountered. Then it will become necessary to use matrix compression by means of fast summation methods. These methods are known under the name of panel clustering [18, Ch. 7], hierarchical matrices [5], adaptive cross approximation [4] or multipole [16, 3].

Another challenge is the case of large wavenumbers $\kappa$, if the scatterer has normalized size 1. Then the surface mesh has to become vary fine just to resolve the spatial oscillations of the field intensities. A remedy currently under investigation is the use of modulation approaches [10, 6, 8, 14].

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# 5

# CSE Research Projects

**Title:** Three-dimensional numerical simulations of cellular jet diffusion flames

**Researchers:** Christos E. Frouzakis
Konstantinos Boulouchos

**Institute/ Group:** Aerothermochemistry and Combustion Systems Laboratory

**Description:**

Recent experimental investigations have demonstrated that the appearance of particular cellular states in circular non-premixed jet flames depends significantly on a number of parameters, including the initial mixture strength, reactant Lewis numbers, and proximity to the extinction limit (Damköhler number). For $CO_2$-diluted $H_2/O_2$ jet diffusion flames, these studies have shown that a variety of different cellular patterns or states can form. For given fuel and oxidizer compositions, several preferred states were found to co-exist, and the particular state realized was determined by the initial conditions. In order to elucidate the dynamics of cellular instabilities, circular non-premixed jet flames are modeled with a combination of three-dimensional numerical simulation and linear stability analysis (LSA). In both formulations, chemistry is described by a single-step, finite-rate reaction, and different reactant Lewis numbers and molecular weights are specified. The three-dimensional numerical simulations show that different cellular flames can be obtained close to extinction and that different states co-exist for the same parameter values. Similar to the experiments, the behavior of the cell structures is sensitive to (numerical) noise. During the transient blow-off process, the flame undergoes transitions to structures with different numbers of cells, while the flame edge close to the nozzle oscillates in the streamwise direction. For conditions similar to the experiments discussed, the LSA results reveal various cellular instabilities, typically with azimuthal wavenumber $m = 1 - 6$. Consistent with previous theoretical work, the propensity for the cellular instabilities is shown to increase with decreasing reactant Lewis number and Damköhler number.

**References:**

C.E. Frouzakis, A.G. Tomboulides, P.F. Fischer, P. Papas, R.M. Rais, P.A. Monkewitz, K. Boulouchos, Three-dimensional numerical simulations of cellular jet diffusion flames, *Proc. Combust. Inst.*, **30**, (in press)

**Title:** Computational Solid State Electronics

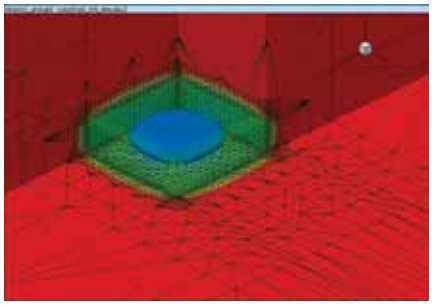
**Researchers:** Wolfgang Fichtner
Andreas Schenk
Bernhard Schmithüsen
Eduardo Alonso
Dölf Aemmer

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

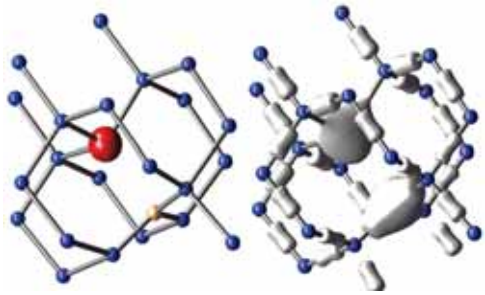
**Description:**

For the development of novel micro- and nano-electronic processes and devices, 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.

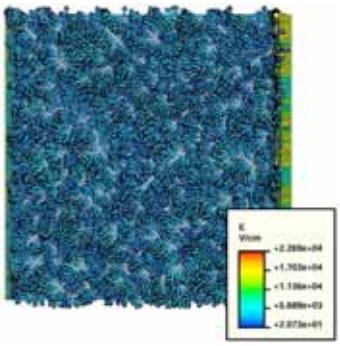
We are performing research in a variety of fields in the computational solid state electronics domain. Current projects include the development and utilization of new simulations tools for molecular dynamics studies in material diffusion, novel devices such as single-electron transistors, and quantum devices. 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 including parallelization on shared and distributed memory architectures. These simulations were carried out on compute-servers of our laboratory and we also use the IBM SP4 system at CSCS Manno in a *Large User Project*. The following pictures illustrate some of our activities:



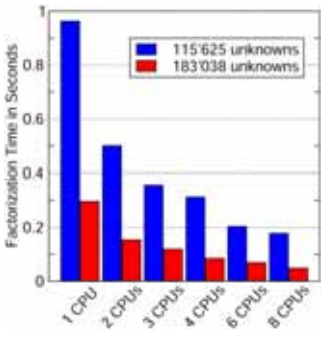
Quantum mechanical charge density: coupled Kohn-Sham/drift-diffusion simulation.



Ab initio study of co-doping in silicon: simulation with the density functional code VASP.



Noise in semiconductor devices: electrical field computed by a transient Monte-Carlo simulation.




Eigenvalue calculation in semiconductor devices: speed-up of the LU-factorization.

T. Höhr, A. Schenk, A. Wettstein, W. Fichtner
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IEICE Transactions on Electronics, vol. E86-C, no. 3, pp. 379-384, 2003.

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IEICE Transactions Electron, vol. E86-B, no 2, 2003, pp. 1060-1957, Oct. 2003.

Ch. Müller, W. Fichtner
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Physical Review B, 70(16), 2004.

D.C. Müller, E. Alonso, W. Fichtner
Arsenic Deactivation in Si: Electronic Structure and Charge States of Vacancy-Impurity Clusters
Physical Review B, vol. 68, no. 4, pp. 045208-1–045208-8, 2003.

A. Schenk, B. Schmithüsen, A. Wettstein, A. Erlebach, S. Brugger, F. M. Bufler, T. Feudel, W. Fichtner
Simulation of RF Noise in MOSFETs Using Different Transport Models
IEICE Trans. Electron, vol. E86-C, no. 3, pp. 481-489, Mar., 2003.

**Title:** SNF SCOPES project: Establishing Computational Science and Engineering in Bulgaria and Macedonia

**Researchers:** Walter Gander, Peter Arbenz[⋆]
Stephan Dodunekov, Svetoslav Markov[†]
Ivan Mirchev[‡]
S. Kapralov[§]
Smile Markovski[◦]
Tomislav Zlatanovski[∞]

**Institute/ Group:** [⋆]Institute of Computational Science
[†]Bulgarian Academy of Science, Maths. and Informatics
[‡]South-West University Blagoevgrad, Dept. Informatics
[§]Technical University Gabrovo, Dept. of Mathematics
[◦]University Saints Cyril and Methodius (UKIM) Skopje, Institute of Informatics
[∞]UKIM Skopje, Faculty of Mechanical Engineering

**Description:**

The initial hope of the project was to introduce CSE curricula at Bulgarian universities along the lines of the CSE courses given at ETH. We however found that that the ETH curriculum cannot be adopted right-away in Bulgaria or Macedonia. So it was necessary to make *local* propositions. It was suggested to try to involve just a few (two or three) departments and develop courses that teach how to execute computationally intensive tasks in the respective areas. Several of the involved institutes have already established some connections in this direction. Such a procedure will be potentially more successful than trying to establish a completely new CSE curriculum. With the Bulgarian Academy of Sciences (BAS) as the leading institution, several master programs with emphasis in CSE could/will be established:

- A master program in "Bio- and medical informatics" at University of Sofia.
- A program "Scientific computing" at the University of Sofia.
- A program "Biomathematics, Ecology and Scientific computing" at the South-West University of Blagoevgrad.
- A program "Computational Mathematics"at the University of Veliko Turnovo.

The partners at the Bulgarian universities in Blagoevgrad and in Gabrovo took great effort in modernizing old courses or in introducing new courses in CS&E that make use of mathematical software, mainly MATLAB and Mathematica.

**References:**

http://www.math.bas.bg/~bio/CSE/

**Title:** Jacobi–Davidson algorithms for the complex symmetric eigenvalue problem

**Researchers:** Oscar Chinellato
Peter Arbenz

**Institute/ Group:** Institute of Computational Science

**Description:**

The development and optimization of modern optoelectronic semiconductor lasers, such as vertically-cavity surface-emitting lasers (VCSELs) require the solution of the three-dimensional homogeneous Maxwell equations describing the optical field. Their numerical discretization by finite element methods (of Nédélec type) lead to large sparse generalized complex-symmetric matrix eigenvalue problems.

The stable and accurate computation of these matrices is investigated. Variants of the Jacobi–Davidson method are derived and implemented that can exploit their complex-symmetric structure. The correction equations are solved by conjugate-gradient-type algorithms preconditioned by a combination of hierarchical basis and domain decomposition preconditioners.

**References:**

O. Chinellato, P. Arbenz, M. Streiff and A. Witzig: *Computation of Optical Modes Inside Axisymmetric Open Cavity Resonators*. June 2003. Accepted for publication in "Future Generation Computer Systems".

P. Arbenz and M. Hochstenbach: *Jacobi–Davidson Method for Solving Complex-Symmetric Eigenvalue Problems*. SIAM J. Sci. Comput. 25 (5): 1655-1673 (2004).

O. Chinellato and W. Gautschi: *Improved and Stabilized Modification Algorithms for Orthogonal Polynomials*. Technical Report, Institute of Computational Science, ETH Zürich, October 2004.

**Title:** CSE-SEP project TH-1/02-4: Large Scale Eigenvalue Problems in Opto-Electronic Semiconductor Lasers and Accelerator Cavities

**Researchers:** Peter Arbenz[⋆]
Wolfgang Fichtner[†]
Hansruedi Fitze[‡]
Olaf Schenk[§]

**Institute/ Group:** [⋆]Institute of Computational Science
[†]Integrated Systems Laboratory
[‡]Paul Scherrer Institute
[§]Department of Informatics, University of Basel

**Description:**

For the development and optimization of both modern and future optoelectronic semiconductor lasers, such as vertically-cavity surface-emitting lasers (VCSELs), and of particle accelerator cavities, computer aided design became an indispensible tool building a tremendous challenge for researchers in physics, computational science, and engineering. Though both problems differ in their technical background and their dimensions by several orders of magnitude (a few micrometers versus a few meters) they both require the solution of the three- dimensional homogeneous Maxwell equations describing the optical and electromagnetic field, respectively. Their numerical discretization by finite element methods lead to large sparse generalized eigenvalue problems which are hard to solve on contemporary computer architectures with respect to memory constraints and simulation time. In laser simulation these eigenvalue problems describe only a part of the physical description, i.e. they are naturally imbedded into a much more complex nonlinearly coupled optoelectronic model.

The aim of this project is the extension of an existing Maxwell equation eigensolver to very lare scale problems and its integration into an semiconductor laser simulator bringing research and development of computational science and engineering together.

**References:**

P. Arbenz, M. Bečka, R. Geus, and U. Hetmaniuk: *Towards a Parallel Eigensolver for Electromagnetic Fields in Cavities.* Proceedings of the PARA'04 Workshop on the State-of-the-Art in Scientific Computing. Lyngby, DK, June 20-23, 2004. (Springer LNCS)

O. Chinellato, P. Arbenz, M. Streiff and A. Witzig: *Computation of Optical Modes Inside Axisymmetric Open Cavity Resonators.* Technical Report 402, Institute of Computational Science, ETH Zürich, June 2003. Accepted for publication in Future Generation Computer Systems.

P. Arbenz and R. Geus: *Multilevel preconditioners for solving eigenvalue problems occuring in the design of resonant cavities*. April 2003. Accepted for publication in "Applied Numerical Mathematics".

R. Geus and P. Arbenz: *PySparse and PyFemax: A Python framework for large scale sparse linear algebra*. Contributed paper at PyCon03, Washington DC, USA, 26-28 March, 2003. `http://www.python.org/pycon/papers/pysparse.html`

**Title:** Novel smoothing techniques and robust QC-cycles.

**Researchers:** Oliver Bröker*

**Institute/ Group:** *Institute of Scientific Computing

**Description:**

Approximate Inverses using Frobenius–norm minimization have been shown to be effective for a braod range of scalar problems that can be treated by algebraic multigrid (see references). The convergence of standard multigrid for problems with discontinuous coefficients or complicated flow patterns can be improved by replacing the ubiquitous Gauss–Seidel iteration with approximate inverse smoothing.

Smoothing with approximate inverses has one obvious drawback: the additional memory and setup–cost involved for computing the inverse. In our new investigations, we improve on this drawbakc by explictly computing the inverse for problems with regula grids and constant coefficients. We improve the perfomence of explicit approximate inverse smoothing by optimizing the cache–efficiency.

Indefinite problems pose an additinal hurdle for multigrid schemes associated with the coarse grid correction. To overcome this problem we do a GMRES-like correction on each level of the multigrid hierarchy, called the QC-cycle. We show for the Helmholtz problem that the QC algorithm converges satisfactorily for high-wavenumbers, while keeping the space needed for the correction small.

**References:**

O. Bröker and M. J. Grote: *Sparse Approximate Inverse Smoothers for Geometric and Algebraic Multigrid*. Appl. Numer. Math. **41** (2002), pp. 61–80.

O. Bröker, M. J. Grote, C. Mayer, and A. Reusken: *Robust Parallel Smoothing for Multigrid via Sparse Approximate Inverses*. SIAM J. Sci. Comput. **23** (2002), pp. 1396–1417.

Grote, M. J. and T. Huckle: *Parallel preconditioning with sparse approximate inverses*. SIAM J. Sci. Comput. **18** (1997), pp. 838–853.

**Title:** Finite Element Mapping for Spring Network Representations of the Mechanics of Solids

**Researchers:** Andrei A. Gusev

**Institute/Group:** Institute of Polymers, Department of Materials, ETH

**Description:**

We present a general finite element mapping procedure for defining spring network representations of solid mechanics. The procedure is rigorous and equally suitable for setting regular and unstructured spring network models of generally anisotropic solids. We use the procedure to define close-packed triangular and simple cubic lattice spring models of isotropic 2D and 3D elastic media, respectively.We extend the study to heterogeneous solids and show that the mapped spring network approach constitutes an appealing route for incorporating subelement level constitutive equations.

**References:** A.A. Gusev, *Phys. Rev. Let*. **2004**, *93*, 034302.

**Title:** Prediction of Elastic Properties of a Poly(styrene-butadiene-styrene) Copolymer Using a Mixed Finite Element Approach

**Researchers:** Stephan A. Baeurle[*,**]
Glenn H. Fredrickson[*]
Andrei A. Gusev[**]

**Institute/Group:** [*]Department of Chemical Engineering & Materials, University of California, Santa Barbara
[**]Institute of Polymers, Department of Materials, ETH

**Description:**

Despite several decades of research, the nature of linear elasticity in microphase-separated copolymers with chemically connected glass-rubber phases is still not fully understood. In this paper we investigate the linear elastic properties of a poly(styrene-butadiene-styrene) triblock copolymer using a mixed finite element approach. The technique permits phases of full incompressibility as well as phases of near incompressibility as they occur in this two-component system to be dealt with. Strikingly and contrary to the common belief, we find that the continuum description is accurate and that no additional detailed molecular information is needed to reproduce the available linear elastic experimental data. Our investigation indicates that the anomalous Poisson ratio of the polybutadiene phase of 0.37, determined by previous authors and attributed to molecular characteristics of the polybutadiene phase, might be related to sample end effects arising in their tensile and torsional experiments. We also test the suitability of several semiphenomenological models in reproducing the experimental measurements. We find that some of the methods provide reliable results of accuracy comparable to results from our mixed finite element approach.

**References:** S.A. Baeurle, G.H. Fredrickson, A.A. Gusev, *Macromolecules* **2004**, *37*, 5784-5791.

**Title:** A new domain-model approach to theoretically predict the stress relaxation of thermoplastic elastomers

**Researchers:** Stephan A. Baeurle[*,**]
Atsushi Hotta[*]
Andrei A. Gusev[**]

**Institute/Group:** [*]Department of Chemical Engineering & Materials, University of California, Santa Barbara
[**]Institute of Polymers, Department of Materials, ETH

**Description:**

In this paper we report on a new theoretical approach to predict the long-time stress relaxation behavior of thermoplastic elastomers. This approach relies on the method of Gurtovenko and Gotlib [J. Chem. Phys. 115 (2001), pp. 6785-6793], which has originally been conceived to describe the relaxation dynamics of inhomogeneously crosslinked polymers forming agglomerations of crosslinks. In this work we demonstrate that the method can be extended to describe the stress relaxation behavior of homogeneously crosslinked thermoplastic elastomers, which are subjected to an extensional strain pertaining to the nonlinear regime of mechanical properties. In our approach thermal fluctuations induce fluctuations in size of domains of crosslinks via a chain-pullout mechanism. We compare our theoretical predictions to the experimental measurements of Hotta et al. [Macromolecules 35 (2002), pp. 271-277] performed on poly-(styrene-isoprene-styrene) triblock copolymers, which are composed of hard domains of polystyrene embedded in a rubbery polyisoprene matrix. Our study confirm the importance of the chain-pullout mechanism in the stress relaxation process and demonstrates the involvement of multiple time- and structural-length-scales.

**References:**

S.A. Baeurle, A. Hotta, A.A. Gusev, *Polymer* (in print)

**Title:** Numerical prediction and optimization of physical and mechanical properties of interpenetrating phase composites

**Researchers:** Martin Heggli
Andrei A. Gusev

**Institute/Group:** Institute of Polymers, Department of Materials, ETH

**Description:**

Interpenetrating phase composites offer improved mechanical and physical properties compared to the monolithic components. In these multiphase materials each phase is three-dimensionally interconnected throughout the structure. This special topology enables the development of materials with multifunctional characteristics. The 3-D microstructure of such interpenetrating composites has been measured by X-ray microtomography. Since the tomography information is represented in a pixelated form it can directly be used to build a 3-D finite element model of the microstructure. Grid based cubic finite elements are used to represent the individual voxels.

Therefore we are able to base our numerical calculations on the real microstructure rather than on simplified model structures. Effective elastic properties as well as physical properties governed by the Laplace equation (e.g. electrical conductivity) are calculated and verified against experimental data of graphite/aluminium and polymer/glass composites. In a second step the numerical procedure is used to explore modifications of the microstructure with the goal to optimize specific properties of the composite material.

**References:** A manuscript is in preparation

**Title:** Matching thermal expansion of mica-polymer nanocomposites and metals

**Researchers:** Olga Guseva[*,**]
Hans Rudolf Lusti[*]
Andrei A. Gusev[*]

**Institute/Group:** [*]Institute of Polymers, Department of Materials, ETH
[**]Laboratory for Corrosion and Materials Integrity, EMPA, Dübendorf

**Description:**

Finite element numerical simulations have been carried out to demonstrate that by the dispersing of a small amount of exfoliated muscovite mica platelets in a solid polymer one can considerably reduce and even match the thermal expansion coefficients of metal and polymer components of hybrid polymer-metal structures. In practice, such mismatch reduction may lead to the extension of the service life of hybrid polymer-metal structures. Computer models comprised of a random dispersion of fully aligned round muscovite mica platelets have been studied. It was found that the decrease of the thermal expansion for such nanocomposites is controlled by the product of the aspect ratio and the volume fraction of the mineral platelets, and that the dependence can be accurately described by a stretched exponential master curve, thus considerably facilitating the task of designing mica-polymer nanocomposites with tailored thermal expansion.

**References:**

O. Guseva, H.R. Lusti, A.A. Gusev, *Model. Simul. Mater. Sci. Eng*. **2004,** *12*, S101–S105.

**Title:** Finite element predictions for the thermoelastic properties of nanotube reinforced polymers

**Researchers:** Hans Rudolf Lusti
Andrei A. Gusev

**Institute/Group:** Institute of Polymers, Department of Materials, ETH

**Description:**

The overall effective thermoelastic properties of nanotube reinforced polymers (NRP) were estimated numerically by using a finite element based procedure. Three-dimensional multi-inclusion periodic computer models were built for three different nanotube orientation states, namely, fully aligned, two-dimensional random in-plane and three-dimensional random states. The enhancement of the Young's modulus as well as the decrease of the thermal expansion coefficient were calculated numerically, assuming technologically relevant combinations of the nanotube aspect ratio and volume fraction. Maximal changes of the thermoelastic properties can be achieved in the longitudinal direction of NRPs with fully aligned carbon nanotubes whereas two-dimensional random in-plane and three-dimensional random composite morphologies exhibit more moderate enhancements but in more than one direction. Numerical predictions for the enhancements of the thermoelastic properties confirmed that carbon nanotubes can be considerably more effective for the reinforcement of polymers than conventional glass or carbon fibres.

**References:** H.R. Lusti, A.A. Gusev, *Model. Simul. Mater. Sci. Eng*. **2004,** *12,* S107-S119.

**Title:** Effect of particle agglomeration on the elastic properties of filled polymers

**Researchers:** Hans Rudolf Lusti
Ilya A. Karmilov
Andrei A. Gusev

**Institute/Group:** Institute of Polymers, Department of Materials, ETH

**Description:**

We conducted a numerical finite-element-based study on the reinforcing effect of particle agglomeration on the stiffness of sphere-filled polymers. Two different types of agglomerates were considered. The first type was made up of 10 nonoverlapping identical spheres, whereas the second type were 10 slightly fused spheres. Numerical results reveal that by using agglomerates with fused spheres, one can significantly increase the composite stiffness, whereas the use of nonfused agglomerates does not allow one to achieve any additional stiffness increase compared to a composite with evenly dispersed nonagglomerating spheres.

**References:** H.R. Lusti, I.A. Karmilov, A.A. Gusev, *Soft Mater*. **2003**, *1*, 115-120.

**Title:** On the possibility of reduced variable predictions for the thermoelastic properties of short fibre composites

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

**Institute/Group:** [*]IRC in Polymer Science and Technology, University of Leeds, UK
[**]Institute of Polymers, Department of Materials, ETH

**Description:**

Computer aided design offers the potential for the rapid development of new advanced structures from short fibre reinforced composites. The advantage of a validated numerical simulation is clear, as it allows a large number of the potential structure's solutions to be studied before proceeding to a manufacturing stage, reducing cost and risk accordingly. In our recent work we have demonstrated that the direct finite-element-based procedure of Gusev could be reliably employed for the prediction of thermoelastic properties of laboratory injection moulded samples, on the basis of Monte Carlo multi-fibre computer models built based on the measured fibre orientation distribution functions. Most injection moulded or extruded structures however, exhibit non-uniform fibre orientation states across the final parts, with a diverging variety of different local fibre orientation states. It Would be impractical to characterize all the possible orientation states by their full distribution functions, and it would be equally impractical to attempt direct numerical property predictions for all the various orientation states. Here we show that real injection moulded and extruded materials show fibre orientation states close to a maximum entropy prediction (i.e. most random) and that local thermomechanical properties can be excellently predicted based on the second order orientation moments and a constant strain assumption between the phases. Our results landmark a practical possibility of computer aided design of advanced structural parts from short fibre reinforced composites.

**References:** P.J. Hine, H.R. Lusti, A.A. Gusev, *Compos. Sci. Technol.* **2004**, *64*, 1081-1088.

**Title:** Voltage breakdown in random composites

**Researchers:** Andrei A. Gusev[*]
Olga Guseva[*,**]

**Institute/Group:** [*]Institute of Polymers, Department of Materials, ETH
[**]Laboratory for Corrosion and Materials Integrity, EMPA, Dübendorf

**Description:**

Voltage breakdown is a critical phenomenon involving a catastrophic increase in the electric conductivity of a dielectric body, induced by an external electric field. Here, we studied the voltage breakdown phenomenon in a composite comprised of a random dispersion of metal spheres in a polymer matrix, based on periodic Monte Carlo realizations with a varying number of spheres. We gradually increased the electric field and collected the individual voltage breakdown estimates, predicted numerically, on the basis of morphology-adaptive unstructured meshes and by using an iterative finite element solver. At all the concentrations studied, the individual estimates obtained with computer models of 1000 spheres were rather uniform. But strikingly, already with a dozen spheres, the ensemble minimum estimates obtained with a given number of spheres were practically the same as those obtained with 1000 spheres. Our results suggest that in random composites the voltage breakdown is a locally controlled phenomenon, and that estimates obtained with incredibly small computer models are representative for much larger, laboratory samples.

**References:** A.A. Gusev, O. Guseva, *Adv. Eng. Mater*. **2003**, *5*, 713-715.

**Title:** Non-additive effects in the elastic behavior of dental composites

**Researchers:** Michael Wissler[*]
Hans Rudolf Lusti[*]
Chantal Oberson[*]
Albert H. Widmann-Schupak[**]
Gianluca Zappini[***]
Andrei A. Gusev[*]

**Institute/Group:** [*]Institute of Polymers, Department of Materials, ETH
[**]MatSim GmbH, Zürich
[***]Ivoclar Vivodent AG, Schaan (Liechtenstein)

**Description:**

Solid polymers have a stiffness of several GPa whereas a natural tooth has a stiffness of about 20 GPa. By putting rigid minerals into a polymer, one matches the composite's stiffness with that of the tooth. Such composites are widely used in various dental medicine applications. For example, they are frequently used for tooth filling. In practice, low aspect ratio fillers are typically used, with a filler content of about 60-70 volume percent. As identical spheres cannot be randomly packed at such high loadings, a mixture of two and more different size fillers is usually employed, with an order- of-magnitude difference in the size of the particles. Based on the additivity premise, it would be tempting to think that one could predict the stiffness of such composites in a series of two-phase homogenization steps. For example, for a composite with a bimodal size distribution, one could first predict the stiffness of a dispersion of small particles in the pure polymer and then the stiffness of a dispersion of big particles in a matrix with the effective properties obtained in the first step. In fact, this additive route would be a classical textbook guideline recommended for designing three and more phase composite materials. Here, for the first time to our best knowledge, we have carried out direct finite element predictions for the stiffness of a dental composite with a bimodal size distribution, and compared the results with those obtained in a two step homogenization series. It appears that the discrepancy between direct and additive predictions is quite substantial and thus no reliable design can be accomplished based on the additivity premise.

**References:** M. Wissler, H.R. Lusti, C. Oberson, A.H. Widmann-Schupak, G. Zappini, A.A. Gusev, *Adv. Eng. Mater.* **2003**, *5*, 113-116.

**Title:** Stable FEM-BEM coupling for Helmholtz transmission problems

**Researchers:** R. Hiptmair
P. Meury

**Institute/ Group** Seminar for Applied Mathemtaics
ETH Zurich

**Description:**

When solving Helmholtz transmission problems we have to tackle a problem which is posed on an unbound domain. By coupling finite element and boundary element methods (symmetric FEM - BEM coupling) the transmission problem can be reduced to a variational problem which is posed on a bounded domain.
However, classical symmetric FEM - BEM coupling suffers from spurious resonances altough the underlying transmission problem is well posed. By using a suitable regularization operator

$$\mathsf{M} : H^{-\frac{1}{2}}(\Gamma) \quad \rightarrow \quad H^{\frac{1}{2}}(\Gamma)$$

and the Calderon projector we obtain a resonance-free variational formulation which is amenable to finite element discretizations. A possible choice for $\mathsf{M}$ is

$$(\mathsf{Id} - \Delta_\Gamma)^{-1} : H^{-1}(\Gamma) \rightarrow H^{1}(\Gamma)$$

where $\Delta_\Gamma$ is the Laplace-Betrami operator. Implementation and numerical testing of this variational formulation is in preparation.

**References:** A SAM Report is in preparation.

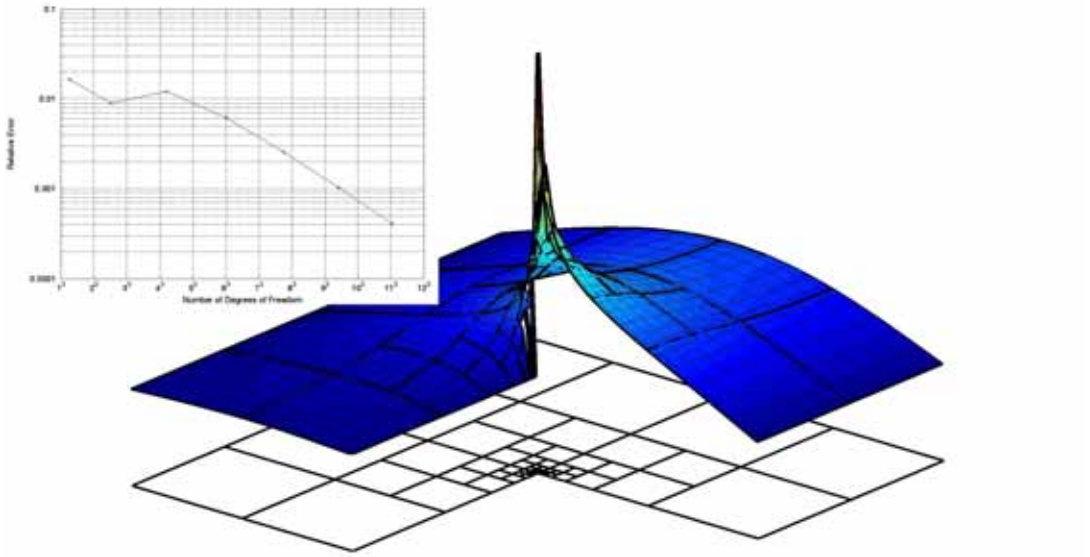
**Title:** *hp*-adaptive FE discretization for time-harmonic Maxwell equations in 2D

**Researchers:** Kersten Schmidt
Philipp Frauenfelder

**Institute/ Group:** Seminar for Applied Mathematics
Department of Mathematics

**Description:**

When solving Maxwell's equations in complex geometries with dielectric media the Finite Element Method with *Edge Elements* is a popular procedure. The basis functions of the Edge Elements lie in the space H(curl) and fullfill the interface boundary conditions. In this project an existing C++ class library is extended to incorporate a fully *hp*-adaptive edge discretisation in 2D, based on quadrilaterials. This includes adaptive refinement in polynomial degree in each direction (anisotropically) and in mesh size. The code allows for independent refinement of elements since conforming as well as non-conforming meshes can be dealt with. Boundary effects can be accuratly resolved at low computational cost. Future work intends to extend the current implementation to include three-dimensional edge element classes.



One component of 1st Maxwell eigenfunction on L-shape domain with PEC boundary condition is well resolved on a geometrically refined mesh (to the re-entrant corner). In the small diagramm the exponential convergence of the belonging eigenvalue is shown.

**Title:** Simulation of VCSEL devices using $hp$–version $\vec{H}(\mathrm{curl})$ and $H^1$ conforming elements.

**Researchers:** P.D. Ledger
R. Hiptmair

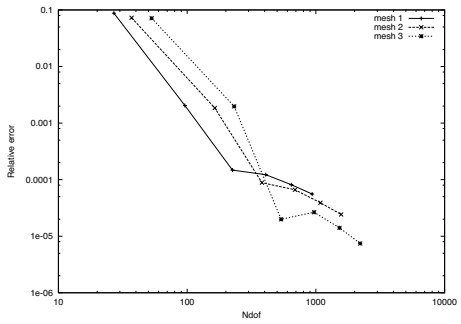
**Institute/ Group:** Seminar for Applied Mathematics
ETH Zürich

**Description:**

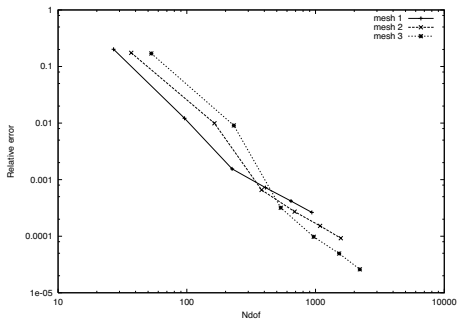
Our interest in Vertical Cavity Side Emitting Laser (VCSEL) devices lies in the accurate calculation of the resonant frequencies $\omega^2$ and the associated electric field intensity vectors $\vec{E}$ of the governing vector wave equation

$$\mathrm{curl}\,\mu^{-1}\mathrm{curl}\,\vec{E} - \omega^2\epsilon\vec{E} = \vec{0} \tag{1}$$

For these devices one can exploit the rotationally symmetric nature of the geometry thanks to a Fourier decomposition of the field. This therefore allows us to reduces the dimension of the problem from three to two. We are currently investigating the approximation of the related closed cavity problem in axisysmmetric coordinates using a $hp$ finite element discretisation with $\vec{H}(\mathrm{curl})$ and $H^1$ conforming basis functions. Ongoing work involves the incorporation of appropriate boundary conditions to truncate the open problem associated with the VCSEL device. Below we show convergence curves for the first two resonant modes of a mushroom–shaped closed cavity solved using a $hp$ discretisation.




$\omega_1^2$




$\omega_2^2$

**References:** R. Hiptmair and P.D. Ledger. Computation of resonant modes for axisymmetric Maxwell cavities using $hp$ version edge finite elements. International Journal for Numerical Methods in Engineering. submitted.

**Title:** Interaction of the disaccharide trehalose with a phospholipid bilayer: A molecular-dynamics study.

**Researchers:** Cristina S. Pereira*
Roberto D. Lins*
Indira Chandrasekhar*
Luiz Carlos G. Freitas**
Philippe H. Hünenberger*

**Institute/ Group:** * Laboratory of Physical Chemistry
** Departamento de Química,Universidade Federal de São Carlos, Brazil

**Description :**

The disaccharide trehalose is well known for its bioprotective properties. Produced in large amounts during stress periods in the life of organisms able to survive potentially damaging conditions, trehalose plays its protective role by stabilizing biostructures such as proteins and lipid membranes. In this study, molecular dynamics simulations are used to investigate the interaction of trehalose with a phospholipid bilayer at atomistic resolution. Simulations of the bilayer in the absence and in the presence of trehalose at two different concentrations (1 or 2 molal) are carried out at 325 K and 475 K. The results show that trehalose is able to minimize the disruptive effect of the elevated temperature and stabilize the bilayer structure. At both temperature, trehalose is found to interact directly with the bilayer through hydrogen bonds. However, the water molecules at the bilayer surface are not completely replaced. At high temperature, the protective effect of trehalose is correlated with a significant increase in the number of trehalose-bilayer hydrogen bonds, predominantly through an increase in the number of trehalose molecules bridging three or more lipid molecules.

**References:** Pereira, C.S., Lins, R.D., Chandrasekhar, I., Freitas, L.C.G. & Hünenberger, P.H.
Biophys. J. **86** (2004) 2273-2285.

**Title:** Explicit-solvent molecular-dynamics simulations of the $\beta(1\rightarrow3)$- and $\beta(1\rightarrow6)$-linked disaccharides $\beta$-laminarabiose and $\beta$-gentiobiose in water.

**Researchers:** David Kony*
Wolfgang Damm**
Serge Stoll***
Philippe H. Hünenberger*

**Institute/ Group:** * Laboratory of Physical Chemistry
** Schrödinger Inc. New York, USA
*** Départment de chimie Inorganique, Analytique et Appliquée, Université de Genève

**Description :**

The conformational preferences about the glycosidic linkages present in $\beta$-laminarabiose and $\beta$-gentiobiose in water are investigated by comparing molecular-dynamics (MD) simulations with results from NMR spectroscopy (coupling constants, NOE-derived distances), X-ray crystallography (structures), and molecular mechanics (adiabatic energy maps). The simulations are performed using the OPLS-AA-SEI force field recently developed for hexopyranoses, and extended to account for the properties of the linkages present in the two disaccharides. The experimental and theoretical results for $\beta$-laminarabiose are very consistent, and reveal a clear correlation between the conformation of the dihedral angle $\psi$ and the presence of an interresidue hydrogen bond (4-hydroxyl group of the reducing residue to the ring oxygen of the non-reducing residue). The solvent (water) plays an essential role in determining the preferential value about $\psi$, by dramatically reducing the strength of this intramolecular hydrogen bond. Application of the OPLS-AA-SEI force field to $\beta$-gentiobiose requires significant adjustments of the torsional parameters and electrostatic scaling scheme. After optimization of the force field based on *ab initio* calculations in vacuum and on the experimental population profile around the dihedral angle $\omega$ in water, the OPLS-AA-SEI force field is able to give a realistic representation of the conformational behavior of the $\beta(1\rightarrow6)$-linkage on the nanosecond time scale. As expected, the glycosidic dihedral angles in this linkage present an enhanced flexibility compared to the $\beta(1\rightarrow3)$-linkage. The results of the two simulations point (in line with previous studies) towards the need of developing a new Karplus-type equation relating hetero-nuclear $^3J_{C,H}$ coupling constants to the glycosidic dihedral angle $\phi$. They also suggest that the Karplus-type equation of Stenutz et al. for the homo-nuclear $^3J_{H,H}$ coupling constant is superior to the widely used equation of Haasnoot et al.

**References:** Kony, D., Damm, W., Stoll, S. & Hünenberger, P.H. J. Phys. Chem. B **108** (2004) 5815-5826.

**Title:** A fast pairlist-construction algorithm for molecular simulations under periodic boundary conditions.

**Researchers:** Tim N. Heinz*
Philippe H. Hünenberger*

**Institute/ Group:** * Laboratory of Physical Chemistry

**Description :**

A new grid–cell algorithm is presented, that permits the construction of cutoff–based non–bonded pairlists in molecular simulations under periodic boundary conditions based on an arbitrary box shape. The key features of the method are (*i*) the use of a one–dimensional mask array (to determine which grid cells contain interacting atoms) that incorporates the effect of periodicity, and (*ii*) the grouping of adjacent interacting cells of the mask array into stripes, which permits the handling of empty cells with a very low computational overhead. Testing of the algorithm on water systems of different sizes (containing about 2000 to 11000 molecules) shows that the method (*i*) is about an order of magnitude more efficient compared to a standard (double–loop) algorithm, (*ii*) achieves quasi–linear scaling in the number of atoms, (*iii*) is weakly sensitive in terms of efficiency to the chosen number of grid cells, and (*iv*) can be easily parallelized.

**References:** Heinz, T.N. & Hünenberger, P.H.
J. Comput. Chem. **25** (2004) 1474-1486.

**Title:** pH-dependent stability of a decalysine $\alpha$-helix studied by explicit-solvent molecular dynamics simulations at constant pH.

**Researchers:** Ulf Börjesson*
Philippe H. Hünenberger*

**Institute/ Group:** * Laboratory of Physical Chemistry

**Description :**

The acidostat method previously developed for performing explicit-solvent molecular dynamics simulations at constant pH (*J. Chem. Phys.* **2001**, *114*, 9706) is applied to polyfunctional compounds, namely 1,4-diaminobutane and a decalysine peptide. The titration behavior of 1,4-diaminobutane is investigated by performing a series of simulations at different pH using the acidostat method. The method accounts at least to some extent for site-site coupling and reproduces the experimental p$K_a$s of the compound within half a p$K$ unit, although the simulations reveal insufficient sampling of the protonation-state variables. In a second step, the ability of the acidostat method to account for correlation s between the solution pH and the structure and dynamics of a biomolecule is tested by studying the pH-dependent stability of an $\alpha$-helical decalysine peptide. To this end, four 32 ns constant-pH simulations at different pH values are performed. The results are compared to those of standard molecular dynamics simulations of a fully-protonated or a fully-deprotonated peptide, and to experimental data on (comparatively longer) polylysine peptides. In agreement with experiment, the peptide predominantly remains in an $\alpha$-helical conformation under high-pH conditions, but becomes disordered under low-pH conditions. The helix-coil transition pH for the peptide is found to be between 9.5 and 10.3, in good agreement with the experimental value for polylysine (10.3). The constant-pH simulations also evidence a clear correlation between the protonation of specific lysine sidechains, and the local loss of backbone hydrogen bonds and partial peptide unfolding, both effects occurring predominantly in the C-terminal region of the peptide.

**References:** Börjesson, U. & Hünenberger, P.H.
J. Phys. Chem. B (2004) in press.

**Title:** Construction of optimized NMR experiments using molecular dynamics in the space of pulse-sequence variables

**Researchers:** Konstantin Pervushin*
Beat Vögeli*
Tim N. Heinz*
Philippe H. Hünenberger*

**Institute/ Group:** * Laboratory of Physical Chemistry

**Description :**

The optimization of coherence-transfer pulse-sequence elements (CTEs) is the most challenging step in the construction of heteronuclear correlation NMR experiments achieving a sensitivity close to its theoretical maximum (in the absence of relaxation) in the shortest possible experimental time and featuring active suppression of undesired signals. As reported in the present article, this complex optimization problem in a space of high dimensionality turns out to be numerically tractable. Based on the application of molecular dynamics in the space of pulse-sequence variables, a general method is proposed for constructing optimized CTEs capable of transferring an arbitrary (generally non-Hermitian) spin operator encoding the chemical shift of heteronuclear spins to an arbitrary spin operator suitable for signal detection. The CTEs constructed in this way are evaluated against benchmarks provided by the theoretical unitary bound for coherence transfer and the minimal required transfer time (when available). This approach is applied for constructing of a set of NMR experiments enabling direct and selective observation of individual 1H-transitions in $^{13}$C-labeled methyl spin systems close to optimal sensitivity.

**References:** Pervushin, K., Vögeli, B., Heinz, T.N. & Hünenberger, P.H. submitted to J. Am. Chem. Soc.

**Title:** Solving Dirichlet Problems Numerically Using the Feynman–Kac Representation

**Researchers:** F.M. Buchmann*
W.P. Petersen*

**Institute:** *Seminar for Applied Mathematics

**Description:**

Many applications, for example, in finance or physics and chemistry applications with a large number of species, the underlying dimensionality of the space may be high. In these cases, the partial differential equations (PDEs) which describe the equilibrium state easily become industrial tasks. In this work, we have used bounded simulated Brownian motion driven stochastic differential equations to study high dimensional elliptic problems. What is required are the first-exit times and first-exit positions of the stochastic paths. Two layers are used near the boundary. One is of size $O(\sqrt{h})$ wherein controlling the stepsize $h$ near the boundary prevents excursions. When a path reaches another, of size $O(h^{p+1})$, it is stopped because the distance to the boundary is smaller than the order of the integration rule, $O(h^p)$. Using this technique, we have sucessfully simulated elliptic problems in dimensions up to 64. Our results show that the sensitivity of our boundary finding algorithm actually decreases in higher dimensions.

Since sub-samples may be computed independently, the ETH Beowulf cluster provides an excellent platform. Inter-CPU communication is small and sub-samples may be computed asynchronously. In consequence, simulations are easily parallelized, fault tolerant, and fairly simple to program.

This project was funded by TH-Gesuch funds 0-20981-2, awarded in May 2002.

**References:**

F.M. Buchmann and W.P. Petersen, *BIT Numerical Mathematics*, **43**, pp. 519-540 (2003).

**Title:** Developing a Divergence Preserving Finite Volume Method for Maxwell Equations

**Researcher:** Paolo Corti
Dr. Manuel Torrilhon
Dr. Michael Fey
Prof. Rolf Jeltsch

**Institute:** Seminar for Applied Mathematics
ETH Zürich

**Description:**

The Maxwell equations describe the motion of electric charges and electromagnetic field in a medium. This set of equations can be subdivided in two groups, a first one that describes the changes in time of the electromagnetic fields, and a second one - an intrinsic constraint - that couples the fields to the charges.
The time dependence of the charge density is not explicitly given through a partial differential equation alone, as for the field equation. In the continuum we can couple the two sets of equations to derive the rules for the evolution of charge density.
In the continuous case with a physical initial condition, using the evolution of the charge equation automatically satisfies the constraint. The opposite is also true: from the constraint we get the physical charge. Finite volume method that solves the field equations have to deal with non physical solutions, which can be eliminate through some artificial steps. This happens if the operators are discretized without taking into account the implicit characteristics that exist in the continuum. This feature has to be mimicked in the discrete case to have a physically relevant result. We are developing a formulation in the framework of the finite volume method of Torrilhon and Fey to obtain a numerical algorithm that retains the desired attributes, without imposing the physical constraint in some artificial way between each time step.

**References:**

M. Torrilhon and M. Fey, *Constraint-preserving Upwind Methods for Multidimensional Advection Equations*, SIAM J. Num. Anal., (2004), in press

**Title:** Multidimensional Numerical Methods for the Regularized 13–Moment Equations

**Researcher:** Miroslav Čada
Dr. Manuel Torrilhon
Dr. Michael Fey
Prof. Rolf Jeltsch

**Institute:** Seminar for Applied Mathematics
ETH Zürich

**Description:**

Thermodynamics of gases is a field theory with the main objective of determing fields of the constitutive variables, density, velocity and temperature of all particles. In order to obtain the fields one needs balance equations, namely the conservation of mass, momentum and energy. However these equations do not consider dissipative effects.

The 13–moment equations, derived from extended thermodynamics, are dissipative, hyperbolic field equations for monatomic gases. The main idea of extended thermodynamics is that for processes with rapid changes, e.g. shock tube experiment where that are more variables than in the classical Euler case, are needed to give an appropriate theoretical description for rarefied gases. However these equations yield a closure problem for the last moment. For this system of equations, the moment in the space derivative of one equation is subsequently needed for the time derivative in the next equation. This system of equations yields to a closure problem, since the very last moment is not described in the system itself.

In recent work a new closure for the 13–moment equations has been presented ([1], [2]). The regularized 13–moment equations obtain two additional equations for the stress tensor and the heat flux. It is the objective of ongoing work to derive appropriate multidimensional numerical methods for their solution.

**References:**

[1] H. Struchtrup, M. Torrilhon *Regularization of Grad's 13 moment equations: Derivation and linear analysis*, Phys. Fluid 15/9, (2003), 26689–2680

[2] M. Torrilhon, H. Struchtrup *Regularized 13–Moment–Equations: Shock Struckture Calcuylations and Comparison to Burnett Models*, J. Fluid Mech. (2004) to appear

**Title:** An exit probability approach to solve high dimensional Dirichlet problems

**Researchers:** F.M. Buchmann*
W.P. Petersen*

**Institute:** *Seminar for Applied Mathematics

**Description:**

In a previous work, *Solving Dirichlet Problems Numerically Using the Feynman-Kac Representation*, we studied a numerical procedure for high dimensional elliptic problems which relied on bounded increments for the driving Brownian motion in stochastic differential equations. There, the bounded increments are not isotropic and may introduce small errors in finding the boundary of the domain. A method for generating random rotation matrices (from G.W. Stewart) in $n-$space is thus required. Since we are only interested in weak solutions of the stochastic equations, another probabilistic procedure became evident. What is important is that the simulated stochastic paths do not exit and come back, that is the first exit times and exit positions are correctly sampled. There are two situations:

- At time $t_k$, the process $X(t_k) \in D$ and also at the end of the timestep, $X(t_{k+1}) \in D$. The probability of an excursion must be estimated and a standard weak test is made. If the test shows an excursion, the exit time is sampled and a bridge process is used to estimate the exit postion.
- While at time $t_k$, the process $X(t_k) \in D$ but at the end of the step, $X(t_{k+1}) \notin D$. In this case, the process clearly exited, so what remains is to estimate when during this timestep. Once the exit time is estimated, a bridge can be used to sample the exit position.

We find extremely good results with this procedure and have simulated model problems in hypercubic and hypersherical domains up to 128 dimensions on the ETH Beowulf machine.

This project was funded by TH-Gesuch funds 0-20981-2, awarded in May 2002.

**References:**

F.M. Buchmann and W.P. Petersen, submitted to *J. Computational Physics*, 2004.

F.M. Buchmann, to be published in *J. Computational Physics*, 2004. Or "Simulation of stopped diffusions," SAM Tech. Rep. 2004-03 (2004).

**Title:** Weak approximations of stopped diffusions

**Researchers:** F.M. Buchmann*
W.P. Petersen*

**Institute:** *Seminar for Applied Mathematics

**Description:**

In a recent paper, Buchmann formulated a procedure for simulating stopped diffusions in one space dimension. This procedure was designed to sample exit times for Monte-Carlo solutions of elliptic partial differential equations. In the current work, we have generalized the one dimensional case to $n-$spaces where boundaries are assumed locally flat relative to the scale $(\sqrt{h})$ defined by the time step of the simulated stochastic path. Except for sharp corners or cusps, this is the usual case.

What is involved is to perform a coordinate transformation to a locally defined system in which the boundary is approximated by a hyperplane orthogonal to a convenient rectangular coordinate direction. Again, two situations are evident:

- At time $t_k$, the process $X(t_k) \in D$ and also at the end of the timestep, $X(t_{k+1}) \in D$. The probability of an excursion must be estimated and a test made. If the test shows an excursion, the exit time is sampled.
- While at time $t_k$, the process $X(t_k) \in D$ but at the end of the step, $X(t_{k+1}) \notin D$. In this case, the process clearly exited, so the exit time $\tau$, $t_k < \tau < t_{k+1}$ (where $h = t_{k+1} - t_k$) must be estimated.

Once an estimate of the exit time is found, a bridge process ($\xi$ is a zero centered normally distributed $n-$vector) of the form

$$\mathbf{X}_{loc}(t) = (1 - t/h)\mathbf{X}_k + (t/h)\mathbf{X}_{k+1} + \sqrt{(1 - t/h)(\tau/h)}\xi$$

is constructed and the intersection of this Wiener "sausage" with the boundary hyperplane sampled. The sample point is an estimate of the exit process value: $\mathbf{X}(\tau) = \mathbf{X}_{loc}(t)$, where $\tau = t_k + t$. This value is what is required for the Feynman-Kac functional which represents the solution to the elliptic PDE problem.

This project was funded by TH-Gesuch funds 0-20981-2, awarded in May 2002.

**References:**

F.M. Buchmann and W.P. Petersen, submitted for the proceedings of the MC2QMC conference, Juan-les-Pins, France, June, 2004.

F.M. Buchmann, to be published in *J. Computational Physics*, 2004. Or "Simulation of stopped diffusions," SAM Tech. Rep. 2004-03 (2004).

**Title:** A Generic Random Number Generator Test Suite

**Researchers:** M. Rütti†
M. Troyer†
W.P. Petersen*

**Institutes:** †Institute for Theoretical Physics, ETH
*Seminar for Applied Mathematics, ETHZ

**Description:**

Random number generators used in Monte-Carlo simulations and a variety of computer science applications are relatively simple modular recurrence formulas. The resulting arithmetic sequences are not truly random but do exhibit most randomness properties desirable for applications. Confidence thus requires randomness testing. There are a number of random number test suites: *DieHard* tests, tests described in D. Knuth's vol. 2, various physical tests, and many new ones. The lack of an organized suite which includes all well known packages meant that tests for properties desired in an application had to be ferreted out by users who know little about the theory or internals of any given generator. There have also been no standard user interfaces, nor standard test result reporting procedures. Our work here attempts to address these issues:

- Establish a standard interface to be used with the **C++** language, but easily adaptable to Fortran and **C**. Hence, well considered Fortran/C wrappers were implemented, and carefully designed calling sequences standardized.
- Integration of known tests and implement mechanisms for adding new ones easily, according to strict **C++** conventions.
- Report results of a suite of tests easily and flexibly. For example: graphical output, LaTeXtables, HTML or XML table production should be available to display the results.

Our test suite achieves these objectives and has been accepted as for **C++** standardization by the JTC1/SC22/WG21 working group and also by the **Boost** framework standards committee.

**References:**

M. Rütti, M. Troyer, and W.P. Petersen, submitted to the proceedings of *MC2QMC* Monte-Carlo simulation meeting, Juan-les-Pins, France, June, 2004.

Test suite accepted by the JTC1/SC22/WG21 - C++ standards WG21 committee for standard random number testing/generation, 2004.

**Title:** Estimation of weak lensing parameters by stochastic integration.

**Researcher:** W.P. Petersen*

**Institute:** *Seminar for Applied Mathematics

**Description:**

Inspired by a project on N–body cosmological simulations which includes W. Petersen from ETH, G. Lake, B. Moore, J. Stadel from the University of Zürich, H.M.P. Couchman from McMaster Univ., and A. Babul from the Univ. of Victoria, the current work examined the statistics of gravitational forces on light rays from high redshift sources. The N–body simulations showed that sums of these forces over several correlation lengths ($\sim$ 7Mpc) look Gaussian. Hence, the light deflection increments for $\Delta z \lessapprox 1/10$ are proportional to two dimensional (or complex) Brownian motion and therefore the light shearing can be modeled by stochastic differential equations. The shear takes on a form

$$\sigma(z) = \int_0^z (D(\xi)/D(z))^2 f(\xi) dw(\xi)$$

where the function $f(z)$ is a smooth deterministic function, $D(z)$ is the angular diameter distance, and $w(z)$ is a complex Brownian motion with redshift parameter $z$. Using this form for the shear, a modified Dyer-Roeder differential equation can be written

$$(1+z)(1+\Omega z)\frac{d^2D}{dz^2} + \ (\frac{7}{2}\Omega z + \frac{\Omega}{2} + 3)\frac{dD}{dz} + \ \frac{|\sigma(z)|^2}{(1+z)^5}D = 0.$$

Here, $\Omega = \rho/\rho_c$ (= 1 in our simulations) is the ratio of average mass density $\rho$ to the critical closure density $\rho_c$. Formally, this version of the Dyer-Roeder equation is the same as S. Seitz and P. Schneider's, with the essential difference that the shear $\sigma(z)$ is a continuous random variable. For our version, an integration method for the above two non-linear stochastic differential equations was constructed. The resultant angular diameter distance ($D(z)$) distribution was computed out to $z = 5$, with $f(z)$ extracted from N–body simulations. From these simulations, $f(z)$ turned out to be extremely simple and has only one fitted parameter, its normalization.

**References:**

W.P. Petersen, Stochastic Analysis and Applications, **22**, No. 4, pp. 989-1008 (2004).

**Title:** Communication strategies for multi-dimensional FFT on distributed memory computers.

**Researchers:** W.P. Petersen*, R. Mooser*
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**Description:**

On distributed memory computers, moving data often becomes a dominant process in multi-dimensional Fast Fourier Transforms. Namely, although $\log(n)$ steps are required to perform the actual arithmetic operations, only two steps of data transposition may take one half of the computer time. The simplest data layout for a three dimensional array is in **slabs**. In this arrangement, $x$ and $y$ direction vectors are locally CPU memory resident, while the $z$ direction vectors are distributed over processors. The $x$ and $y$ vectors are transformed "on board." To perform the $z$ direction transforms, a transposition "between boards" is needed to make $z-$direction vectors locally memory resident. A second transposition returns the transformed data to their original ordering.

Many familiar packages have built-in transposition procedures, but our experiments showed these generic routines inefficient. The generic implementations use the `MPI` command `MPI_Alltoall`. We find that `MPI_Sendrecv_replace` faster by using a direct index-digit permutation. For $p$ processors, where $0 \leq b \leq p-1$ counts the blocks of size $(N_Z/p) \times (N_Y/p) \times N_X$ `complex` data in any slab numbered `CPU`, $B$ numbers the blocks in the $y$-$z$ plane,

$$B = \texttt{CPU} \times p + b,$$

and $0 \leq \texttt{CPU} \leq p-1$. Block $B$ must be exchanged with permuted block $B'$,

$$B' = b \times p + \texttt{CPU}.$$

**References:**

A. Adelmann, A. Bonelli, W. P. Petersen, C. W. Überhuber, *Communication Efficiency of Parallel 3D FFTs*, Proceedings of VECPAR, Valencia, Spain (2004).

W.P. Petersen, *Some FFT tests of network and chip performance with implications for the ETH Beowulf cluster Asgard upgrade*, SAM Internal Tech. Report, Feb. 15, 2004.

W.P. Petersen, *Beowulf-Cluster, Phase 2, 3-D FFT Benchmark Results*, SAM Internal Tech. Report, July 5, 2004.

**Title:** Repetition test for pseudo-random number generators

**Researchers:** G.H. Gonnet†
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W.P. Petersen*

**Institutes:** †Institute for Computational Science, Informatik, ETHZ
*Seminar for Applied Mathematics, ETHZ

**Description:**

For a uniform random number generator with integer range, say $0 < RNG < 2^w$, the expectated step $k$ at which some number in the sequence repeats can be shown to be approximately

$$\mathbb{E}[k] = \sqrt{\frac{\pi}{2}} 2^{w/2} + O(1)$$

steps. Linear congruential (LC) methods, $u_n = a \cdot u_{n-1}$ **mod** $2^w$, cannot repeat any number $u_k$ before $k = 2^w$. Otherwise, the entire sequence repeats since the recurrence is a one-step whose period is $2^w$. Lagged Fibonacci (LF) sequences, or their generalizations, have vastly longer periods. For example, the simple recurrence $u_n = u_{n-p} + u_{n-q}$ **mod** $2^w$ has a period of approximately $2^w \cdot 2^{p \vee q}$ for suitably chosen $p, q$. If $\max(p, q) = p \vee q$ is large enough, the period of the sequence is astronomically large. However, numbers in LF sequences do re-appear at the above expected rate $\mathbb{E}[k]$. For pattern matching algorithms, satisfying the expected repetition time is very important.

With this in mind, a RNG test called the **repetition test** was implemented and included in the Rütti et al test suite. Since a repetition is expected to occur at roughly $O(2^{w/2})$ steps, not $2^w$, keeping a history of which values have already been generated becomes possible. Recall that IEEE standard double precision uses $w = 53$. A hashing procedure which requires storage of only $O(2^{w/2})$ numbers serves this purpose. We tested various popular RNGs. For example, James' version of `RANLUX`, the Mersenne Twister of Matsumoto et al, and several others were tested. Many popular generators fail. In particular, although integer versions of some pass, floating point implementations of them may fail.

**References:**

G. H. Gonnet, *Repeating time test for $U(0, 1)$ random number generators*, Technical Report, Dept. Informatik, ETH, Zürich, May, 2003.
`http://www2.inf.ethz.ch/~gonnet/RepetitionTest`.

G. H. Gonnet, M. Gil, and W. P. Petersen, submitted for the proceedings of MC2QMC conference, Juan-les-Pins, France, 2004. Proceedings to be published by Springer-Verlag.

**Title:** Efficient Finite-Volume Schemes for Atmospheric Modeling

**Researchers:** William Sawyer*,**
Rolf Jeltsch*
Atsumu Ohmura**
Arthur A. Mirin***

**Institute/ Group:** * Seminar for Applied Mathematics, ETHZ
** Institute for Atmospheric and Climate Science, ETHZ
*** Lawrence Livermore National Laboratory, USA

We investigate the use of pentagonal/hexagonal grids for the solution of the shallow water equations on the sphere (SWES). Such grids avoid problems due to converging points near the pole. In the numerical scheme used to solve the SWES, we ensure that key physical quantities, such as mass and angular momentum, are conserved in the discrete sense. This makes the scheme useful as a building block for atmospheric dynamics on time scales of months to years, where conservation properties are crucial. The resulting algorithm has shown to be viable for long term simulations. Moreover, due to the use of radial basis functions with compact support, the data dependencies of the finite volumes are limited to immediate neighbors, thus limiting communication and allowing scalability on massively parallel computers.

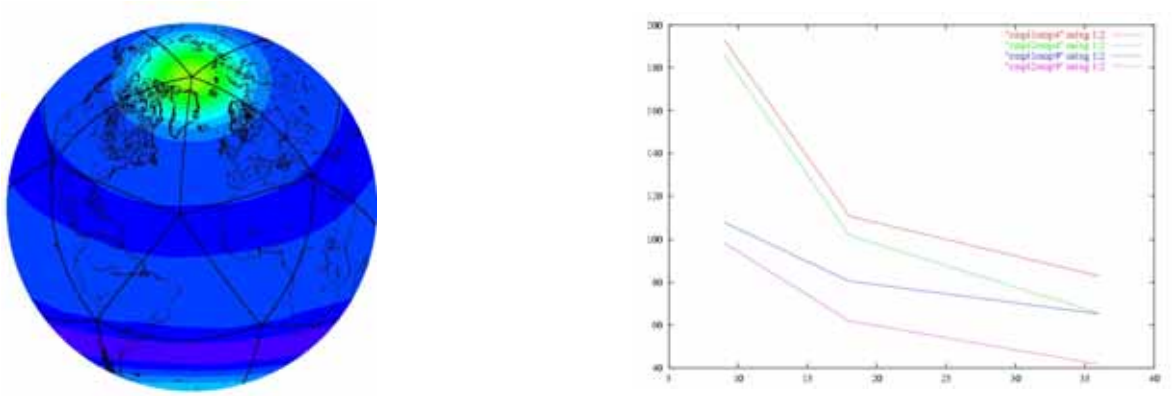

Figure 1: *On left, a 14-day SWES simulation illustrates that the Coriolis effect keeps part of the initial mass near the north pole, while allowing the remainder to flow (concentric rings) from pole to pole. The grid resolution is four refinement levels higher than the depicted icosahedron. On right, timings (in seconds) are given from our parallel implementation of the Lin/Rood dynamical core as a function of the number of (multithreaded) processes. The results for 4 and 9 threads indicate that communication can be improved by multithreading communication with new Message-Passing Interface (MPI-2) functionality, as opposed to MPI-1.*

**References:**

[1] W. Sawyer and R. Jeltsch, A Finite-Volume Mass- and Vorticity-conserving Solver of the Shallow-Water Equations on the Sphere using Penta-/Hexagonal Grids, *Numerical Mathematics and Advanced Applications*, pp. 746–755, Springer-Verlag, 2004.

[2] W. Sawyer and A. A. Mirin, A scalable implementation of a finite-volume dynamical core in the Community Atmosphere Model, *Parallel and Distributed Computing and Systems*, Acta Press, accepted.

**Title:** A Model for the Light arc Simulations

**Researcher:** Harish Kumar
Dr. Manuel Torrilhon
Prof. Rolf Jeltsch

**Institute:** Seminar for Applied Mathematics
ETH Zürich

**Description:**

A light arc phenomenon occurs when a sudden change in the electric field takes place which in turn charges the fluid particles around it so that the fluid starts behaving like plasma. Hence current starts flowing in the fluid and a large amount of energy is generated. Due to the current flow, a magnetic field also devlops.

In this project we try to model this phenomenon. We consider magnetohydrodynamics(MHD) equation (which governs the plasma flow in the magnetic field) in a cylinder. The cylinder is filled with some fluid. When we change the electric field suddenly, the temperature in the cylinder rises, due to generation of the energy and increases the conductivity of the fluid, and a strong current starts flowing in the domain. Also a magnetic field devlops. We observe that the temperature first rises very fast due to fast change in electric field, and then slowly decreases and attains a stable state as the electric field stabilizes. The strong current generated initially also attains a stable state.

**References:**

[1] M. Torrilhon *Zur Numerik der Idealen Magnetohydrodynamics*, Shaker Verlag, Aachen(2004)

**Title:** Finite element characterization of the human myometrium derived from ex vivo uniaxial compression tests

**Researchers:** Stephan Weiss
Peter Niederer

**Institute/ Group:** Institute for Biomedical Engineering
Biomechanics

**Description:**

The construction of a computer based training simulator for hysteroscopy requires models of the uterus that run in real-time. Significant simplifications with respect to the mechanical formulation are however necessary to meet this requirement with presently available computer hardware. A detailed Finite Element model of the uterus which is based on a continuum mechanics' approach is intended to serve for calibration and validation purposes of such simplified models.
The internal structure of the uterine wall has to be considered along with the necessary measurements for the formulation of a comprehensive model. The uterine wall is about 1 – 2 cm thick and consists of three layers: the endometrium (mucous membrane of the body of the uterus), the myometrium (muscle layer) which is by far the thickest layer and the perimetrium (peritoneum of the uterus).
The objective of this study is the determination of material parameters from ex vivo uniaxial compression tests of the myometrium with the help of an optimization process in a Finite Element analysis.

**Title:** A Finite Element study relating to the rapid filling phase of the human ventricles

**Researchers:** Diane-Elise Bettendorff
Peter Schmid
Peter Niederer

**Institute/ Group:** Institute of Biomedical Engineering
Group for Biomechanics and medical Optics

**Description:**

The main cavities of the healthy human heart, called ventricles, double in volume during the rapid filling phase of the diastole. This study aims at investigating to what extent the ventricular pressures are responsible for such an important augmentation in the internal volumes of the cavities. For this purpose, a quasi-incompressible, three-dimensional Finite Element (FE) model of both ventricles of the human heart has been developed, using MSC Marc Mentat. The geometry of the human heart was derived from 32 slices of Magnetic Resonance images. To study the influence of ventricular filling pressures on the rapid filling phase, nonlinear elastic FE analyses with different types of cavity pressure functions applied as boundary conditions were performed. Moreover, the effect of the viscoelasticity of the cardiac tissue on the mechanical behavior of the heart was investigated by comparing elastic and viscoelastic FE simulations. We arrive at the conclusion that under normal conditions the influence of the viscoelasticity of the tissue should not be disregarded in ventricular mechanics. Furthermore, this study has shown that the ventricular pressure measured during the rapid filling phase cannot be the single cause of the rise of the observed left ventricular volume. Our assumption, which will be verified in a future project, is that an elastic recoiling mechanism of the ventricular muscle might account for this volume increase.

**Title:** A three-dimensional model of the fibre architecture of the human left ventricle

**Researchers:** Farshad Dorri
Peter Niederer
Paul P. Lunkenheimer (University of Münster, Germany)

**Institute/ Goup:** Institute of Biomedical Engineering
Group for Biomechanics and Medical Optics

**Description:**

The Fibre Strand Peel-Off Technique (SPOT) was used to determine the spatial architecture of the muscle fibres in a healthy adult human *post mortem* heart. The epicardial and endocardial surfaces as well as the pathway in space of several thousand ventricular muscle fibre strands were digitised and a corresponding computer model of the left ventricle was constructed.

During the gradual peeling process, the fibre strands were chosen as densely as possible, however, for practical reasons, they were not evenly distributed throughout the myocardium such that the pattern had to be completed accordingly by an interpolation scheme. As a result, the local anisotropy of a human post mortem heart was described by a homogeneous unit vector field from which the statistical distribution of the orientation angles was derived. It was found that the myocardium exhibits local inhomogeneities with respect to the fibre orientation pattern, and that an appreciable amount of fibre strands has a non surface-parallel orientation. A subsequent Finite Element analysis allowed to simulate ventricular contraction by choosing an appropriate constitutive law for the myocardium to which a stress tensor modelling active contraction was added.

**References:** A manuscript is in press in *Progress in Biophysics and molecular Biology*

| | |
|---|---|
| **Title:** | Intensity-based 2D-3D Registration of Medical Images |
| **Researchers:** | Xinhui Yang<br>Wolfgang Birkfellner (University of Vienna)<br>Peter Niederer |
| **Institute /**<br>**Group:** | Institute for Biomedical Engineering<br>Group for Biomechanics and Medical Optics |

**Description:**

Under clinical conditions, a registration in real time between a prerecorded 3D computed tomography (CT) data set of a patient and his or her actual position which is determined by way of 2D x-ray projection is often necessary (e.g., exact patient positioning in radiation therapy, calibration of surgical robots, pose estimation in computer-aided surgery). This task requires the determination of a transformation that maps two coordinates systems by comparing a projection image rendered from CT with a real x-ray projection image. Iterative variation of the CT's position between rendering steps finally leads to exact registration. The aim of our work was to develop and validate a technique to register the intra-operative 2D x-ray images with pre-operative 3D CT images in a clinical scenario. We proposed a novel class of similarity measures based on Tchebichef moments, which utilizes the decomposition of the X-ray and the associated digital reconstructed radiography (DRR) into linearly independent orthogonal Tchebichef moments. The results show that the new similarity measure performs more efficiently and accurately on phantom images than well-established methods. A crucial step in the entire process consists of the production of digitally reconstructed radiographs (DRR) from CT data. The standard approach for this purpose is based on the ray-casting technique which however is extremely time consuming due to the need to process each voxel and to perform interpolations. With the aid of the splatting technique, we are developing a rapid algorithm for the generation of DRRs without compromising their quality.

**References:**


1. W. Birkfellner, X. Yang, W. Burgastaller, *et al*, 2D/3D registration using a rotation-invariant cost function based on Zernike moments, Proceeding of SPIE Medical Imaging 2004 – Image Processing, Fitzpatrick JM & Sonka M (Eds.) Volume 5370, Part I 2004: 321-327 (2004).

2. X. Yang, W. Birkfellner, P. Niederer, A similarity measure based on Tchebichef moments for 2D/3D medical image registration, Proceedings of CARS 2004 - Computer Assisted Radiology and Surgery Volume 1268, 2004: 153-158

**Title:** A Concerted variational strategy for investigating rare events

**Researchers:** Daniele Passerone*
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**Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

**Description:**

A strategy for finding transition paths connecting two stable basins is presented. The starting point is the Hamilton principle of stationary action; we show how it can be transformed into a minimum principle through the addition of suitable constraints like energy conservation. Methods for improving the quality of the paths are presented: for example, the Maupertuis principle can be used for determining the transition time of the trajectory and for coming closer to the desired dynamic path. A saddle point algorithm (conjugate residual method) is shown to be efficient for reaching a "true" solution of the original variational problem.

**References:** J. Chem. Phys. 118, 2025 (2003)

**Title:** Water structure as a function of temperature from X-ray scattering experiments and *ab initio* molecular dynamics

**Researchers:** Greg Hura*
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Robert M. Glaeser*/***
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****Computational Science, Department of Chemistry and Applied Biosciences, ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

**Description:**

We present high-quality X-ray scattering experiments on pure water taken over a temperature range of 2 to 77 °C using a synchrotron beam line at the advanced light source (ALS) at Lawrence Berkeley National Laboratory. The ALS X-ray scattering intensities are *qualitatively* different in trend of maximum intensity over this temperature range compared to older X-ray experiments. While the common procedure is to report both the intensity curve and radial distribution function(s), the proper extraction of the real-space pair correlation functions from the experimental scattering is very difficult due to uncertainty introduced in the experimental corrections, the proper weighting of OO, OH, and HH contributions, and numerical problems of Fourier transforming truncated data in *Q*-space. Instead, we consider the direct calculation of X-ray scattering spectra using electron densities derived from density functional theory based on real-space configurations generated with classical water models. The simulation of the experimental intensity is therefore definitive for determining radial distribution functions over a smaller *Q*-range. We find that the TIP4P, TIP5P and polarizable TIP4P-Pol2 water models, with DFT-LDA densities, show very good agreement with the experimental intensities, and TIP4P-Pol2 in particular shows quantitative agreement over the full temperature range. The resulting radial distribution functions from TIP4P-Pol2 provide the current best benchmarks for real-space water structure over the biologically relevant temperature range studied here.

**References:** Phys. Chem. Chem. Phys. 5 (10), 1981 (2003)

**Title:** Efficient exploration of reactive potential energy surfaces using Car-Parrinello molecular dynamics

**Researchers:** Marcella Iannuzzi*
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**Description:**

The possibility of observing chemical reactions in *ab initio* molecular dynamics runs is severely hindered by the short simulation time accessible. We propose a new method for accelerating the reaction process, based on the ideas of the extended Lagrangian and coarse-grained non-Markovian metadynamics. We demonstrate that by this method it is possible to simulate reactions involving complex atomic rearrangements and very large energy barriers in runs of a few picoseconds.

**References:** Phys. Rev. Lett. 90, 238302 (2003)

**Title:** *Ab initio* simulation of $H_2S$ adsorption on the (100) surface of pyrite

**Researchers:** András Stirling*
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**Description:**

The adsorption properties of $H_2S$ on the (100) surface of pyrite have been studied by Car–Parrinello simulations. The predicted adsorption properties have been contrasted to those of water on the same surface. It was found that $H_2S$ prefers molecular adsorption on the surface iron sites while the dissociative adsorption is highly unfavorable. The binding of the $H_2S$ and $HS^-$ species to the Fe sites results from a coordinative covalent bond from the ligand sulfur atom. The adsorption energy at full coverage is much lower than at partial coverage due to steric repulsion among the adsorbates. As opposed to water adsorption, hydrogen bonding plays a marginal role in $H_2S$ adsorption.

**References:** J. Chem. Phys. 119, 4934 (2003)

**Title:** Insights into the electronic dynamics in chemical reactions

**Researchers:** D. Aktah*
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***Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

**Description:**

We study with an ab initio molecular dynamics method the bond-breaking and bond-forming processes in chemical reactions. To obtain reactive trajectories, we use a newly developed method based on the optimization of a suitably defined action. The Hellmann-Feynman forces, which are needed to optimize the action, are calculated within density-functional theory. We contrast a concerted [4+2] cycloaddition of cyclopentadiene and ethylene with the nonconcerted [2+2] cycloaddition of two ethylene molecules. We find that the duration of the bond-breaking and bond-forming processes due to the nuclear motion is ~100 fs. Moreover the electronic delocalization, as well as the HOMO-LUMO energy gap during the two reactions, allows us to distinguish clearly between the concerted and the nonconcerted mechanism.

**References:** J. Phys. Chem. A, 108, 848 (2004)

**Title:** Hydrogen bond driven chemical reactions: Beckmann rearrangement of cyclohexanone oxime into ε-caprolactam in supercritical water

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Division of Frontier Research, Creative Research Initiative "Sousei", Hokkaido University, Kita 21, Nishi 10, Kita-ku, Sapporo 001-0021, Japan

**Description:**

Recent experiments have shown that supercritical water (SCW) has the ability to accelerate and make selective synthetic organic reactions, thus replacing the common but environmentally harmful acid and basic catalysts. In an attempt to understand the intimate mechanism behind this observation, we analyze, via first-principles molecular dynamics, the Beckmann rearrangement of cyclohexanone oxime into ε-caprolactam in supercritical water, for which accurate experimental evidence has been reported. Differences in the wetting of the hydrophilic parts of the solute, enhanced by SCW, and the disrupted hydrogen bond network are shown to be crucial in triggering the reaction and in making it selective. Furthermore, the enhanced concentrations of $H^+$ in SCW play an important role in starting the reaction.

**References:** J. Am. Chem. Soc., 126, 6280 (2004)

**Title:** Proton transfer in heterocycle crystals

**Researchers:** Marcella Iannuzzi*
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**Description:**

We study the proton diffusion process in imidazole-based molecular crystals, which are new candidate materials for fuel cell membranes. These materials are characterized by hydrogen bonded networks of molecules, which provide viable routes for the long-range diffusion of protons. By the application of a recently developed, powerful technique to determine reaction pathways in complex systems, we are able to reproduce the diffusion process in the imidazole crystal and in the more complicated and rigid structure of imidazole 2-ethyleneoxide. Our results cast new light on the atomistic details of the molecular rearrangements sustaining the ionic diffusion.

**References:** Phys. Rev. Lett. 93, 025901 (2004)

**Title:** Polyamorphism of ice at low temperatures from constant-pressure simulations

**Researchers:** Roman Martonak
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**Institute/ Group:** Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

**Description:**

We report results of molecular dynamics simulations of amorphous ice in the pressure range 0– 22.5 kbar. The high-density amorphous (HDA) ice prepared by compression of $I_h$ ice at $T$ = 80 K is annealed to $T$ = 170 K at intermediate pressures in order to generate relaxed states. We confirm the existence of recently observed phenomena, the very high-density amorphous ice, and a continuum of HDA forms. We suggest that both phenomena have their origin in the evolution of the network topology of the annealed HDA phase with decreasing volume, resulting at low temperatures in the metastability of a range of densities.

**Referneces:** Phys. Rev. Lett. 92, 225702 (2004)

**Title:** Dispersion corrections to density functionals for water aromatic interactions

**Researchers:** Urs Zimmerli*
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Petros Koumoutsakos*

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**Description:**

We investigate recently published methods for extending density functional theory to the description of long-range dispersive interactions. In all schemes an empirical correction consisting of a $C_6 r^{-6}$ term is introduced that is damped at short range. The coefficient $C_6$ is calculated either from average molecular or atomic polarizabilities. We calculate geometry-dependent interaction energy profiles for the water benzene cluster and compare the results with second-order Møller–Plesset calculations. Our results indicate that the use of the B3LYP functional in combination with an appropriate mixing rule and damping function is recommended for the interaction of water with aromatics.

**References:** J. Chem. Phys. 120, 2693 (2004)

**Title:** Effective force fields for condensed phasesystems from abinitio moleculardynamics simulation: A new method for force-machting

**Researchers:** Sergei Izvekov*
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**Description:**

A novel least-squares fitting approach is presented to obtain classical force fields from trajectory and force databases produced by *ab initio* (e.g., Car–Parrinello) molecular dynamics (MD) simulations. The method was applied to derive effective nonpolarizable three-site force fields for liquid water at ambient conditions from Car–Parrinello MD simulations in the Becke–Lee–Yang–Parr approximation to the electronic density functional theory. The force-matching procedure includes a fit of short-ranged nonbonded forces, bonded forces, and atomic partial charges. The various parameterizations of the water force field differ by an enforced smooth cut-off applied to the short-ranged interaction term. These were obtained by fitting to the trajectory and force data produced by Car–Parrinello MD simulations of systems of 32 and 64 $H_2O$ molecules. The new water force fields were developed assuming both flexible or rigid molecular geometry. The simulated structural and self-diffusion properties of liquid water using the fitted force fields are in close agreement with those observed in the underlying Car–Parrinello MD simulations. The resulting empirical models compare to experiment much better than many conventional simple point charge (SPC) models. The fitted potential is also shown to combine well with more sophisticated intramolecular potentials. Importantly, the computational cost of the new models is comparable to that for SPC-like potentials.

**References:** J. Chem. Phys. 120, 10896 (2004)

**Title:** Liquid Water from First Principles: Investigation of Different Sampling Approaches

**Researchers:** I-Feng W. Kuo, Christopher J. Mundy, Matthew J. McGrath, J. Ilja Siepmann Joost VandeVondele, Michiel Sprik, Jürg Hutter, Bin Chen, Michael L. Klein, Fawzi Mohamed, Matthias Krack, Michele Parrinello

**Institute/ Group:** Chemistry and Materials Science Directorate, Lawrence Livermore National Laboratory, Livermore, California 94550; Departments of Chemistry and of Chemical Engineering and Material Science, University of Minnesota, 207 Pleasant Street SE, Minneapolis, Minnesota 55455-0431; Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, United Kingdom; Physical Chemistry Institute, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich, Switzerland; Department of Chemistry, Louisiana State University, Baton Rouge, Louisiana 70803-1804; Center for Molecular Modeling and Department of Chemistry, University of Pennsylvania, 231 South 34th Street, Philadelphia, Pennsylvania 19104-6323; Laboratory of Physical Chemistry, ETH Zurich, USI-Campus, Via Giuseppe Buffi 13, 6904 Lugano, Switzerland

**Description:**

A series of first principles molecular dynamics and Monte Carlo simulations were carried out for liquid water to investigate the reproducibility of different sampling approaches. These simulations include Car-Parrinello molecular dynamics simulations using the program CPMD with different values of the fictitious electron mass in the microcanonical and canonical ensembles, Born-Oppenheimer molecular dynamics using the programs CPMD and CP2K in the microcanonical ensemble, and Metropolis Monte Carlo using CP2K in the canonical ensemble. With the exception of one simulation for 128 water molecules, all other simulations were carried out for systems consisting of 64 molecules. Although the simulations yield somewhat fortuitous agreement in structural properties, analysis of other properties demonstrate that one should exercise caution when assuming the reproducibility of Car-Parrinello and Born-Oppenheimer molecular dynamics simulations for small system sizes in the microcanonical ensemble. In contrast, the molecular dynamics and Monte Carlo simulations in the canonical ensemble appear to be more reliable**.** Furthermore, in the case of canonical Car-Parrinello molecular dynamics simulations the application of Nosé-Hoover chain thermostats allows the use of larger fictitious electron masses. For the Becke-Lee-Yang-Parr exchange and correlation energy functionals and norm-conserving Troullier-Martins or Goedecker-Teter-Hutter pseudopotentials, these simulations at a fixed density of 1.0 g/cm3 and a temperature close to 315 K point to an overstructured liquid with a height of the first peak in the oxygen-oxygen radial distribution function of about 3.0, an underestimated value of the classical constant-volume heat capacity of about70 J/(mol K), and an underestimated self-diffusion constant of about 0.04 Å2/ps.

**References:** J. Phys. Chem. B, 108 (34), 12990-12998, (2004)

**Title:** Ab initio study of dehydroxylation – cabonation reaction on brucite surface

**Researchers:** S. V. Churakov*
Marcella Iannuzzi*
Michele Parrinello**

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**Description:**

The possibility of forming magnesite from brucite crystallites, in a $CO_2$-rich environment, has attracted large interest as a possible industrial procedure to store $CO_2$ in the form of carbonate minerals. The reaction mechanisms responsible for such processes are, however, not very well-known. In this work we first consider the compatibility of the magnesite and brucite structures, along specific crystallographic directions. In the second part we describe the sequence of events that leads to the formation of a magnesite layer, via the dehydroxylation of brucite and consequent adsorption and diffusion of carbon complexes. To observe these thermally activated events, we employ a method recently developed in our group[1,2] for finding complex reaction pathways and reproducing the related free energy surface. We find that the $(1\bar{1}00)$ brucite surface can be dehydroxylated quite easily. The formation of vacancies in the hydroxyl layers might favor the diffusion of OH and protons through the channels between two neighboring (0001) OH planes, which characterize the brucite structure. This mechanism creates the necessary conditions for further dehydroxylation and formation of magnesite layers.

**References:** J. Phys. Chem. B 108, 11567, (2004)

**Title:** Reconstructing the density of states by history-dependent metadynamics

**Researchers:** C. Micheletti*
Alessandro Laio**
Michele Parrinello**

**Institute/ Group:** * International School for Advanced Studies (SISSA) and INFM, Via Beirut 2-4, 34014 Trieste, Italy
**Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi13, Lugano, Switzerland

**Description:**

We present a novel method for the calculation of the energy density of states $D(E)$ for systems described by classical statistical mechanics. The method builds on an extension of a recently proposed strategy that allows the free-energy profile of a canonical system to be recovered within a preassigned accuracy [A. Laio and M. Parrinello, Proc. Natl. Acad. Sci. U.S.A. **99**, 12562 (2002)]. The method allows a good control over the error on the recovered system entropy. This fact is exploited to obtain $D(E)$ more efficiently by combining measurements at different temperatures. The accuracy and efficiency of the method are tested for the two-dimensional Ising model (up to size 50×50) by comparison with both exact results and previous studies. This method is a general one and should be applicable to more realistic model systems.

**References:** Phys. Rev. Lett. 92 (17), 170601 (2004)

**Title:** Microscopic Mechanism of antibiotics translocation through a porin

**Researchers:** Matteo Ceccarelli*
Christophe Danelon**
Alessandro Laio*
Michele Parrinello*

**Institute/ Group:** *Computational Science, Department of Chemistry and Applied Biosciences, ETH Zurich, USI Campus, Lugano, Switzerland
**Institut Pharmacologie et Biologie Structurale, 31077 Toulouse, France

**Description:**

OmpF from the outer membrane of *Escherichia coli* is a general porin considered to be the main pathway for *ß*-lactam antibiotics. The availability of a high-resolution crystal structure of OmpF and new experimental techniques at the single-molecule level have opened the way to the investigation of the microscopic mechanisms that allow the passage of antibiotics through bacterial pores. We applied molecular dynamics simulations to investigate the translocation process of ampicillin (Amp) through OmpF. Using a recent algorithm capable of accelerating molecular dynamics simulations we have been able to obtain a reaction path for the translocation of Amp through OmpF. The mechanism of passage depends both on the internal degrees of freedom of Amp and on interactions of Amp with OmpF. Understanding this mechanism would help us design more efficient antibiotics and shed light on nature's way of devising channels able to enhance the transport of molecules through membranes.

**References**: Biophysical Journal, 87, 58-64 (2004)

**Title:** Correlations among hydrogen bonds in liquid water

**Researchers:** Paolo Raiteri
Alesandro Laio
Michele Parrinello

**Institute/ Group:** Computational Science, Department of Chemistry and Applied Biosciences
ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

**Description:**

By performing computer simulations of water with the TIP5P potential we show that structures formed by two or more hydrogen bonds affect the dynamical and static properties of water, especially in the vicinity of freezing temperature. In particular, the short time correlation between two coupled hydrogen bonds cannot be predicted assuming the statistical independence of the single hydrogen bonds. This introduces an additional relaxation time of ~9 ps close to the freezing point. We also find that the time persistence of structures formed by several hydrogen bonds (the first solvation shell) correlates with the local density, which is smaller around water molecules with a long-living environment.

**References:** Phys. Rev. Lett. 93 (8), 87801 (2004)

**Title:** Reactivity of Osmium Tetraoxide Toward Nitrogen Heterocycles. Implications for the Molecular Recognition of DNA Mismatch

**Researchers:** Dirk V. Deubel

**Institute/ Group:** Computational Science, Department of Chemistry and Applied Biosciences
ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland
and Academia Sinica, Taipei, Taiwan, R.O.C.

**Description:**

The transition structures and activation energies for the [3+2] addition of osmium tetraoxide across the C=C bond of N-containing heterocycles were predicted and rationalized using density functional theory. A "genealogical tree" of 20 substrates from ethylene to 1-methyl-protected pyrimidines and 9-methyl-protected purines was designed to study systematically the effects of endocyclic substitution, exocyclic substitution, and the loss of aromaticity upon cyclization and ring fusion. An initial screening was performed by calculating the energies of hydrogenation at the C=C double bond in all model substrates. Based upon this evaluation, promising N-heterocyclic targets of osmium tetraoxide were selected for an investigation of the kinetic reaction profile of the metalla-analogous cycloadditions. In contrast to considerable differences in the thermodynamics of the osmylation of pyrimidine derivatives, similar activation energies between 15 and 17 kcal/mol were predicted for the [3+2] addition of osmium tetraoxide across the C5=C6 bonds of 1-methylthymine, 1-methyluracile, and 1-methylcytosine. Interestingly, the reaction with the rare N4-imino tautomer of 1-methylcytosine shows the smallest activation energy. The analysis of donor-acceptor interactions between substrate and metal oxide in the transition states elucidates the asynchronous formation of the two C-O bonds upon the metal-oxide addition to pyrimidines and reveals that osmium tetraoxide is either an electrophilic or a nucleophilic oxidant, depending on substrate. The results of this study contribute to the rationalization of bioanalytical methods that use the heavy-metal oxide, in particular the molecular recognition and cleavage of DNA mismatch.

**References**: Angew. Chem., 115, 2019-2022 (2003); Angew. Chem. Int. Ed., 42, 1974-1977 (2003)

**Title:** The Surprising Nitrogen-Analogue Chemistry of the Methyltrioxorhenium-Catalyzed Olefin Epoxidation

**Researchers:** Dirk V. Deubel

**Institute/ Group:** Computational Science, Department of Chemistry and Applied Biosciences
ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

**Description:**

Density functional theory calculations at the B3LYP level have been carried out to investigate the mechanism of the reaction of ethylene with $[Re(O)_2(O\text{-}NH)Me]$, a formal hydroxylamine derivative of the industrial epoxidation catalyst methyltrioxorhenium(VII) (MTO). A variety of reaction pathways has been considered, including the concerted heteroatom-transfer mechanism postulated by Sharpless and the stepwise mechanism via a five-membered "organometallacycle" postulated by Mimoun. Ethylene has been found not to coordinate directly at the metal. The calculations reveal similar activation free enthalpies for the concerted nitrene transfer event (aziridination) and for the formation of an organometallic rhena-2,3-oxazolidine via [2+2] addition of ethylene across the Re-N bond of the metallaoxaziridine moiety. The fragmentation of the organometallacycle is faster than its formation and gives ethylideneazane rather than aziridine. An additional pathway has a lower activation free enthalpy and leads to a rhena-3,2-oxazolidine. The formation of this organometallacycle proceeds via an intermediate ring-opening product, $[Re(O)_2(\square^1\text{-}O\text{-}NH)Me]$, which undergoes [3+2] cycloaddition across the C=C bond of ethylene. Analysis of its electronic structure reveals that the $\square^1$ species should be considered a metalla-analog nitrosonium ylide rather than a metalla-analog imine oxide. Fragmentation of the rhena-3,2-oxazolidine liberates acetaldehyde. The discovery of favorable pathways leading to organometallacycles upon reaction of C=C bonds with $[Re(O)_2(O\text{-}NH)Me]$ stands in sharp contrast to the strong preference of the concerted mechanism in the olefin epoxidation with rhenium peroxo complexes. The calculations show the multiple mechanisms to be distinguishable by four different products, calling for further experimental studies. The successful search for the five-membered organometallacycles parallels the computational prediction of four-membered organometallacycles derived from d0 metal oxo complexes (*Acc. Chem. Res.* 2003, *36*, 645) and the indirect observation of metalla-2-oxetanes in recent gas-phase experiments (*Angew. Chem 2003, 115, 3928).*

**References**: J. Am. Chem. Soc., 125, 15308-15309, (2003)

**Title:** AM/MM Car-Parrinello molecular dynamics study of the solvent effects on the ground state and on the first excited single state of acetone in water

**Researchers:** Ute F. Röhring*
Irmgard Frank**
Jürg Hutter***
Alessandro Laio*
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***Institute of Physical Chemistry, University of Zurich, 8057 Zurich, Switzerland
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**Description:**

We present a hybrid Car-Parrinello quantum mechanical/molecular mechanical (QM/MM) approach that is capable of treating the dynamics of molecular systems in electronically excited states in complex environments. The potential energy surface in the excited state is described either within the restricted open-shell Kohn-Sham (ROKS) formalism or within time-dependent density functional theory (TDDFT). As a test case, we apply this technique to the study of the solvent effects on the ground state and on the first excited singlet state of acetone in water. Our results demonstrate that for this system a purely classical description of the solvent is sufficient, since inclusion of the first solvent shell of 12 water molecules into the quantum system does not show a significant effect on this transition. The excited-state energies calculated with ROKS are red shifted by a constant value compared to the TDDFT results, while the relative variations of the excitation energy for different configurations are in very good agreement. The experimentally observed blue shift of the excitation energy in going from gas phase to condensed phase is well reproduced. Excited-state dynamics carried out with ROKS yield the relaxation of the solute and the rearrangement of the solvent structure on a picosecond timescale. The calculated Stokes shift is in reasonable agreement with experimental data.

**References**: Chem. Phys. Chem., 4 (11), 1177-1182 (2003)

**Title:** Reaction mechanism of caspases: Insights from QM/MM Car-Parrinello Simulations

**Researchers:** M Sulpizi
Alessandro Laio
Joost Vande Vondele
A Cattaneo
Ursula Röthlisberger
Paolo Carloni

**Institute/ Group:**

**Description:**

**References**: Proteins-Structure Function and Genetics, 52 (2), 212-224 (2003)

**Title:** Road Maps for Nitrogen Transfer Catalysis. The Challenge of the Osmium(VIII)-Catalyzed Diamination

**Researchers:** Dirk V. Deubel*
Kilian Muñiz**

**Institute/ Group:** *Computational Science, Department of Chemistry and Applied Biosciences ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland
**Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität, D-53121 Bonn, Germany

**Description:**

Although the Sharpless dihydroxylation has been used on laboratory and industrial scales for several decades, an analogous osmium-catalyzed diamination is unknown. To explore the reaction of osmium(VIII) oxo-imido complexes with C=C bonds, density functional calculations have been performed. The calculations predict a chemoselective and perispecific 3+[2] addition of the NH=Os=NH moiety of diimidodioxoosmium(VIII) to ethylene, yielding dioxoosma-2,5-diazolidine. From first sight, this metallacycle seems extremely stable, more stable than diimidoosma-2,5-dioxolane by 40 kcal/mol. However, a comparison of the thermodynamic reaction profiles for catalytic model cycles of dihydroxylation, aminohydroxylation, and diamination reveals that, contrary to common belief, the instability of the metal=N bond in the osmium(VIII) imido complex rather than the stability of the metal-N bond in the osmium(VI) intermediate causes most of the energy difference between the metallacycles. Substituents on the substrate have a small effect on the thermodynamic reaction profiles, whereas substituents on the imido ligands allow for a steric and electronic control of the reaction free enthalpies in the range of up to 25 kcal/mol. The results of this study help identify potential challenges in the development of the as-yet hypothetical title reaction and provide a modular concept for exploring novel catalytic routes.

**References**: Chem. Eur. J., 10, 2475-2486 (2004)

**Title:** From Evolution to Green Chemistry: Rationalization of Biomimetic Oxygen-Transfer Cascades

**Researchers:** Dirk V. Deubel

**Institute/ Group:** Computational Science, Department of Chemistry and Applied Biosciences
ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

**Description:**

Thermodynamic electron-transfer potentials from biology textbooks elucidate the sequence of electron-transfer events in the respiratory chain in mitochondria. In this study, thermodynamic and kinetic oxygen-transfer potentials have been defined and predicted for oxidants and substrates using density functional theory, aiming to rationalize multiple oxygen-transfer events in chemical catalysis, particularly in current developments of the Sharpless dihydroxylation. Key transition states for competing mechanisms in a recent dihydroxylation method containing the olefin, osmium tetraoxide, methyltrioxorhenium(VII), a chiral tertiary amine, and the green terminal oxidant hydrogen peroxide have been investigated rigorously. The calculations show the amine to function as an oxygen-transfer mediator between rhenium peroxides and osma-2,5-dioxolanes, in addition to its role as a carrier of chiral information. Unique mechanistic and stereoelectronic patterns in this oxygen-transfer cascade explain the unexpected failure of reactivity predictions using simpler models such as Marcus theory.

**References:** J. Am. Chem. Soc. 2004, 126, 996-997

**Title:** Factors Governing the Kinetic Competition of Nitrogen and Sulfur Ligands in Cisplatin Binding to Biological Targets

**Researchers:** Dirk V. Deubel

**Institute/ Group:** Computational Science, Department of Chemistry and Applied Biosciences, ETH Zürich, USI Campus, 6900 Lugano, Switzerland

**Description:**

The kinetic competition of sulfur and nitrogen nucleophiles L in the substitution reactions of cisplatin derivatives, *cis*-$[Pt^{II}(NH_3)_2(X)(OH_2)]^{n+}$ + L --> *cis*-$[Pt^{II}(NH_3)_2(X)(L)]^{m+}$ + $H_2O$ (X = $Cl^-$, $H_2O$), has been studied using density functional theory and continuum dielectric calculations. The calculations reveal an intrinsic kinetic preference of platinum(II) for nitrogen over sulfur ligands. However, biologically relevant substituents can mask this preference for nitrogen nucleophiles. Investigation of the activation free energies of the substitution reactions in dependence of the dielectric constant (epsilon) demonstrates the microenvironment to be crucial in the binding of cisplatin to its intracellular targets. The fused aromatic heterocycle of guanine stabilizes the transition state for platination at a smaller (epsilon) more efficiently than do the functional groups of amino acid residues. The results of this work suggest a relatively facile platination of guanine-N7 sites of DNA in regions of low (epsilon), particularly in the proximity of histone cores.

**References:** J. Am. Chem. Soc., 126, 5999-6004 (2004)

**Title:** A Variational Definition of Electrostatic Potential Derived Charges

**Researchers:** Alessandro Laio*
Francesco Luigi Gervasio*
Joost VandeVondele**
Marialore Sul pizi***
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*** LCBC, EPFL Lausanne, Switzerland

**Description:**

In a recent work [Laio, A., VandeVondele, J., Rothlisberger, U. *J. Phys. Chem. B* **2002** *106*, 7300] a novel method has been proposed to define dynamical electrostatic potential derived (D-RESP) charges for systems described within a quantum mechanics/molecular mechanics (QM/MM) scheme. Here, we derive the analytic dependence of these charges on the quantum charge density and on the atomic positions. This *variational* property can be exploited for defining interaction potentials between the quantum and the classical subsystems that depend explicitly on the value of the D-RESP charges. Such potentials can be used for a multitude of different purposes, such as improving the computational efficiency of the electrostatic coupling between the QM and the MM subsystems and for defining a QM/MM analogue of the exclusion schemes commonly used in classical biomolecular force fields.

**References:** J. of Phys. Chem. B, 108 (23), 7963-7968 (2004)

**Title:** Constant pressure reactive molecular dynamics simulations of phase transitions under pressure: The graphite to diamond conversion revisited

**Researchers:** F. Zipoli*
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**Computational Science, Department of Chemistry and Applied Biosciences, ETH Zurich, USI Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland

**Description:**

We have introduced a new technique for constant-pressure molecular dynamics by combining the idea behind the Parrinello-Rahman scheme and the method by Iannuzzi, Laio and Parrinello [Phys. Rev. Lett. 90, 238302 (2003)], recently devised to deal with rare events. The new scheme is suitably devised to describe solid-solid phase transitions for which the primary order parameter is not the cell shape, but some internal structural coordinate. The method has been demonstrated by simulating the conversion of graphite into diamond at high pressure within a tight-binding model.

**References:** The European Physical Journal B, 39, 41, (2004)

**Title:** Evolution of the Ge/Si(001) wetting layer during Si overgrowth and crossover between thermodynamic and kinetic behavior

**Researchers:** D.B. Migas*
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***INFM and L-NESS, Dipartimento di Fisica, Politecnico di Milano, Polo Regionale di Como, Via Anzani 52, I-22100 Como, Italy

**Description:**

By comparing the scanning tunnel microscope images of the morphological evolution in Ge/Si(001) during Si overgrowth with the results of classical molecular-dynamic simulation and *ab initio* calculations for Si distribution in the wetting layer, we conclude that the disappearance of the ($M\times N$) reconstruction is determined by Si-Ge intermixing in the third and fourth layers in the Ge wetting layer. The subsequent evolution of the ($2\times N$) pattern, where $N$ increases with further Si deposition, is shown to be produced by Si-Ge intermixing in the second layer. We suggest that this process corresponds to a crossover between thermodynamic behavior and kinetic behavior, which eventually leads to the Si capping.

**References:** Phys. Rev. B, 69 (23), 235318, (2004)

**Title:** Olefin Epoxidation with Inorganic Peroxides. Solutions to Four Long-Standing Controversies on the Mechanism of Oxygen Transfer

**Researchers:** Dirk V. Deubel*
Gernot Frenking**
Philip Gisdakis***
Wolfgang A. Herrmann***
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Jörg Sundermeyer**

**Institute/ Group:** *Computational Science, Department of Chemistry and Applied Biosciences, ETH Zürich, USI-Campus, Via Giuseppe Buffi 13, 6900 Lugano, Switzerland
**Department of Chemistry, Philipps Universität Marburg, 35032 Marburg, Germany
***Department of Chemistry, Technische Universität München, 85748 Garching, Germany

**Description:**

Four controversies on the mechanism of the olefin epoxidation with Mimoun-type complexes, $[MoO(O_2)_2(OPR_3)]$, Herrmann-type complexes, $[ReO(O_2)_2Me]$, and related inorganic peroxides have inspired industrial and academic researchers in the last three decades: First, is the oxygen transfer from the peroxo complex to the olefin concerted or stepwise? Second, does the oxidant act as an electrophile or a nucleophile? Third, is the mechanism of the stoichiometric reaction also valid for catalytic protocols? Fourth, how can stereochemical information be transferred between oxidant and substrate? In this Account, we discuss answers to the long-standing questions, focusing on recent contributions from quantum chemical calculations.

**References:** Acc. Chem. Res. 2004, 37, 645-652.

**Title:** The influence of temperature and density functional models in ab initio molecular dynamics simulation of liquid water

**Researchers:** Joost VandeVondele*
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Matthias Krack**
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**Description:**

Application in an ab initio molecular dynamics study of liquid water is a crucial test of density functional theory methods for the modeling of condensed aqueous systems. In order to assess the reliability of these tests, the effect of temperature on the structure and dynamics of liquid water has been characterized with 16 simulations of 20 ps in the temperature range of 280K to 380K. We find a pronounced influence of temperature on the pair correlation functions and on the diffusion constant including non-ergodic behaviour on the time scale of the simulation in the lower temperature range (which includes ambient temperature). These observations were taken into account in a consistent comparison of a series of density functionals (BLYP, PBE, TPSS, OLYP, HCTH120, HCTH407). All simulations were carried out using a new ab initio molecular dynamics approach in which wave functions are represented using Gaussians with a plane wave basis as auxiliary basis to expand the density. Whereas the first three functionals show similar behaviour, it is found that the latter three functionals yield more diffusive dynamics and less structure.

**References:** Preprint submitted to Jornal of Chemical Physics, June 2004

**Title:** Automatic tests of the compatibility of 1D and 2D NMR spectra and chemical structures

**Researchers:** Lóránt Bódis
Ernö Pretsch

**Institute/ Group:** Laboratory of Organic Chemistry
Group of Prof. E. Pretsch
In cooperation with
Dr. H. Senn, F. Hoffmann-La Roche Ltd.
Dr. P Portmann, Upstream Solutions, Zürich

**Description:**

Today, different one- and two-dimensional NMR spectra can be automatically recorded with such a high rate that more and more, their interpretation has become a bottle-neck. In this project, we make use of our $^{1}H$ and $^{13}C$ NMR spectra prediction programs to estimate the corresponding 1D and 2D NMR spectra. Various strategies of comparing the measured and predicted spectra are being developed and tested. They are optimized for detecting both structure incompatibilities and the presence of impurities.

**Title:** Modeling, Analysis and Numerics of Ferromagnetism

**Researcher:** Andreas Prohl

**Institute:** Seminar for Applied Mathematics
ETH Zürich

**Description:** Micromagnetics is a continuum variational theory describing magnetization pattern in ferromagnetic media. Its multiscale nature due to different inherent spatio-temporal physical and geometric scales, together with nonlocal phenomena and a nonconvex side-constraint leads to a rich behavior and pattern formation. This variety of effects is also the reason for severe problems in analysis, model validation and reductions, and numerics, which are only accessed recently.

**References:**

[1] M. Kruzik and A. Prohl, *Recent Delopments in Modeling, Analysis and Numerics of Ferromagnetism*, SIAM Reviews (2004), submitted.

**Title:** The NH and ND stretching fundamentals of $^{14}ND_2H$

**Researchers**: M. Snels**
H. Hollenstein*
M. Quack*

**Institute/Group:** * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Istituto di Fisica dell' Atmosfera, Area di Ricerca di Roma Tor Vergata

**Description:**

High resolution (0.004 $cm^{-1}$ instrumental bandwidth) interferometric Fourier transform infrared spectra (FTIR) of $^{14}ND_2H$ were obtained on a BOMEM DA002 spectrometer under essentially Doppler limited conditions. We report the analysis of the ND and NH stretching fundamentals of $^{14}ND_2H$ with term values for the symmetric (*s*) and antisymmetric(*a*) sublevels with respect to the inversion plane of the planar geometry $T_v(s)$ = 2430.7990(7) $cm^{-1}$ and $T_v(a)$ = 2434.6222(8) $cm^{-1}$ for the $\nu_{3a}$ fundamental, $T_v(s)$ = 2559.8069(8) $cm^{-1}$ and $T_v(a)$ = 2559.9630(9) $cm^{-1}$ for the $\nu_{3b}$ fundamental and $T_v(s)$ = 3404.238(5) $cm^{-1}$ and $T_v(a)$ = 3404.316(5) $cm^{-1}$ for the $\nu_1$ fundamental. The two modes $\nu_3$ which are degenerate in $ND_3$ and whose degeneracy is lifted in $ND_2H$, are distinguished by the subscripts 3*a* or 3*b*, being symmetric (3*a*) or antisymmetric (3*b*) with respect to the $C_s$ plane of symmetry of the equilibrium geometry of $ND_2H$. Up to 20 molecular parameters of the effective S-reduced Hamiltonian could be determined accurately for each fundamental. In particular, the inversion-rotation interaction parameter could be determined for the two ND-stretching modes. Assignments were established with certainty by means of ground state combination differences. The results are important for the mode selective inhibition or catalysis of inversion at the nitrogen atom by exciting ND and NH stretching vibrations, for treatments of isotope effects on inversion of ammonia by means of effective Hamiltonians as well as true molecular Hamiltonians on high dimensional potential hypersurfaces. Extensive numerical calculations are carried out in the analysis of the experiments [1]. The results are also important in relation to quantum dynamical wavepacket calculations during and after coherent laser excitation of this molecule [2].

**References:**

[1] M. Snels, H. Hollenstein, M. Quack, J. Chem. Phys. **119**, 7893–7902 (2004)
[2] R. Marquardt, M. Quack, I. Thanopulos, D. Luckhaus, J. Chem. Phys. **118**, 643-658 (2003).

**Title:** Isotopomer-selective overtone spectroscopy of jet-cooled benzene by ionization detected IR + UV double resonance: The $N = 2$ CH-chromophore absorption of $^{12}C_6H_6$ and $^{13}C^{12}C_5H_6$ near 6000 $cm^{-1}$.

**Researchers**: M. Hippler*
R. Pfab**
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**Institute/Group:** * Group for Molecular Kinetics and Spectroscopy
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** Physical Chemistry, ETH Zürich

**Description:**

Employing our recently introduced IR+UV double-resonance scheme for obtaining mass-resolved infrared spectra, the isotopomer selected $N$=2 CH-chromophore absorption of $^{12}C_6H_6$ and $^{13}C^{12}C_5H_6$ near 6000 $cm^{-1}$ has been recorded in a supersonic jet expansion of the benzene isotopomer mixture at natural abundance. The $^{13}C^{12}C_5H_6$ spectra are the first of this kind reported in the literature. The $^{12}C_6H_6$ spectrum is compatible with a proposed model of intramolecular vibrational redistribution with a distinct hierarchy of time scales: the CH-stretching state is the IR chromophore state coupled to the IR field. With a decay time of $\tau \approx$ 100 fs, vibrational excitation is redistributed to a first tier of vibrational states, probably CH-stretching/bending combination bands coupled by strong Fermi resonances. Vibrational excitation is then further redistributed with $\tau \approx 0.35$ ps to a second tier of states, possibly by weaker higher order anharmonic resonances. The observed line widths give a lower bound for the decay time into the dense background manifold, $\tau > 1.3$ ps. Although the experimental jet spectra are in qualitative agreement with previously published calculated spectra, they clearly disagree in finer details [1,2]. The results are of importance for our understanding of intramolecular vibrational redistribution in polyatomic molecules [3,4,5,6].

**References:**

[1] M. Hippler, R. Pfab, and M. Quack, **107**, 10743 – 10752 (2003)
[2] M. Hippler, R. Pfab, and M. Quack, Proc. 18th Coll. High Resol. Mol. Spectroscopy, Dijon 2003, paper D14, p. 118
[3] M. Quack, Chimia **57**, 147-160 (2003).
[4] M. Quack, Akademie-Journal der Union der deutschen Akademien der Wissenschaften (Themenschwerpunkt Chemie), 38-44 (2003).
[5] M. Quack, Chimia **55**, 753-758 (2001).
[6] M. Quack, in *Femtosecond Chemistry, Proc. Berlin Conf. Femtosecond Chemistry*, Berlin (March 1993) (Eds.: J. Manz, L. Woeste), Verlag Chemie, Weinheim (1995), Chapter 27, 781-818.

**Title:** A global electric dipole function of ammonia and its isotopomers in the electronic ground state

**Researchers**: R. Marquardt**
M. Quack*
I. Thanopulos***
D. Luckhaus****

**Institute/Group:**
* Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Laboratoire de Chimie Théorique, Université de Marne-la-Vallée
*** University of British Columbia, Vancouver (present address)
**** Institut für Physikalische Chemie, Universität Göttingen (present address)

**Description:**

A global analytical representation of the electric dipole hypersurface for ammonia and isotopomers is developed as a function of bond lengths and bond angles. Its simple and general form allows for the simultaneous description of all three dipole moment components using a small number of parameters. The parameter values are determined by adjustment to dipole moment values obtained from *ab initio* calculations at the MP2 and MCSCF level of theory. The dipole function is used to calculate six dimensional transition moments for $NH_3$, using wave functions obtained from a variational calculation and a global analytical representation of the potential hypersurface. The comparison with experiment demonstrates a fairly reliable description of the electric dipole hypersurface for molecular structures with potential energy equivalent to up to 10000 $cm^{-1}$. At higher excitations a qualitatively correct asymptotic behavior of the dipole function is assured by construction.

**References:**

R. Marquardt, M. Quack, I. Thanopulos, D. Luckhaus, J. Chem. Phys. **119**, 10724 – 10732 (2003)

**Title:** Combined Multidimensional Anharmonic and Parity Violating Effects in CDBrClF

**Researchers**: Martin Quack*
Jürgen Stohner*, **

**Institute/Group:** * Group for Molecular Kinetics and Spectroscopy
Physical Chemistry, ETH Zürich
** Zürich University of Applied Sciences (ZHW), Institute of Chemistry and Biotechnology ICB, Winterthur

**Description:**

Parity violation causes rovibrational frequency shifts in infrared and microwave spectra between the corresponding lines of enantiomers of chiral molecules. In previous theoretical treatments of this effect simple harmonic and anharmonic adiabatic approximations were used which assumed that the vibrational potential as well as the parity violating potential are separable in normal (or local) coordinates. In the present work we investigate in detail the influence of nonseparable anharmonic couplings on vibrational frequency shifts caused by the parity violating potential in CDBrClF. We use the strongly coupled four dimensional CD- and CF-chromophore subspaces and discuss how relative frequency shifts are influenced by coupling in the pure vibrational potential as well as in the parity violating potential. A four dimensional parity violating potential energy hypersurface has been determined ab initio and fitted to a polynomial expansion. We analyse the nonseparable multidimensional representation of the parity violating potential in a chiral molecule. The effects of the multidimensional anharmonic couplings provide the dominant corrections. They are found to be about 20 % for the expectation value of the parity violating energy difference $\Delta E_{pv}$ between enantiomers (coupled $\Delta_{pv}E/hc \approx 1.76 \times 10^{-12}$ cm$^{-1}$ compared to $1.96 \times 10^{-12}$ cm$^{-1}$ uncoupled). The corrections due to anharmonic multidimensional coupling can be more than a factor of two for vibrational frequency shifts, depending on the mode considered [1,2].

**References:**

[1] M. Quack, J. Stohner, J. Chem. Phys. **119**, 11228 – 11240 (2003)
[2] J. Stohner, M. Quack, Proc. 18th Coll. High Resol. Mol. Spectroscopy, Dijon 2003, paper J13, p. 287.

**Title:** Parity violating potentials for the torsional motion of methanol and its isotopomers ($CH_3OH$, $CD_3OH$, $^{13}CD_3OH$, $CH_3OD$, $CH_3OT$, $CHD_2OH$ and CHDTOH)

**Researchers**: R. Berger**
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A. Sieben*
M. Willeke*

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

**Description:**

We present calculations on the parity conserving, and the parity violating potentials in several methanol isotopomers for the torsional motion by the newly developed methods of electroweak quantum chemistry from our group. The absolute magnitudes of the parity violating potentials for methanol are small [1] compared to $H_2O_2$ and $C_2H_4$ [2, 3], but similar to $C_2H_6$, which is explained by the high (threefold) symmetry of the torsional top in $CH_3OH$ [1] and $C_2H_6$ [2]. Chiral and achiral isotopic substitution in methanol leads to small changes only, but vibrational averaging is discussed to be important in all these cases. Simple isotopic sum rules are derived to explain and predict the relationships between parity violating potentials in various conformations and configurations of the several investigated isotopomers. The parity violating energy difference $\Delta_{pv}E = E_{pv}(R) - E_{pv}(L)$ between the enantiomers of the chiral methanol CHDTOH first synthesized by Arigoni and coworkers [4] is for two conformers about $-3.66 \cdot 10^{-17}$ ($hc$) $cm^{-1}$ and for the third one $+7.32 \cdot 10^{-17}$ ($hc$) $cm^{-1}$. Thus for $\Delta_{pv}E$ the conformation is more important than the configuration (at the equilibrium geometries without vibrational averaging). Averaging over torsional tunneling may lead to further cancellation and even smaller values.

**References:**

[1] R. Berger, M. Quack, A. Sieben, and M. Willeke, Helv. Chim. Acta, **86**, 4048–4060 (2003)
[2] A. Bakasov, T. K. Ha, and M. Quack, J. Chem. Phys. **109** (17), 7263-7285 (1998).
[3] R. Berger and M. Quack, J. Chem. Phys. **112** (7), 3148-3158 (2000).
[4] D. Arigoni, Topics in Stereochemistry, **221**, 1213 (1969); J. Lüthy, J. Retey, and D. Arigoni, Nature **221** (5187), 1213 (1969).

**Title:** Very high resolution studies of chiral molecules with a Bruker IFS 120 HR: the rovibrational spectrum of CDBrClF in the range 600–2300 $cm^{-1}$

**Researchers**: S. Albert *
K. K. Albert
M. Quack*

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

**Description:**

The infrared spectrum of the chiral molecule CDBrClF has been measured with a resolution of 0.001 $cm^{-1}$ and analysed in the $\nu_5$, $\nu_4$, $\nu_3$ and $2\nu_4$ regions. The results are discussed in relation to molecular parity violation and are analyzed with the aid of extensive numerical simulations [1].

**References:**

[1] S. Albert, K. K. Albert, M. Quack, Trends in Optics and Photonics **84**, 177–180 (2003)

**Title:** Mode-selective stereomutation tunneling as compared to parity violation in hydrogen diselenide isotopomers $^{1,2,3}H_2{}^{80}Se_2$

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

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

**Description:**

We present quantitative calculations of the mode selective stereomutation tunneling in the chiral hydrogen diselenide isotopomers $X_2Se_2$ with X = H, D, and T [1]. The torsional tunneling stereomutation dynamics were investigated with a quasi-adiabatic channel quasi-harmonic reaction path Hamiltonian approach which treats the torsional motion anharmonically in detail and all remaining coordinates as harmonic (but anharmonically coupled to the reaction coordinate). We also investigated the influence of the excitation of fundamental modes on the stereomutation dynamics and predict which modes should be promoting or inhibiting. Our stereomutation dynamics results and the influence of parity violation on these are discussed in relation to our recent investigations for the analogous molecules $H_2O_2$, HSOH, $H_2S_2$ and $Cl_2S_2$. The electronic potential energy barrier heights for the torsional motion of hydrogen diselenide are similar to those of HSOH, whereas the torsional tunneling splittings are similar to the corresponding values of HSSH. The evaluated ground state values for the torsional tunneling splittings for $D_2Se_2$ are of the same order as the parity-violating energy difference reported in a recent paper of Laerdahl and Schwerdtfeger, whereas for $T_2Se_2$ the corresponding tunneling splitting is about three orders of magnitude smaller (see also a recent review [2]).

**References:**

[1] M. Gottselig, M. Quack, and M. Willeke, Israel Journal of Chemistry, **43**, 353-363 (2003)
[2] M. Quack, Chimia **57** (4), 147-160 (2003).

**Title:** Mode-selective stereomutation tunneling and parity violation in $HOClH^+$ and $H_2Te_2$

**Researchers**: M. Gottselig
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J. Stohner
M. Willeke

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

**Description:**

We investigate the stereomutation tunneling processes in the axially chiral prototype ion $HOClH^+$ and in $H_2Te_2$ isotopomers in their relation to parity violation using quantum chemical calculations including our recently developed MC-LR approach to electroweak quantum chemistry and the quasiadiabatic channel reaction path Hamiltonian (RPH) approach. All the molecules dealt with here exhibit intermediate barriers to stereomutation (in the range from 0.1 to 0.3 eV depending on the molecule and cis- or trans-type of transition structure considered). Whereas tunneling dominates the quantum dynamics of stereomutation in all isotopomers of $HOClH^+$, the ground-state torsional tunneling splittings for hydrogen ditelluride isotopomers $D_2Te_2$, and $T_2Te_2$, are calculated to be much smaller than the parity violating energy differences $\Delta E_{pv}$ between the enantiomers of these molecules. We present a systematic investigation of the dependence of tunneling splittings upon the excitation of various vibrational modes and we identify some strongly promoting and some weakly inhibiting modes as well as essentially inactive modes. A comparison of the new results for $HOClH^+$ with our previous results for the isoelectronic HSOH shows some similarities but also some striking differences. $HOClH^+$ is predicted to have sufficient kinetic stability for a spectroscopic observation, as a barrier of more than 1 eV separates it from the more stable isomer $H_2OCl^+$. We also provide a summary comparing the whole series of axially chiral $HXYH^+$ isotopomers with X, Y = O, S, Se, Te, Cl and discuss the outlook for experiments on molecular parity violation in this series of molecular and ionic species. For the hydrogenic compounds $D_2Te_2$ is the only non-radioactive compound, in which parity violation is predicted to dominate over tunneling, similar to the chlorinated species $Cl_2S_2$, which we had investigated earlier [2].

**References:**

[1] M. Gottselig, M. Quack, and M. Willeke, Int. J. Mass Spectrometry **233**, 373-384 (2004)
[2] R. Berger, M. Gottselig, M. Quack, M. Willeke, Angew. Chem.-Int. Edit. **40**, 4195-4198 (2001).

**Title:** Global analytical potential hypersurface for large amplitude nuclear motion and reactions in methane. II. Characteristic properties of the potential and comparison to other potentials and experimental information.

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Physical Chemistry, ETH Zürich
** Lab. de Chimie Théorique, Université de Marne-la-Vallée, France

**Description:**

The global analytical potential surface for the electronic ground state of methane developed in [1] is analyzed and discussed in detail [2]. A new determination of the experimental potential surface for the CH chromophore in $CHD_3$, obtained from more recently measured line positions and integrated absorption coefficients, is also reported. The complete, nine-dimensional calculation of the vibrational ground state by diffusion quantum Monte Carlo on the fully anharmonic potential surface allows the determination of the equilibrium structure with a high level of certainty from comparison with experimental values of rotational constants for methane and isotopomers. Other results regarding properties of the anharmonic potential surface close to the equilibrium configuration are theoretical values for the vibrationally induced electric dipole moments in $CH_3D$, $CH_2D_2$, and $CHD_3$, which are obtained in conjunction with a nine-dimensional, vector-valued representation of the electric dipole moment in this molecule and agree well with the experimental data. The accuracy regarding the description of spectroscopic data [3] pertaining to highly excited vibrational states and the global character of the proposed potential surface representation render it a powerful instrument for the theoretical treatment of chemical reaction dynamics. A relation to reaction kinetics can be established through calculation of the lowest adiabatic channel on the complete nine-dimensional potential hypersurface for methane using quasiadiabatic channel quantum Monte Carlo techniques. The adiabatic channel model parameter thus derived is consistent with empirical results obtained from experiment [4].

**References:**

[1] R. Marquardt, M. Quack, J. Chem. Phys. **109**, 10628-10643 (1998).
[2] R. Marquardt, M. Quack, J. Phys. Chem. **108**, 3166–3181 (2004)
[3] M. Lewerenz, M. Quack, J. Chem. Phys. **88**, 5408-5432 (1988).
[4] M. Quack, J. Troe, in *Encyclopedia of Computational Chemistry*, Vol. 4 (Eds.: P. von Ragué Schleyer, N. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, H. F. I. Schaefer, P. R. Schreiner), John Wiley & Sons (1998), 2708-2726.

**Title:** Rovibrational analysis of the $\nu_4$ and $\nu_5 + \nu_9$ of $CHCl_2F$

**Researchers**: S. Albert
K. K. Albert
M. Quack

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

**Description:**

The infrared spectrum of $CHCl_2F$ has been measured with a new, very high resolution Fourier transform infrared spectrometer, the Bruker IFS 120 HR Zurich Prototype (ZP) 2001. The spectrum was recorded with a resolution of 0.0007 $cm^{-1}$ in the range 600–2300 $cm^{-1}$ at room temperature. The assignment of the rovibrational transitions has been carried out with the Giessen interactive Loomis-Wood program developed by Winnewisser et al. and the least squares adjustment has been performed with the Zurich WANG program [2]. The spectrum has been analyzed in the $\nu_4$ region of $CH^{35}Cl_2F$ (744.474 $cm^{-1}$) and the $\nu_5 + \nu_9$ regions of $CH^{35}Cl_2F$ (829.084 $cm^{-1}$) and $CH^{35}Cl^{37}ClF$ (825.027 $cm^{-1}$) using an effective Hamiltonian. Both bands are important to understand the absorption behavior of the fluorochlorohydrocarbon $CHCl_2F$, important in the context of atmospheric pollution as well as in laser chemistry. Local perturbations have been identified in both bands. The results are discussed in relation to molecular parity violation in the case of the chiral isotopomer $CH^{35}Cl^{37}ClF$ and are analyzed by means of extensive numerical simulations.

**References:**

[1] S. Albert, K. K. Albert, and M. Quack, J. Mol. Struct. **695-696**, 385–394 (2004)
[2] D. Luckhaus, M. Quack, Mol. Phys. **68**, 745-758 (1989).

**Title:** Ab initio calculation of parity violating potential energy hypersurfaces of chiral molecules

**Researchers**: A. Bakasov*
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** Chemistry Department, Technical University Berlin (present address)

**Description:**

We introduce the explicit concept of parity violating potential energy hypersurfaces, which govern the rotation-vibration tunneling dynamics as well as the time dependent parity violation in chiral molecules. Calculations are reported for sections of the hypersurfaces of $H_2O_2$ and $H_2S_2$ at various levels of electroweak quantum chemistry, including CIS-RHF, CIS-LR, and CASSCF-LR [1]. Important findings concern the observed increase of the parity violating potentials ($E_{pv}$) with increasing bond lengths $r_{OO}$ and $r_{ss}$, the confirmation of lines and surfaces of "accidentally" zero $E_{pv}$ at chiral geometries and the absence of a precise, simple scaling law for observables such as the measurable parity violating energy difference between enantiomers $\Delta E_{pv}$. The latter is due to the complicated geometry dependent $E_{pv}$, although a rough scaling on the order of $Z^{(5\pm1)}$ with nuclear charges of the two heavy centers can be confirmed. The results are discussed in relation to possible experiments on molecular parity violation and in relation to earlier results using various theoretical techniques [2–5].

**References:**

[1] A. Bakasov, R. Berger, T. K. Ha, M. Quack, Int. J. Quantum Chem. **99**, 393-407 (2004)
[2] A. Bakasov, T. K. Ha, and M. Quack, in *Chemical Evolution, Physics of the Origin and Evolution of Life, Proc. of the 4th Trieste Conference (1995)*, edited by J. Chela-Flores and F. Raulin (Kluwer Academic Publishers, Dordrecht, 1996), 287-296.
[3] A. Bakasov, T. K. Ha, and M. Quack, J. Chem. Phys. **109** (17), 7263-7285 (1998).
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[5] R. Berger and M. Quack, J. Chem. Phys. **112** (7), 3148-3158 (2000).

**Title:** Femtosecond Intramolecular Dynamics After Near-IR Excitation of $CH_3I$, $C_2H_5I$, $CF_3CHFI$, and $C_7H_8$ Molecules in the Gas Phase and in Solution.

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Physical Chemistry, ETH Zürich
** State Optical Institute, St. Petersburg

**Description:**

The rapid flow of vibrational energy within a molecule is central for reaction control and for the theory of unimolecular reactions. It defines the lifetime of vibrationally excited states and thus the time during which a specific vibrational excitation can control the outcome of chemical reactions [1]. Times for intramolecular vibrational energy redistribution (IVR) [2,3] can be deduced either indirectly from time-independent high resolution infrared(IR) spectra or measured directly in kinetic pump-probe experiments. We have applied delayed ultraviolet(UV) absorption spectroscopy with a time resolution of 150 fs to measure intramolecular vibrational energy redistribution after near-IR excitation of the CH-stretching vibration around 5900 $cm^{-1}$ in $CF_3CHFI$, $CH_3I$, $C_2H_5I$, and $C_7H_8$. Intramolecular relaxation time $\tau_{IVR}$ between 3 and 7 ps have been found in the gas phase. For $CH_3I$ an additional short time of 250 fs has been measured. In the liquid phase IVR is followed by a fast collisional energy transfer of the excitation energy to the solvent molecules. Assuming a two step kinetic mechanism intermolecular relaxation times $\tau_{Transfer}$ between 10 and 30 ps have been determined.

**References:**

[1] V. Krylov, M. Nikitchenko, M. Quack, and G. Seyfang, Proc. SPIE Vol. 5337, pages 178-189 (Nonlinear Frequency Generation and Conversion: Materials, Devices and Applications III, ed. by K. L. Schepler and D. D. Lowenthal, SPIE, Bellingham, WA, 2004)
[2] M. Quack, in *Femtosecond Chemistry, Proc. Berlin Conf. Femtosecond Chemistry, Berlin (March 1993)* (Eds.: J. Manz, L. Woeste), Verlag Chemie, Weinheim **(**1995**)**, Chapter 27, 781-818.
[3] M. Quack, Chimia **55**, 753-758 (2001).

**Title:** Doppler-limited FTIR spectrum of the $\nu_3(a')$/ $\nu_8(a'')$ Coriolis resonance dyad of $CHClF_2$: Analysis and comparison with ab initio calculations

**Researchers**: S. Albert
H. Hollenstein
M. Quack
M. Willeke

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

**Description:**

The Doppler-limited FTIR spectrum of the band system in the region 1070–1170 $cm^{-1}$ (Doppler width ≈ 0.0015 $cm^{-1}$, FWHM) was measured with our new Bruker IFS 120 HR Zürich prototype (ZP2001) spectrometer. This instrument allows for an unapodized resolution of 0.0007 $cm^{-1}$ (FWHM). Up to now, this is the highest resolution realized by a commercial FTIR spectrometer system. It allows a high resolution analysis of the room temperature spectra of the strongly coupled modes $\nu_3(a')$ and $\nu_8(a'')$, corresponding to the symmetric and antisymmetric CF-stretching vibrations, including also further couplings not analyzed previously. The present analysis is based on effective rotational Hamiltonians for the $v_3 = 1$ and $v_8 = 1$ states including all terms up to sextic, and involves the full first order Coriolis interaction operator. The final analysis involves both chlorine isotopomers and includes all hybrid components wich are allowed by symmetry. It results in the band centers $\nu_3^0$ = 1108.7274 $cm^{-1}$, $\nu_8^0$ = 1127.282 $cm^{-1}$, $3\nu_9^0$ = 1098.5 $cm^{-1}$ and $(\nu_6 + 2\nu_9)^0 = 1144.32$ $cm^{-1}$. The main Coriolis interaction parameters are $\xi_a^{3,8} = 0.385$ $cm^{-1}$, $\xi_c^{3,8} = -0.095$ $cm^{-1}$. In addition, smaller interactions could be determined quantitatively as well [1,2]. Our results are in essential agreement with the original analysis by Luckhaus and Quack [3], which was, however, much less complete and precise.
We report *ab initio* calculations for this molecule on the MP2 level of theory with an aug-cc-pVDZ or a aug-cc-pVTZ basis set. Various subspaces of the potential energy and electric dipole moment hypersurfaces have been calculated in reduced normal coordinates including up to three dimensions. With these hypersurfaces we determined the corresponding vibrational absorption spectra, comprising transition wavenumbers and intensities. An analysis of the vibrational levels with an effective Hamiltonian was used to derive anharmonic constants.

**References:**

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[2] S. Albert, H. Hollenstein, M. Quack, M. Willeke, Proc. 18th Coll. High Resol. Mol. Spectroscopy, Dijon 2003, p. 87
[3] D. Luckhaus, M. Quack, Mol. Phys. 68, 745-758 (1989).

**Title:** Modeling Weather and Climate on European and Alpine scales

**Researchers:** Christoph Frei, Olivier Fuhrer, Sophie Fukutome, Joachim Gurtz, Cathy Hohenegger, Jan Kleinn, Daniel Lüthi, Christoph Schär, Jürg Schmidli, Sonia Seneviratne, Pier Luigi Vidale, André Walser

**Institute/Group**: Institute for Atmospheric and Climate Science, ETH Zürich
Group of Prof. Christoph Schär

**Description:**

Our research revolves around the study of continental and Alpine-scale weather and climate, with special focus on the water cycle, over a continuum of spatial and temporal scales. Regional climate processes are investigated with the help of a regional climate model (RCM), the Climate High-Resolution Model (CHRM). The dynamics of dry and moist atmospheric flow past realistic and idealized topography are investigated with the help of a hierarchy of hydrostatic and non-hydrostatic atmospheric models (e.g. HRM, ARPS, LM). Hydrological processes in intermediate and major catchments in the Alpine region are investigated with the help of hydrological models (e.g. WASIM).

Research on climate aspects is dedicated to the study of natural and anthropogenic climate variations on seasonal to centennial time scales. This work involves conducting comprehensive RCM numerical simulations at horizontal resolutions between 14 and 56 km, driven by the output of intermediate-resolution general circulation models and reanalysis data sets. The research aims at better understanding our climate system and at developing regional climate change scenarios. Recent research from our group considers the variability of the European summer climate in response to anthropogenic greenhouse gas forcing. Our simulations suggest that there are intricate physical interactions between the climate system and the water cycle, which may give rise to changes in variability, in addition to the anticipated mean warming. The research is funded by the Swiss National Science Foundation (NCCR Climate) and the European Commission (projects PRUDENCE and ENSEMBLES).

Research on weather aspects is motivated by the emergence of high-resolution cloud-resolving models. Such models offer promising prospects in numerical weather prediction as well as quantitative precipitation and flood forecasting. Our research uses state-of-the-art non-hydrostatic models to address predictability issues. We are using ensemble (Monte Carlo) experiments to isolate the sensitivity of simulated weather evolutions with respect to initial conditions, with special consideration being given to moist atmospheric convection. We are also conducting idealized high-resolution experiments of flow past topography to study the dynamics of embedded convection, and are involved in the formulation of future atmospheric prediction models.

**References**: See list of publications.

**Title:** Efficient pricing under multiscale stochastic volatility models

**Researchers:** N. Hilber*
A.-M. Matache**
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**Institute/ Group:** *Seminar of Applied Mathematics
Department of Mathematics
** Seminar of Applied Mathematics and RiskLab

**Description:**

The fast numerical valuation of financial derivatives under stochastic volatility is addressed.
In the standard Black-Scholes model the volatility of the risky asset is assumed to be constant or a function of time and explicit pricing formulas are available for European Vanillas. Such models are generally too crude to match observed log-return prices well. A more flexible class of models assumes that the volatility is a stochastic process. Such models lead to degenerate parabolic partial differential equations in $d \geq 2$ space dimensions, which, in general, cannot be solved in closed form. Standard discretizations suffer form the so-called curse of dimension, i.e. the number of degrees of freedom grows like $O(h^{-d})$, where $h$ is the mesh-width in one dimension. To reduce the number of the degrees of freedom, wavelet based sparse tensor product Finite Element spaces are used. We apply *hp*-discontinuous Galerkin time stepping to discretize in time, where the wavelet basis is used to precondition the iterative solver of the corresponding matrix equations in each time step. The resulting algorithm has log-linear complexity comparable to that of the best FFT-based methods for the usual Black-Scholes type model.

**References:** N. Hilber, A.-M. Matache and C. Schwab, *Sparse Wavelet Methods for Option Pricing under Stochastic Volatility* , submitted, available also as Research Report 2004-07, Seminar of Applied Mathematics, ETH Zürich
http://www.sam.math.ethz.ch/reports/2004/07

**Title:** Generalized *hp*-FEM for Lattice Structures

**Researchers:** A. W. Rüegg
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**Institute:** Seminar for Applied Mathematics
**Group:** Department of Mathematics
ETH Zürich

**Description:**
Progress in manufacturing techniques allows the production of *lattice materials* of increasing complexity that are of growing importance in mechanical engineering, optoelectronics, etc.
Typically, when trying to characterize the physical properties of such materials, one has to take into account *three different length scales*: the macroscopic size $l$ of the material block, the microscopic scale of the heterogeneities $\varepsilon$ and finally the thickness of the bars $\delta$. Taking the limit $\delta \to 0$, the remaining dimensionally reduced structures can be modeled by *networks* consisting of one-dimensional curves periodically arranged in a higher dimensional space.
A high order *generalized Finite Element Method* (gFEM) is developed to solve numerically elliptic *partial differential equations* (PDE's) on periodic lattice structures (see [2]). The standard polynomial spaces are replaced by conforming function spaces that are adapted to the micro-scale dependent coefficients of the differential operator, i.e. information much smaller than the macro mesh size $H \gg \varepsilon$ is built into the shape functions. These two-scale FE-spaces are obtained by augmenting the standard piecewise polynomial FE spaces with non-polynomial, periodic micro shape functions that are solutions of suitable unit cell problems on the reference network.
Taking into consideration the periodicity of the micro shape functions, the computation of the stiffness matrices to solve the discrete two scale problem can be realized with *work independent of the micro scale length* $\varepsilon$.
This method is implemented in C++ within the programming framework described in [2].

This Research is supported under the project "Homogenization and multiple scales" HMS2000 of the EC (HPRN-CT-1999-00109), by the Swiss Federal Government under Grant BBW 01.0025-01 and by the Swiss National Science Foundation under Project "Hierarchic FE-Models for periodic lattice and honeycomb materials" with Number SNF 200020-100017/1.

**References:**

[1] A.W. Rüegg, *Implementation of Generalized Finite Element Methods for Homogenization Problems*, Journal of Scientific Computing, (2002) **17**, 671–681

[2] A.W. Rüegg. A. Schneebeli, R. Lauper, *Generalized hp-FEM for Lattice Structures*, SAM-Research Report 2002-23

**Title:** FEM for Elliptic Problems with Stochastic Data

**Researchers:** Christoph Schwab
Radu Alexandru Todor

**Institute/ Group:** Seminar for Applied Mathematics
Department of Mathematics

**Description:**

Often the data (load vector) of a PDE is either incompletely known or uncertain to some extent which makes its description as a random field more realistic. The problem itself becomes then a stochastic differential equation (SDE), whose solution is, in general, a random field taking values in a suitable function space. Complete description of this random field requires knowledge of its joint probability densities, so that in applications one is often only interested in the first (expectation), second (correlation) and sometimes even higher order moments of the random solution. Deterministic PDEs for the moments of the random solution can be derived, but solving them proves difficult due to their high-dimensional character. The project aims at reducing the apparent huge numerical complexity of such problems. More precisely,

a) for the problem with deterministic coefficients, but stochastic right hand side, we develop efficient FEM for the numerical solution of the deterministic boundary value problems in high-dimensional, tensorized domains. The goal is here to achive essentially the same scalability of the solution algorithm for the second (and higher) order moments as for the solution of the deterministic problem.

b) for the problem with stochastic coefficients, the stochastic Galerkin method will be used, which discretizes the stochastic PDE simultaneously in physical and probability space. Since the latter is infinite-dimensional, this strategy will lead to potentially extremely high dimensional deterministic problems to be solved; also here we will develop strategies for complexity reduction in the presence of high dimensions by *sparse interpolands* and by *adaptive approaches*.

**References:**

C. Schwab, R.A. Todor, *Sparse finite elements for stochastic elliptic problems with Stochastic Loading*, SAM Report 2002-05, Numer. Math. 95 (2003), no. 4, 707–734.
C. Schwab, R.A. Todor, *Sparse finite elements for stochastic elliptic problems - higher order moments*, SAM Report 2003-04, Computing 71 (2003), no. 1, 43–63.
P. Frauenfelder, C. Schwab and R.A. Todor, *Finite elements for elliptic problems with stochastic coefficients*, SAM Report 2004-12 (to appear in Computer Methods in Applied Mechanics and Engineering).

**Title:** Domain decomposition preconditioners for *hp* finite elements on anisotropically stretched meshes

**Researchers:** Dr. Andrea Toselli (Project Leader)
Dr. Xavier Vasseur

**Institute:** Seminar for Applied Mathematics
**Group:** Department of Mathematics
ETH Zürich

**Description:**

In order to make the iterative solution of very large algebraic systems of finite element equations possible and efficient on parallel architectures, domain decomposition techniques (DD) have been used extensively in recent years. These methods are by now well-understood for standard equations (e.g., simple diffusion or viscous flow problems at moderate Reynolds number in regular 2-d or 3-d domains), with subdomains and meshes of regular shape. In this case, optimal or nearly optimal convergence of iterative solution techniques based on domain decomposition is by now well-established. This pertains to low order standard finite element discretizations as well as to high-order $p$-version or spectral element discretizations. However, their performance in general degrades drastically whenever anisotropic meshes or very thin subdomains are employed and their generalization to less standard finite element approximations (edge elements, for instance) is far from being straightforward.

The purpose of this project is to extend some of the most popular and powerful DD methods to finite element approximations on anisotropic meshes of a wide class of equations. In addition it aims at developing robust DD strategies for three dimensional electromagnetic problems. It consists of a theoretical part, where efficient methods are devised and analyzed, and a programming part, where these novel methods are implemented and tested on some real life problems.

Extensive numerical tests showing the performance and robustness of domain decomposition preconditioners for the solution of algebraic linear systems arising from *hp* finite element approximations of scalar elliptic problems on geometrically refined boundary layer meshes in two and three dimensions have been performed. In addition, a novel dual-primal FETI strategy has been developed for three-dimensional edge element approximations.

This project is sponsored by the Swiss National Foundation under Grant 20-63397.00.

**Title:** Frustrated Quantum Spin Systems

**Researchers:** G. Schmid, S. Wessel, M. Troyer, M. Sigrist [*]
A. Läuchli[**]

**Institute/Group:** [*]Theoretische Physik, ETH Zürich
[**] Université de Toulouse

**Description:**

Frustrated quantum spin systems offer the possibility to study the appearance of unusual quantum phases, driven by competing interactions and large fluctuations. In recent experiments on insulating cuprate materials evidence for substantial cyclic four-spin exchange interactions was accumulated. Higher order spin interactions are poorly understood in general. We investigated the overall phase diagrams of systems with such interactions and witnessed a surprisingly rich phase diagram already on the simple ladder structure. Among the different phases we discover the long sought staggered spin current phase.
We are also interested in the phase diagram of the generalized Shastry-Sutherland model (which seems to be realized in $SrCu_2(BaO_3)_2$ ). Our results indicate that the phase between the usual Neel order and the exact dimmer phase is actually a Valence Bond Crystal with a plaquette covering.

**References:**

- A. Läuchli, G. Schmid and M. Troyer, Phys. Rev. B **67**, 100409 (R) (2003)

**Title:** Numerical investigation of strongly correlated systems

**Researchers:** M. Indergand, U. Ledermann, S. Wessel, M. Sigrist, M. Troyer, T.M. Rice[*]
A. Läuchli [**], H.-D. Chen,, S.-C. Zhang, [***], S. Capponi[****]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] IRRMA, EPF Lausanne
[***] Stanford University, USA
[****] Université de Toulouse

**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 analyze 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:**

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- M. Matsumoto, B. Normand, T.M. Rice and M. Sigrist, Preprint, submitted to Phys. Rev. B
- A. Läuchli, C. Honerkamp and T.M. Rice, Preprint, submitted to Phys. Rev. Lett.
- C. Honerkamp and T.M. Rice, J. Low Temp. Phys. 131, 159 (2003).
- H.-D. Chen, S. Capponi, F. Alet, S.-C. Zhang, Phys. Rev. B **70**, 024516 (2004)

**Title:** Quantum Antiferromagnetism in Quasicrystals

**Researchers:** S. Wessel, I. Milat [*]
A. Jagannathan [**]
S. Haas [**]

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

**Description:**

Quantum magnetic phases of low-dimensional antiferromagnetic Heisenberg systems show various degrees of disorder caused by zero-point fluctuations. In our study we explore how non-perodic environments, such as provided in quasicrystal structures, further affect the magnetic properties of quantum magnets. In particular we study the Heisenberg model on a two-dimensional bipartite quasiperiodic lattice. The distribution of local staggered magnetic moments is determined, using the stochastic Series Expansion Quantum Monte Carlo method. A non-trivial inhomogeneous ground state is found. For a given local coordination number, the values of the magnetic moments are spread out, reflecting the fact that no two sites in a quasicrystal are identical. A hierarchical structure in the values of the moments is observed which arises from the self-similarity of the quasiperiodic lattice. Furthermore, the computed spin structure factor shows antiferromagnetic modulations that can be measured in neutron scattering and nuclear magnetic resonance experiments. Our generic model is a first step towards understanding magnetic quasicrystals such as the recently discovered Zn-Mg-Ho icosahedral structure.

**References:**

S. Wessel, A. Jagannathan and S. Haas, Phys. Rev. Lett. 90, 177205 (2003).
S. Wessel, I. Milat, Preprint, submitted to Phys. Rev. B

**Title:** Phase Diagrams of 2D Bosonic Systems

**Researchers:** F. Alet**,** G. Schmid, M. Troyer [*]
E.S. Sørensen [**]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] McMaster University, Canada

**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. We also studied the generic superfluid/insulator transition at incommensurate filling and found a good agreement with theoretical predictions, albeit at very large system sizes.

**References:**

- G. Schmid and M. Troyer, Phys. Rev. Lett. **93**, 067003 (2004)
- F. Alet and E.S. Sørensen, Phys. Rev. B **70**, 024513 (2004)

**Title:** Quantitative modeling of quantum magnets

**Researchers:** A. Läuchli, M. Troyer, F. Alet [*]
D.C. Johnston [**]
C. Yasuda, S. Todo, K. Hukushima, H. Takayama[***]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] Ames Laboratories, Ames, Iowa
[***] University of Tokyo, Japan

**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

C. Yasuda, S. Todo, K. Hukushima, F. Alet, M. Keller, Matthias Troyer, H. Takayama, Preprint, submitted to Phys. Rev. Lett.

B. Pedrini, J. L. Gavilano, D. Rau, H. R. Ott, S. M. Kazakov, J. Karpinski, S. Wessel, Preprint, to appear in Phys. Rev. B

J. Das, A.V. Mahajan, J. Bobroff, H. Alloul, F. Alet, E. Sorensen, Phys Rev. B **69**, 144404 (2004)

N. Fukushima, A. Honecker, S. Wessel, W. Brenig, Phys. Rev. B **69**, 174430 (2004)

N. Fukushima, A. Honecker, S. Wessel, S. Grossjohan, W. Brenig, Conference Proceeding, to appear in Physica B.

**Title:** Quantum criticality

**Researchers:** S. Wessel M. Troyer [*]
M. Vojta [**]
S. Sachdev [***]
O. Nohadani, S. Haas [****]

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

**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:**

- K. Harada, N. Kawashima and M. Troyer, Phys. Rev. Lett. **90**, 117203 (2003)
- M. Troyer, Sup. Prog. Theor. Phys. (2003)
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**Title:** Topologically protected quantum bits

**Researchers:** D. Ivanov, P. Dayal, 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

Our most recent work concentrates on a more practical device which still has some of the valuable topological features preserved. We propose a design for a qubit involving four superconducting islands in the topology of a symmetric tetrahedron, uniformly frustrated with one-half flux-quantum per loop and one-half Cooper-pair per island. This structure emulates a noise-resistant spin-1/2 system in a vanishing magnetic field. The flux-frustration boosts quantum fluctuations and relieves the constraints on junction fabrication. Variability of manipulation and optimized readout through single-shot measurements are additional benefits of this design. For specific limits, the spectrum of this `3-body' quantum system can be found analytically using quasi-classical methods, but an accurate and general determination requires numerical solution. This has been implemented successfullyusing exact diagonalization techniques (Lanczos) both in the charge and phase representation of the Hamiltonian.

**References:**

- L. Ioffe, M.V. Feigel'man, A. Ioselevich, D. Ivanov, M. Troyer and G. Blatter
  Nature **415**, 507 (2002).
- M.V. Feigel'man, L.B. Ioffe, V.B. Geshkenbein, P. Dayal, and G. Blatter, Phys. Rev. Lett. **92**, 098301 (2004)

**Title:** New Quantum Monte Carlo Algorithms

**Researchers:** M. Troyer [*]
A. Dorneich [**]
F. Alet [*]
S. Wessel [*]
E. Sorensen [***]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] Universität Würzburg, Germany
[***] Mc Master University, Canada

**Description:**

Great algorithmic progress for quantum Monte Carlo simulations has been achieved in the past years, shadowing the growth of processor power by many orders of magnitude. Still, many problems remain intractable and further algorithmic progress is needed. We have developed an algorithm to measure offdiagonal and time-dependent Green's function in the Stochastic Series Expansion (SSE) Quantum Monte Carlo algorithm.

A break-through was achieved by an adaptation of Wang-Landau sampling to quantum systems. This algorithm has the potential of overcoming the problems associated with tunneling through energy barriers at first order transitions and for disordered and glassy systems.
We also investigated the generalization of detailed balance equations required during the Quantum Monte Carlo simulations. We obtain accordingly improved "directed loop" algorithms, which are shown to be more efficient than conventional ones.

**References:**

M. Troyer, S. Wessel and F. Alet, Phys. Rev. Lett. **90**, 120201 (2003).

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P. Hitchcock, E. S. Sørensen, F. Alet, Phys. Rev. E **70**, 016702 (2004)

S. Wessel, S. Trebst, and M. Troyer, SIAM J. on Multiscale Modeling and Simulation, in print

**Title:** Flat-Histogram Algorithms

**Researchers:** P. Dayal, S. Trebst, M. Troyer, S. Wessel, D. Wuertz [*]
S. Sabhapandit, S. Coppersmith [**]
D. Huse [***]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] Department of Physics, University of Madison, USA
[***] Princeton University, USA

**Description:**

When studying phase transitions the traditional Metropolis algorithm becomes inefficient when the temperature approaches the critical temperature of the transition. For second order phase transitions the problem of ``critical slowing down'' -- a rapid divergence of the number of Monte Carlo steps needed to obtain a subsequent uncorrelated configuration -- was solved more than a decade ago by cluster update algorithms. At first order transitions and in systems with many local minima of the free energy, such as frustrated magnets or spin glasses, there exists the similar problem of long tunneling times between local minima. Recently proposed flat histogram methods produced promising results to effectively study first order phase transitions in these systems as well.

By studying the optimal scaling of flat-histogram methods with system size for classical 2D and 3D Ising models we determined a lower algorithmic bound for all flat-histogram methods such as Wang-Landau sampling, multicanonical sampling, tempering and broad histograms. For the 2D spin glass we found severe limitations in the form of exponential scaling and fat-tailed Frechet distributions of the tunneling time, the relevant time scale when sampling the full energy range in a multicanonical simulation.

We then developed an optimized ensembles, gaining orders of magnitude over the flat histogram and multicanonical ensembles.

**References:**

- P. Dayal, S. Trebst, S. Wessel, D. Wuertz, M. Troyer, S. Sabhapandit, S.N. Coppersmith, Phys. Rev. Lett. **92**, 097201 (2004); AIP Conf. Proc. 690, 400 (2003).
- S. Alder, S. Trebst, A. Hartmann and M. Troyer, JSTAT P07008 (2004)
- D. Huse, S. Trebst and M. Troyer, Phys. Rev. E **70**, 046701 (2004).

**Title:** Simulations of novel exotic phases of matter

**Researchers:** F. Alet. S. Trebst, M. Troyer

**Institute/Group:** Theoretische Physik, ETH Zürich

**Description:**

Novel states of matter with fractional quantum numbers, where an electron effectively splits up into smaller parts, each carrying only parts of the mass or charge of the original electron, have been a vivid research topic within condensed matter physics, propelled by the discovery of high temperature superconductivity and the fractional quantum hall effect.

The central role of excitations carrying a fractional charge in these novel quantum phases has been addressed in theoretical works over the years. Related topological states have recently been found to be promising candidates for the physical implementation of qubits, the elementary building units of a quantum computer. What has been missing so far are detailed numerical investigations if these proposed exotic phases are actually realized in realistic model.

We develop novel quantum simulation algorithms to study microscopic models and search for these fractionalized states with explicit macroscopic topological order to obtain the needed definitive proof of existence of these phases through high-performance numerical work.

**Title:** NP-hardness of the negative sign problem of quantum Monte Carlo simulations

**Researchers:** M. Troyer [*]
U.-J. Wiese [**]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] Universität Bern

**Description:**

Quantum Monte Carlo simulations, while being efficient for bosons and non-frustrated quantum magnets, suffer from the infamous ``negative sign problem'' when applied to fermions or frustrated magnets -- causing an exponential increase of the computing time with the number of particles. A polynomial time solution to the sign problem is highly desired, since it would provide an unbiased and numerically exact method to simulate correlated quantum systems. Here we argue, however, that such a solution is almost certainly unattainable, by showing that it is NP-hard, implying that a generic solution of the sign problem would also solve all NP-complete problems in polynomial time.

**References:**

- M. Troyer and U.-J. Wiese, Preprint

**Title:** Simulations of trapped ultra-cold atoms

**Researchers:** F. Alet, S. Wessel, S. Trebst, M. Troyer [*]
G.G. Batrouni [**]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] Université de Nice, France

**Description:**

In order to study the Mott-transition observed in trapped atomic gases within an optical lattice we perform Monte Carlo simulations of the bosonic Hubbard model, which is an appropriate lattice model in the strongly interacting regime. The numerical technique which we are using, the stochastic series expansion quantum Monte Carlo, allows us to study local properties of the system and to measure quantities of direct relevance for the experimental situation, such as the momentum distribution function. We have improved the efficiency of the underlying algorithm, by using a directed loop scheme, which is has bounce-free regions also for the soft-core bosonic case. In addition to studying trapping geometries in various dimensions (1, 2, and 3), we are also investigating the dimensional crossover observed within optical lattices with anisotropic hopping matrix elements.

**References:**

M. Rigol, A. Muramatsu, G.G. Batrouni, V. Rousseau, R.T. Scalettar, P.J.H. Denteneer, and M. Troyer, AIP Conf. Proc. **678**, 283 (2003)

S. Wessel, F. Alet, M. Troyer, G.G. Batrouni, Advances in Solid State Physics **44**, 265 (2004).

S. Wessel, F. Alet, M. Troyer, G.G. Batrouni, Phys. Rev. A (2004) in print

S. Wessel, F. Alet, S. Trebst, M. Troyer, G.G. Batrouni, Preprint, submitted J. Phys. Soc. Jpn.

**Title:** Simulations of dissipative quantum systems

**Researchers:** P. Werner, M. Troyer [*]
S. Chakravarty [**]
S. Sachdev [***]

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

**Description:**

Dissipation effects due to coupling to the environment can substantially alter the nature and universality class of a quantum phase transition. In this project we develop new quantum Monte Carlo algorithms for the simulation of dissipation-driven quantum phase transitions, exceeding the performance of standard methods by orders of magnitudes. This allows for the first time the accurate investigation of these quantum phase transitions in systems such as dissipative spin chains, quantum wires, single electron boxes or shunted Josephson junctions.

**References:**

S. Sachdev, P. Werner, M. Troyer, Phys. Rev. Lett. **92**, 237003 (2004)

P. Werner, K. Völker, M. Troyer and S. Chakravarty, Preprint, submitted to Phys. Rev. Lett.

P. Werner, M.Troyer and S. Sachdev, Preprint, submitted J. Phys. Soc. Jpn.

P. Werner and M. Troyer, Preprint, submitted to Phys. Rev. Lett.

P. Werner and M. Troyer, Preprint, submitted to JSTAT

**Title:** The ALPS project

**Researchers:** F. Alet, P. Dayal, M. Körner, S. Trebst, M.Troyer, P. Werner [*]
M. Rütti, W.P. Petersen [**]
and the ALPS collaboration (http://alps.comp-phys.org/) [***]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] SAM, ETH Zürich
[***] and many other institutions

**Description:**

Unlike in other physics communities there have been no "community codes" available to study strongly correlated quantum mechanical systems with researchers writing individual codes, adjusting them for specific needs of new projects and thereby investing weeks to months in software development. The ALPS project (Algorithms and Libraries for Physics Simulations) is an open source effort aiming at simplifying the development of simulation codes for strongly correlated quantum mechanical systems. A set of libraries of differing technical level have been implemented to support researchers to develop model independent, generic software, including basic libraries for lattice structures, quantum models, error analysis, parallelization of simulations and XML tools. On top, generic application programs are offered to non-experts, such as Monte Carlo for classical magnets, Quantum Monte Carlo for quantum magnets and bosons (stochastic series expansion (SSE), continuous time worm algorithm) as well as exact and full diagonalization. Future applications will include Density Matrix Renormalization Group (DMRG) and Linked Cluster Series Expansions.

**References:**

F. Alet, P. Dayal, H.G. Evertz, A. Grzesik, A. Honecker, M. Körner, A. Läuchli, S. Manmana, I. McCulloch, R. Noack, G. Schmid, U. Schollwöck, S. Todo, S. Trebst, Matthias Troyer, P. Werner, S. Wessel (ALPS collaboration), submitted J. Phys. Soc. Jpn.

M. Rütti, M. Troyer and W.P. Petersen, submitted to MCM2004

http://alps.comp-phys.org/

**Title:** Simulation of Electron Source
for Next-Generation X-ray Free Electron Laser

**Researchers:** A. Candel, M. Troyer [*]
M. Dehler, R. Eichler [**]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] Paul Scherrer Institut, PSI Villigen

**Description:**

Advanced next-generation synchrotron radiation sources are needed for future scientific research. To keep costs low, while delivering highest possible brilliance beams, elaborate compact setups are necessary. A new type of compact X-ray free electron laser under consideration at PSI demands very high quality standards of the electron beam. This is far beyond current possibilities and expected only to be realizable with a new generation of electron source, consisting of nanostructured microcathodes, paired with extremely high accelerating gradients.
In order to gain theoretical understanding of this physically extreme regime, we need unpreceded simulation accuracy. We have developed a massive parallel relativistic 3D particle-in-cell code, based on the finite integration technique. First studies on the optimal electron source setup have been conducted and show the suitability of the code for our purposes.

**References:**

A. Candel, M. Dehler, M. Troyer, Preprint, Submitted to Nuclear Instruments and Methods in Physics Research

**Title:** Understanding the Vortex Glass Phase

**Researchers:** H. G. Katzgraber, G. Blatter, D. Würtz [*]
A. P. Young[**]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] University of California Santa Cruz

**Description:**

There have been conflicting claims as to whether the superfluid density vanishes in the vortex glass phase, with Fisher, Fisher and Huse arguing that it is finite and Korshunov predicting that it is zero. As the vortex glass is commonly described by the gauge glass model, we have numerically computed the superfluid density of this model by Monte Carlo simulations. Because the average free energy is independent of a twist angle, it is expected that the average superfluid density vanishes. This is not necessarily the case for the typical (median) value, which is non-zero, because the distribution of the superfluid density among different disorder realizations is very asymmetric. We have shown that the data for the superfluid density is well described by a generalized extreme value distribution with a nonzero "location parameter". The study of more realistic vortex glass models is planned in the future.

**Title:** Nature of the Spin Glass State

**Researchers:** H. G. Katzgraber[*]
A. P. Young[**]

**Institute/Group:** [*] Theoretische Physik, ETH Zürich
[**] University of California Santa Cruz

**Description:**

Two theories attempt to describe the low-temperature properties of spin glasses: the droplet model proposed by Fisher and Huse, and the replica symmetry breaking picture of Parisi. More recently an intermediate scenario, known as TNT (for trivial-nontrivial) has been suggested by Krzakala, Martin, Palassini and Young. We have done a numerical study of the one-dimensional Ising spin glass with power-law interactions, using parallel tempering Monte Carlo, to test these scenarios. A one-dimension model has the advantage that a large range of system sizes can be studied. Our data agree well with replica symmetry breaking, although we cannot fully rule out the intermediate picture.

We have also studied the three-dimensional Edwards-Anderson Ising spin glass in the presence of a (random) field and show, by means of a finite-size study of the correlation length, that there is no Almeida-Thouless line for short-range Ising spin glasses.

In the future we intend to study further properties of spin glasses such as the ultrametric structure of space as well as the concept of universality.

**References:**

H. G. Katzgraber and A. P. Young, Phys. Rev. B 67, 134410 (2003)

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A. P. Young and H. G. Katzgraber, Phys. Rev. Lett., in press

**Title:** Electromagnetic simulations of complex structures with the Finite-Volume Time-Domain method.

**Researchers:** Christophe Fumeaux
Dirk Baumann
Pascal Leuchtmann
Rüdiger Vahldieck

**Institute/ Group**: Laboratory for Electromagnetic Fields and Microwave Electronics

**Description:**

The Finite-Volume Time-Domain (FVTD) method has been applied in computational electromagnetics since the end of the 1980's. It has been inspired from finite-volume techniques used in computational fluid dynamics. The FVTD method is characterized by a great geometrical flexibility since it is applied in unstructured meshes made of arbitrary polyhedrons (typically tetrahedrons). Complex structures that include curved or oblique surfaces are modeled advantageously using such conformal meshes since the boundaries can be handled very accurately. In addition, the use of unstructured mesh permits to vary the size of the cells according to local geometrical requirements: Small details in close proximity to larger structures, for example, can be resolved without explosion of the computational cost, or different mesh finenesses can be applied on both sides of material interfaces with large dielectric contrast.
In this project, the FVTD algorithm is further developed in the perspective of its application to challenging real-world electromagnetic problems. The efficiency of the FVTD computations in inhomogeneous meshes has been drastically improved by the implementation of a generalized time-stepping scheme. In addition, a novel definition of ports has been developed, resulting in improved accuracy in the computation of the scattering parameters of microwave circuits. These techniques enabled the successful simulation of complicated 3D antenna problems: Among them a cavity-backed spiral antenna including balun and honeycomb absorber, various horns with complex geometries, as well as dielectric resonator antennas including detailed feeding mechanisms. The simulation results have been validated through comparison with measurements and/or with results obtained with other methods.

**References:**

- A paper was published in IEEE Transactions on Microwave Theory and Techniques
- A paper was published in the International Journal of Numerical Modelling
- A paper was accepted for publication in the ACES Journal

**Title:** Application of Model Order Reduction in the Optimization of Microwave Filters and Diplexers

**Researchers:** Klaus Krohne
Rüdiger Vahldieck

**Institute/ Group:** Laboratory for Electromagnetic Fields and Microwave Electronics (IFH)
Field Theory Group

**Description:**

The application of general purpose electromagnetic field solvers in the optimization of microwave filters and diplexers is often impeded by an excessive computational effort despite the progress made in the performance of computer hardware and solver software over the last years. The limiting factors are the high number of necessary simulation runs as well as the deteriorated efficiency of those solvers when applied to highly resonant structures, such as filters. In addition to that, most optimizers show a low robustness i.e. a high sensitivity to the initial choice of geometry parameters.
These issues can be addressed with application of Model Order Reduction (MOR) in the optimization scheme. A significant reduction of necessary simulation runs and therewith a decrease in CPU time can be achieved along with a gain in robustness. The optimization focuses on the scattering matrix poles and zeros, which are computed from a reduced order state-space model of the structure, making its computational effort comparable to a surrogate model optimization that is commonly employed. The method has been tested successfully on various examples including high-end problems such as a 16-resonator *E-plane* diplexer with a total of 23 designable geometry parameters.
While the fine, i.e. unreduced, state-space model has originally been obtained from a commercial EM modeler, which is based in the Finite Integration Technique, current research activities focus on state-space models which are obtained from a Finite Volume discretization, that has been developed in-house, and on the numerical issues that arise with these models.

**References:**

A paper was published in IEEE Transactions of Microwave Theory and Techniques

**Title:** Simulation and Optimization of Photonic Crystals

**Researchers:** Christian Hafner
Jasmin Smajic
Cui Xudong

**Institute/ Group**: Laboratory for Electromagnetic Fields and Microwave Electronics
Computational Optics

**Description:**

We have developed a software package for the simulation and optimization of photonic crystals. The field solver is based on the Multiple Multipole Program (MMP) contained in the MaX-1 software. This semi-analytic method provides high accuracy, robustness, and numerical efficiency. It allows us to perform all tasks associated with the design of arbitrary structures within a photonic crystal, namely 1) computation of band diagrams of pure photonic crystals (eigenvalue solver for periodic structures), 2) computation of modes of waveguide within a photonic crystal (complex eigenvalue solver that takes radiation and material losses of imperfect structures into account), 3) computation of the scattering matrix of arbitrary waveguide structures including coupling of photonic crystal waveguides with other types of waveguides or free space (photonic crystal antenna), filters, power dividers, modulators, etc. Because of the high accuracy and robustness, this solver is very well suited for the optimization of structures within a photonic crystal, namely for the design of the defects that are responsible for the main physical effects and for the fine tuning of existing designs. For the latter we have developed an algorithm that is based on gradient search and on the sensitivity analysis of photonic crystal structures. For the former we have developed special procedures based on the concepts of micro genetic algorithms and binary evolutionary strategies that include unique features based on a table of known designs. These optimizers outperform traditional ones by far.

**References:**

- A book chapter has been published by World Scientific Publishing Co., Singapore.
- Two papers were published in Optics Express
- Two Papers were published in the ACES Journal
- A chapter was accepted for publication by Marcel Dekker/CRC Press
- Two chapters were accepted for publication in the Handbook of Theoretical and Computational Nanotechnology, American Scientific Publishers
- A paper was accepted for publication in the Journal of the Optical Society of America A, accepted for publication (July 2004).

**Title:** Reverberation chamber simulation, measurement, and optimization

**Researchers:** Christian Bruns
Pascal Leuchtmann
Rüdiger Vahldieck

**Institute/ Group:** Laboratory for Electromagnetic Fields and Microwave Electronics (IFH)
Field Theory Group

**Description:**

Reverberation chambers offer a new method for electromagnetic compatibility (EMC) tests, usable for radiated emissions and immunity testing of electronic products. The testing principle is based on the idea to have spatially homogeneous and isotropic electromagnetic fields within the volume of the equipment under test (EUT). This is achieved by using one or more so-called mode tuning stirrers which rotate inside an overmoded, metallic cavity.
A numerical model was developed in the IFH field theory group to understand the complex electromagnetic fields inside the reverberation chamber. The model consists of the chamber itself, several mode stirrers, various excitations (dipole, biconical, logarithmic-periodic antennas) and a canonical EUT. Our simulation uses a hybrid method of moments (MoM) / multi-level fast multipole method (MLFMM) approach to compute and visualize the currents, electric and magnetic near and far fields. Simulating such a realistic, finitely conducting chamber with irregular stirrers over a 80 MHz...2 GHz frequency range is computationally very challenging and therefore carried out on a distributed machine cluster with up to 8 processors and 32 GByte RAM. The simulation results are benchmarked against measurements, parameters such as the field correlation and anisotropy coefficients are extracted for different stirrer positions and statistically analyzed. This study allows us to propose guidelines for the design and optimization of reverberation chambers.

**References:**

- Two papers were published in *IEEE Trans. on Electromagnetic Compatibility*
- A paper was published in *IEEE Trans. on Antennas and Propagation*

**Title:** Design and analysis of high-speed traveling-wave photodetectors

**Researchers:** Damir Pasalic
Rüdiger Vahldieck

**Institute/ Group**: Laboratory for Electromagnetic Fields and Microwave Electronics

**Description:**

Traveling wave photodetectors (TWPDs) are opto-electrical transducers, especially suitable for modern ultra-wide-band optical communication systems. The TWPDs' ability to maintain high efficiency and broad bandwidth even under high-power optical illumination is important in microwave fiber optic links, especially since optical pre-amplification is utilized more widely.
TWPDs combine the microwave and optical propagation mechanisms on the same multilayered guiding structure. The optical waveguide is a mesa-type PIN structure consisting of a light-absorbing intrinsic core sandwiched by the P- and N-type light-transparent semiconductor layers. The RF-propagation is guided by the metallic electrodes lying on the multilayered structure, resembling a CPW line. The bandwidth of TWPDs is not RC time constant limited, which is an advantage over vertically illuminated and waveguide photodetectors. Instead, the TWPDs' bandwidth is limited by velocity mismatch between the optical and RF signals, and microwave losses. Therefore, the microwave propagation parameters are of key importance for optimum bandwidth design of TWPDs.
In this project, we developed en efficient hybrid method for the rigorous analysis of traveling-wave photodetectors. Such method was needed, since the already existing equivalent circuit models could not describe accurately the complex physical mechanisms in the TWPD structures. Our method is a combination of a 2D drift-diffusion based semiconductor simulation and a full-wave electromagnetic (EM) analysis of the overall structure. The drift-diffusion semiconductor simulation is performed to describe the optical generation of the distributed current sources in the active (absorbing) region of the photodetector. The obtained current sources are used in the full-wave EM analysis to obtain microwave parameters of interest, such as: RF phase velocity and attenuation, bandwidth, interaction with the embedding microwave circuit, etc. The full-wave EM simulation is performed using time-domain TLM method. The hybrid method developed in our institute was tested on several different structures and the obtained data were in much better agreement with the experiment than the data obtained with the equivalent circuit model.

A paper is submitted to the IEEE Transactions of Microwave Theory and Techniques

**Title:** On the transferability of the SPC/L water model to biomolecular simulation

**Researchers**:
Alice Glättli
Chris Oostenbrink
Xavier Daura*
Daan P. Geerke
Haibo Yu
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland
*Universitat Auto¡noma de Barcelona, Bellaterra, Spain

**Description:**

We investigated the performance of the recently developed SPC/L model for liquid water, as a pure liquid, in binary mixtures with DMSO, and as a solvent model in a peptide folding simulation. Additionally, in order to test the compatibility with the GROMOS biomolecular force field, free energies of hydration of a set of representative compounds were computed. The results are compared to those for the well-established SPC water model, which is generally used as a solvent model in conjunction with the GROMOS force field already for more than two decades. It turns out that as a pure liquid and in binary mixtures with DMSO the SPC/L model outperforms SPC, whereas as solvent in combination with the GROMOS force field both models perform equally well.

**References:** Brazilian J. of Phys. **34** (2004) 116-125

**Title:** Principles of Carbopeptoid Folding:
A Molecular Dynamics Simulation Study

**Researchers**: Riccardo Baron
Dirk Bakowies
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg,
Zurich, Switzerland

**Description:**

The conformational spaces of five oligomers of tetrahydrofuran-based carbopeptoids in chloroform and dimethyl sulfoxide were investigated through nine molecular dynamics simulations. Prompted by nuclear magnetic resonance experiments which indicate various stable folds for some but not all of these carbopeptoids, we have investigated their folding behaviour as function of stereochemistry, chain length, and solvent. The conformational distributions of these molecules are analysed in terms of occurrence of hydrogen bonds, backbone torsional-angle distributions, conformational clustering and solute configurational entropy. While a *cis*-linkage across the tetrahydrofuran ring favours right-handed helical structures, a *trans*-linkage results in a larger conformational variability. Intra-solute hydrogen bonding is reduced with increasing chain length and with increasing solvent polarity. Solute configurational entropies confirm the picture obtained: they are smaller for *cis*- than for *trans*-linked peptides, for chloroform than for dimethyl sulfoxide as solvent and for shorter peptide chains. The simulations provide an atomic picture of molecular conformational variability that is consistent with the available experimental data.

References: manuscript in press (*J. Peptide Sci*.).

**Title:** Charge-on-spring polarizable water models revisited: From water clusters to liquid water to ice

**Researchers**: Haibo Yu
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland

**Description:**

The properties of two improved versions of charge-on-spring (COS) polarizable water models (COS/G2 and COS/G3) that explicitly include non-additive polarization effects are reported. In COS models, the polarization is represented via a self-consistently induced dipole moment consisting of a pair of separated charges. A previous polarizable water model (COS/B2), upon which the improved versions are based, was developed by Yu, Hansson and van Gunsteren [J. Chem. Phys. 118, 221 (2003)]. To improve the COS/B2 model, which overestimated the dielectric permittivity, one additional virtual atomic site was used to reproduce the water monomer quadrupole moments besides the water monomer dipole moment in the gas phase. The molecular polarizability, residing on the virtual atomic site, and Lennard-Jones parameters for oxygen-oxygen interactions were varied to reproduce the experimental values for the heat of vaporization and the density of liquid water at room temperature and pressure. The improved models were used to study the properties of liquid water at various thermodynamic states as well as gaseous water clusters and ice. Overall, good agreement is obtained between simulated properties and those derived from experiments and *ab initio* calculations. The COS/G2 and COS/G3 models may serve as simple, classical, rigid, polarizable water models for the study of organic solutes and biopolymers. Due to its simplicity, COS type of polarization can straightforwardly be used to introduce explicit polarization into (bio)molecular force fields.

**References:** manuscript in press (*J. Chem. Phys*.)

**Title:** Characterisation of the denaturation of human α-lactalbumin in urea by molecular dynamics simulations

**Researchers**: Lorna J. Smith*
Rachel M. Jones*
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland
* Dept of Chemistry, University of Oxford, Oxford, U.K.

**Description:**

Molecular dynamics simulations have been run to characterise the non-cooperative denaturation of the molten globule A-state of human α-lactalbumin by urea. A solvent of explicit urea and water molecules has been used corresponding to a urea concentration of approximately 6M. Three simulations have been performed at temperatures of 293K, 360K and 400K with lengths of 2ns, 8ns and 8ns respectively. The simulations have been compared with experimental data from NMR studies of human α-lactalbumin and related peptides. During the simulations hydrogen bonds form from the protein to both urea and water molecules as intra-protein hydrogen bonds are lost. Urea competes efficiently with water as both a hydrogen bond donor and acceptor. Radial distribution functions of water and urea around hydrophobic side chain atoms show a significant increase in urea molecules in the solvation shell as the side chains become exposed during denaturation. A considerable amount of native-like secondary structure persists throughout the simulations. However, in the simulations at 360K and 400K there are substantial changes to the packing of aromatic and other hydrophobic side chains in the protein and many native contacts are lost. The results suggest that during the non-cooperative denaturation of the molten globule, secondary structure elements are being stabilised by non-specific, non-native interactions.

**References:** manuscript submitted (*Proteins*)

**Title:** Carbopeptoid folding: effects of stereochemistry, chain length and solvent

**Researchers**: Riccardo Baron
Dirk Bakowies
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland

**Description:**

The folding of a polypeptide chain into the stable threedimensional structure of a biologically active protein is still not understood in atomic detail. However, several research groups have recently reported successful atomistic simulations of secondary-structure formation, including the formation of helices of different types, β turns and β sheets of α- and β-peptides. Insight into the nature of both the folding process and the unfolded state has been obtained from various studies simulating the reversible folding of peptides. This development is encouraging and indicates that the biomolecular force fields in use are approaching the accuracy required to predict folding equilibria, although this has so far been demonstrated only for short polypeptides. Experimentally, significant progress has been made in the design and synthesis of peptide analogues that mimic secondary-structure elements of proteins, such as a helices, turns, and β sheets. For example, carbopeptoids, homooligomers of sugar-containing amino acids, have been prepared with both furanose and pyranose residues. These carbopeptoids are members of the family of δ-peptides, which may formally be constructed from α-peptides by replacement of every second peptide fragment with a substituted tetrahydrofuran (THF) or tetrahydropyran ring. These molecules have potential applications as drugs that block protein–protein interactions and inhibit enzyme catalysis.

**References:** Angew. Chem. Int. Ed., 43 (2004) 4055
Angew. Chem. 116 (2004) 4147-4151

**Title:** Alpha- and beta-polypeptides show a different stability of helical secondary structure

**Researchers**: Thereza Soares
Markus Christen
Kaifeng Hu
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland

**Description:**

β-polypeptides are known to adopt helical secondary structure in organic solvents, even for rather short chain lengths. It is investigated whether a short α-polypeptide with amino-acid side chains that enable β-peptides to adopt helical structures, can maintain or adopt stable helical structure in methanol or in water. The molecular dynamics simulations do not predict a particular fold, which indicates an essential role for the additional methylene moiety in the backbone of β-peptides regarding helix stability.

**References:** Tetrahedron **60** (2004) 7775-7780

**Title:** Are NMR-derived model structures for peptides representative for the ensemble of structures adopted in solution? Probing the fourth helical secondary structure of β-peptides by molecular dynamics simulation

**Researchers**: Alice Glättli
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland

**Description:**

Two methods for the conformational interpretation of NMR data of beta-hexapeptide are compared: Conventional structure determination by simulated annealing in vacuo applying NOE distances and dihedral-angle restraints and unrestrained molecular dynamics (MD) simulation using a thermodynamically calibrated force field. Both ensembles of structures fulfill the available NMR data, but are structurally rather different. While the simulated annealing procedure suggests the formation of a 2_8-P-helix, the unrestrained MD simulations indicate that the experimental data can also be described by a much broader conformational ensemble where 2.5_12-P-helical conformations are significantly present.

**References:** Angew. Chem. Int. Ed. Engl. (2004) accepted

**Title:** Do valine side-chains have an influence on the folding behavior of β-substituted β-peptides?

**Researchers**: Alice Glättli**
Dieter Seebach*
Wilfred F. van Gunsteren**

**Institute/Group:** *Laboratory of Organic Chemistry, ETH Hönggerberg, Zürich, Switzerland
**Laboratory of Physical Chemistry, ETH Hönggerberg, Zürich, Switzerland

**Description:**

The influence of the presence of valine side-chains on the folding-unfolding equilibrium and in particular on the $3_{14}$-helical propensity of $\beta^3$-peptides is investigated by means of molecular dynamics simulation. To that end the valine side-chains in two different $\beta^3$-peptides were substituted by leucine side-chains. The resulting four peptides, of which three have never been synthesized, were simulated for 150 to 200 ns at 298 and 340 K starting from a fully extended conformation. The simulation trajectories obtained are compared with respect to their structural preferences and folding behavior. All four peptides show a similar folding behavior and are found to predominantly adopt $3_{14}$-helical conformations, irrespective of the presence of valine side-chains. No other well-defined conformation was observed at significant population in any of the simulations. Our results imply that $\beta^3$-peptides show a structural preference for $3_{14}$-helices independent of the branching nature of the side-chains, in contrast to what has been previously proposed on the basis of circular dichroism measurements.

**References:** Helv. Chem. Act. (2004) accepted

**Title:** Estimating entropies from molecular dynamics simulations

**Researchers**: Christine Peter
Chris Oostenbrink
A. van Dorp
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland

**Description:**

While the determination of free-energy differences by MD simulation has become a standard procedure for which many techniques have been developed, total entropies and entropy differences are still hardly ever computed. An overview of techniques to determine entropy differences is given, and the accuracy and convergence behavior of five methods based on thermodynamic integration and perturbation techniques was evaluated using liquid water as a test system. Reasonably accurate entropy differences are obtained through thermodynamic integration in which many copies of a solute are desolvated. When only one solute molecule is involved, only two methods seem to yield useful results, the calculation of solute–solvent entropy through thermodynamic integration, and the calculation of solvation entropy through the temperature derivative of the corresponding free-energy difference. One-step perturbation methods seem unsuitable to obtain entropy estimates.

**References:** J.Chem.Phys. **120** (2004) 2652-2661

**Title:** A biomolecular force field based on the free enthalpy of hydration and solvation: the GROMOS force-field parameter sets 53A5 and 53A6

**Researchers**: Chris Oostenbrink
A. Villa*
A.E. Mark*
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland
*Groningen Biomolecular Sciences and Biotechnology Institute (GBB), University of Groningen, Groningen, The Netherlands

**Description:**

Successive parameterizations of the GROMOS force field have been used successfully to simulate biomolecular systems over a long period of time. The continuing expansion of computational power with time makes it possible to compute ever more properties for an increasing variety of molecular systems with greater precision. This has led to recurrent parameterizations of the GROMOS force field all aimed at achieving better agreement with experimental data. Here we report the results of the latest, extensive reparameterization of the GROMOS force field. In contrast to the parameterization of other biomolecular force fields, this parameterization of the GROMOS force field is based primarily on reproducing the free enthalpies of hydration and apolar solvation for a range of compounds. This approach was chosen because the relative free enthalpy of solvation between polar and apolar environments is a key property in many biomolecular processes of interest, such as protein folding, biomolecular association, membrane formation, and transport over membranes. The newest parameter sets, 53A5 and 53A6, were optimized by first fitting to reproduce the thermodynamic properties of pure liquids of a range of small polar molecules and the solvation free enthalpies of amino acid analogs in cyclohexane (53A5). The partial charges were then adjusted to reproduce the hydration free enthalpies in water (53A6). Both parameter sets are fully documented, and the differences between these and previous parameter sets are discussed.

**References:** J. Comp. Chem. **25** (2004) 1656 - 1676

**Title:** Amine hydration: A united-atom force field solution

**Researchers**: Chris Oostenbrink
Daniel Juchli
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland

**Description:**

The free energies of hydration for ammonia and mono-, di-, and trimethylated amines experimentally show an unexpected trend that has in the past been difficult to reproduce computationally. Absolute and relative free energies of hydration of these compounds were calculated using the OPLS all-atom and the united-atom GROMOS force fields. Both force fields reproduce the relative free energy of hydration, but the absolute free energies of hydration were only reproduced within $k_BT$ when using the newly developed GROMOS parameter set 53A6. Relative free energies of solvation in chloroform could also be reproduced, indicating a proper partitioning of the compounds between polar and apolar media. Overall we conclude that it is possible to resolve the amine hydration problem using a simple united atom force field.

**References:** manuscript submitted (*JACS*)

**Title:** Validation of the 53A6 GROMOS force field

**Researchers**: Chris Oostenbrink
Thereza A. Soares
Nico F.A. van der Vegt*
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland
*****Max-Planck-Institute, Mainz, Germany

**Description:**

The quality of biomolecular dynamics simulations relies critically on the force field that is used to describe the interactions between particles in the system. Force fields, which are generally parameterized using experimental data on small molecules, can only prove themselves in realistic simulations of relevant biomolecular systems. In this work we begin the validation of the new 53A6 GROMOS parameter set by three test cases. Simulations of the well-studied 129 residue protein hen egg-white lysozyme, of the DNA dodecamer d(CGCGAATTCGCG)$_2$, and of a proteinogenic $\beta^3$-dodecapeptide were performed and analysed. It was found that the new parameter set performs as good as the previous parameters sets in terms of protein (45A3) and DNA (45A4) stability and that it is better at describing the folding – unfolding balance of the peptide. The latter is a property that is directly associated with the free enthalpy of hydration, to which the 53A6 parameter set was parameterized.

**References:** manuscript submitted (*Eur. Biophys. J*)

**Title:** Computer simulation studies on the solvation of aliphatic hydrocarbons in 6.9 M aqueous urea solution

**Researchers**: Daniel Trzesniak
Nico F.A. van der Vegt*
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland
*Max-Planck-Institute, Mainz, Germany

**Description:**

We report solvation free energies for six aliphatic hydrocarbons in 6.9 M urea–water mixture obtained by molecular dynamics simulations. Hydrocarbon transfer free energies from water to the urea solution are also presented. Our calculations predict that, except for methane, aliphatic hydrocarbons are more soluble in 6.9 M urea than in water, in satisfactory agreement (deviations smaller than 2 kJ $mol^{-1}$) with experimental transfer free energies reported in the literature. An analysis of solute–solvent contributions to the solvation enthalpies and entropies indicates that urea enhances the solvation of hydrocarbons compared to pure water due to a favourable van der Waals interaction with the solute whereas the solute–solvent entropy opposes the hydrocarbon transfer. Radial distribution functions between the solute and the solvent are examined and together with an analysis based on Kirkwood–Buff theory indicate a weak preferential urea–hydrocarbon binding. The entropic penalty related with solute urea association is discussed in terms of the molecular interactions in solution.

**References:** Phys. Chem. Chem. Phys. **6** (2004) 697-702

**Title:** Comparison of properties of Aib-rich peptides in crystal and solution: A molecular dynamics study

**Researchers**: Haibo Yu
Maaike Ramseier
Roland Buergi,
Wilfred F. van Gunsteren

**Institute/Group:** Laboratory of Physical Chemistry, ETH Hönggerberg, Zurich, Switzerland

**Description:**

In order to study the differences of the structural properties of Aib-rich peptides in solution and in crystalline state, molecular dynamics (MD) simulations of the Aib-containing peptide II (*p*BrBz-$(Aib)_5$-Leu-$(Aib)_2$-OMe) were performed in crystalline state starting from two different conformers obtained experimentally by X-ray diffraction. The structural properties as derived from X-ray crystallography (*e.g.* torsional angles and hydrogen bonds) are well reproduced in both, constant-volume and constant-pressure simulations, although the force-field parameters used result in a too high density of the crystals. Through comparison with the results from previous MD and nuclear magnetic resonance (NMR) studies of the very similar peptide I (Z-$(Aib)_5$-Leu-$(Aib)_2$-OMe) in dimethylsulfoxide (DMSO) solution, it is found that in the crystal simulation the conformational distribution of peptide II is much narrower than that in the solution simulation of peptide I. This leads to a significant difference in $^3J$(HN, HCα) coupling constant values in agreement with experimental data, whereas the NOE intensities or proton-proton distance bounds appear insensitive to the difference in conformational distribution. For small peptides the differences between their conformational distribution in the crystalline form and in solution may be much larger than for proteins, which should be kept in mind when interpretating molecular properties in the solution state using X-ray crystallographic data.

**References:** ChemPhysChem **5** (2004) 633-641

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

**Researchers:** Martin Wild
Andreas Roesch
Peter Tschuck
Christian Schneeberger
Martin Schraner
Atsumu Ohmura

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

**Description:**

Human induced climate change is, by its nature, a problem of global dimensions. The most powerful tools to investigate the potential impact of human activities on the Earth's climate are three dimensional numerical models of the global climate system. Such models are used in our projects to investigate the response of the Earth's climate to natural and human induced perturbations. The emphasis is on the simulation of present and future climate, using the latest model version of the global climate model developed at the Max Planck Institute for Meteorology in Hamburg (ECHAM5). With this institution, the ETH group has been collaborating in the field of global climate modeling over more than a decade. Due to the generous computational resources allocated to this by the National Center for Scientific Computing (CSCS) in Manno, scenario runs with a very high global resolution of 1.1° can be carried out. Scenarios for the late 21th century have been completed at CSCS during the reporting period, with increased levels of atmospheric greenhouse gases as given in the Special Report on Emission Scenarios (SRES) A2 an B2 provided by IPCC (Intergovernmental Panel on Climate Change).
The focus of the ETH group in this context is on the near surface climate, from global down to European and Alpine scales. Particular emphasis is placed on the surface energy and water exchange processes, and their potential changes under increased greenhouse forcing (Wild et al. 2004). Of interest in this context is, for example, the change in the atmospheric thermal emission downwelling to the surface, which is the most direct effect felt at the surface from a change in atmospheric greenhouse gas composition. GCM estimated changes of this greenhouse forcing can be related to worldwide surface measurements, which are collected at ETH within the Baseline Surface Radiation Network (BSRN). This allows an early detection of the greenhouse effect from a surface perspective (Wild 2004). A further challenge for the models are the simulation of significant trends in surface insolation, which largely affect climate change (Wild et al. 2004).
A further research focus is on the impact of greenhouse warming on the cryosphere (snow, mountain glaciers, polar ice sheets and their effects on sea level). The high spatial resolution of the scenarios allows unprecedented estimates of the cryospheric contribution to sea level changes, resulting in interesting new outcomes for the future contribution of Greenland to sea level (Wild et al. 2003, Huybrechts et al.2004).

**References:** See separate list

**Title:** Computational Optoelectronics

**Researchers:** Bernd Witzigmann
Matthias Streiff
Biju Jacob
Dölf Aemmer

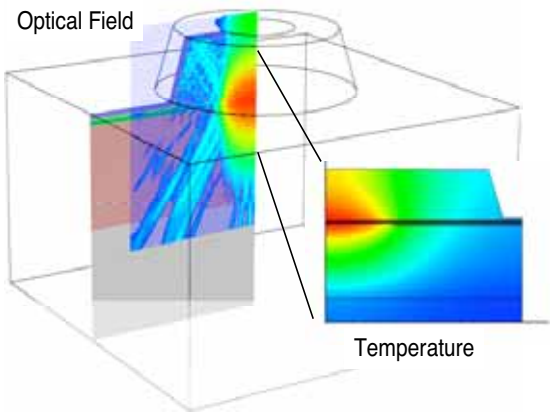
**Institute/ Group:** Integrated Systems Laboratory/
Computational Optoelectronics Group

**Description:**

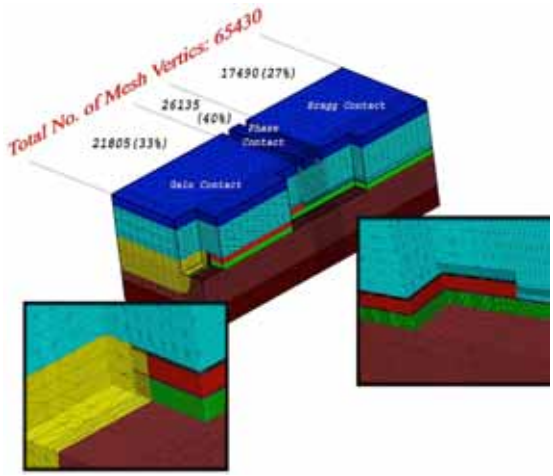
The Computational Optoelectronics group aims to develop models and state-of-the-art simulation tools for optoelectronic devices and systems. Present commercial grade devices routinely draw on material properties engineered on an atomic scale, utilizing advanced physics concepts such as quantum effects both in electronics and optics. Novel applications in lighting, optical sensing and processing technologies drive exciting research in the field of novel materials and device concepts.

Detailed physics-based simulations allow to study the optical, electronic and thermal aspects systematically and to contribute substantially to these research activities. The computational tools only reach a predictive level if the microscopic equations are solved in multiple spatial dimensions and the coupling of electronic, optical, and thermal mechanisms are taken into account. As a natural consequence, high-performance computing is utilized in order to solve the underlying coupled systems of equations.

Our current projects include electro-opto-thermal simulation of Vertical Cavity Surface Emitting Lasers (VCSELs), Simulation of Integrated Tunable Lasers, Electromagnetic Simulation of Microcavities, and a first-principle calculation of the optical properties of composite materials. The simulations are run on compute-servers at Integrated Systems Laboratory, as well as the IBM SP4 system at CSCS Manno in a *Large User Project*. The figures below illustrate some of the project results.




Electro-Opto-Thermal Simulation of a Vertical-Cavity Surface Emitting Laser (VCSEL).




Mesh for fully 3-dimensional Simulation of an Integrated Tunable Laser.

**Title:** Automated NOESY spectral analysis and NMR structure determination using the new software RADAR

**Researchers:** Torsten Herrmann
Francesco Fiorito
Pascal Bettendorff
Kurt Wüthrich

**Institute:** Institut für Molekularbiologie und Biophysik

**Description:**
This project is focused on automated NMR data analysis for three-dimensional structure determination of biological macromolecules in solution, with the prime objectives of increasing the efficiency and the reliability of protein structure determination by NMR. In this process, the presently used software for interactive analysis of multidimensional NMR spectra is being replaced by the fully automated routine RADAR. The software package RADAR will combine and tightly merge the functionalities of the two algorithms ATNOS for automated NOESY peak picking and CANDID for automated NOE assignment, and it should enable direct refinement of NMR structures of proteins against the raw NMR data.
RADAR is based on an input of experimental 2D and heteronuclear-resolved 3D [1H,1H]-NOESY spectra and a chemical shift list from previous, independently performed sequence-specific resonance assignment.
Further developments will include attempts to add automated sequence-specific assignment from minimal sets of NMR spectra.

**References:**
Herrmann, T., Güntert, P. & Wüthrich, K
Protein NMR structure determination with automated NOE assignment using the new software CANDID and the torsion angle dynamics algorithm DYANA.
J. Mol. Biol. **319**(1) (2002) 209-227

Herrmann, T., Güntert, P. & Wüthrich, K.
Protein NMR structure determination with automated NOE-identification in the NOESY spectra using the new software ATNOS.
J. Biomol. NMR **24**(3) (2002) 171-189

**Title:** Structural studies of prion proteins

**Researchers:** Dominik Lysek
Barbara Christen
Daniel Roberto Perez Lagos
Francesco Fiorito
Christine von Schroetter
Simone Hornemann
Kurt Wüthrich

**Institute:** Institut für Molekularbiologie und Biophysik

**Description:**
The prion protein (PrP) is an indispensable factor in the development of transmissible spongiform encephalopathies (TSEs), such as Creutzfeldt-Jakob disease in humans, BSE ("mad cow disease") in cattle, and scrapie in sheep. The prion protein is a highly conserved glycoprotein in mammals, where it is predominantly expressed in neuronal tissue, and which has also been found in birds and reptiles. We have solved three-dimensional structures of the normal recombinant form of a selection of mammalian prion proteins, and are analyzing similarities and differences that might bear on the species barrier for infectious transmission of TSEs. Further we are extending these studies to birds and reptiles in search of new insight into the physiological role of normal PrPs. With the same goal in mind we have recently started a program of studies of intermolecular interactions with PrPs to extend and supplement the structure determinations. An important part of these projects is the cloning and expression of wild-type and variant prion proteins with and without isotope labeling for NMR studies.

**References:**

Lührs, T., Riek, R., Güntert, P. and Wüthrich, K.
NMR structure of the human doppel protein.
J. Mol. Biol. **326** (2003) 1549-1557

Zahn, R., Güntert, P., von Schroetter, C. and Wüthrich, K.
NMR structure of a variant human prion protein with two disulfide bridges.
J. Mol. Biol. **326** (2003) 225-234.

Lysek DA, Wüthrich K.
Prion protein interaction with the C-terminal SH3 domain of Grb2 studied using NMR and Optical Spectroscopy.
Biochemistry **43** (2004) 10393-10399

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**Title:** Structural studies of pheromone-binding protein from Bombyx mori (BmPBP)

**Researchers:** Fred Damberger
Erich Michels
Reto Horst
Kurt Wüthrich

**Institute:** Institut für Molekularbiologie und Biophysik

**Description:**
Odorant-binding proteins (OBPs) occur at high concentrations in the lymph of insect olfactory sensilla and transport the hydrophobic odorant molecules from the periphery of the sensillum to the olfactory receptors. The pheromone binding proteins (PBPs) are a subclass of the OBPs which bind pheromones used in insect communication. Our work so far shows that the pheromone binding protein from the silkmoth Bombyx mori, (BmPBP), undergoes a pH-dependent conformational transition between two forms (BmPBPA observed at pH 4.5 and BmPBPB at pH 6.5) which is likely to relate to biological function. To obtain a more complete picture of the function of BmPBP, we have determined the solution structure of BmPBPA at pH 4.5. Strikingly, a conformationally extended dodecapeptide which is on the surface in the crystal structure of the BmPBP-bombykol complex forms a regular a-helix which inserts into the core of the protein and occupies the ligand binding site. This explains the absence of binding observed for BmPBP at pH 4.5. BmPBP represents a novel mechanism of intramolecular protein regulation involving regions distant in the sequence. We are following up on these initial results with further study of BmPBP under different solution conditions to provide insight into structure-function correlations, which might be applicable to an entire class of proteins with pheromone-binding function.

**References:** Manuscripts are in preparation.

**Title:** Structural aspects of the type-1 pilus assembly

**Researchers:** Reto Horst
Pascal Bettendorff
Torsten Herrmann
Rudi Glockshuber
Kurt Wüthrich

**Institute:** Institut für Molekularbiologie und Biophysik

**Description:**
Type-1 pili ("Fimbrae") are large, heterooligomeric protein filaments of uropathogenic E. coli strains that are required for the attachment of the bacteria to host cell surfaces and that enable survival inside of macrophages. These pili are constituted by up to 2000 protein subunits, where FimA is the most abundant one (>98%), with FimF, FimI, FimG and the mannose-binding subunit FimH making up the rest. We aim at contributing to the understanding of the mechanisms of pilus assembly, which involve additional proteins in the periplasm and the bacterial membrane. Thus, in a previous collaboration with the group of Prof. R. Glockshuber, we solved the solution structure of FimC, a periplasmic assembly factor which is not a structural component of the pili but is required for pilus assembly in vivo. The actual pilus assembly on the cell surface is performed by the membrane protein FimD, which is another target for obtaining structural information. The application of new, TROSY-based NMR techniques will provide insights into the interactions of the different proteins involved and their structures.

**References:** Manuscripts are in preparation.

# 6

# High-performance Hardware

## 6.1 Competence Center for Computational Chemistry

The following resources are available:

- a cluster of 40 dual-processor PC's
- two Compaq Alpha Servers with 6 and 8 EV6/525 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 2003/2004, which is published in November 2004.

Information: http://www.igc.ethz.ch/c4

6.2 Swiss Center for Scientific Computing (CSCS)

## 1. Preface

2003 was a year of fundamental changes at CSCS. The new organizational setting as an autonomous unit of ETH Zurich led by performance mandate and global budget are the most visible expressions of these changes. In this framework, the new CSCS management under the direction of General Manager Dr. Marie-Christine Sawley has the operational freedom and responsibility to realise the strategic guidelines set by the CSCS Steering Board for developing and establishing a world-class high-performance computing centre. In March 2003, former director Prof. Michele Parrinello chose to resign from this position in order to concentrate on his research as a professor of ETH Zurich in computational science. The ETH Board commissioned a taskforce to define the future direction, organisation and framework of the centre. By the middle of the year, Marie Christine Sawley had taken over the position of executive manager of CSCS. She worked out and proposed a business plan for CSCS to the working group,which outlines the scientific and technological strategy, the budget and the management that will enable CSCS to become a leading-edge HPC centre of international scale. The final proposals by the working group, which were based on the functioning principles of the FLAG institutions of the federal administration, were accepted by ETH Board and ETH Zurich by the end of 2003 and took effect in 2004. Whilst these fundamental changes were being planned and unfolded, CSCS continued to serve the Swiss scientific community with its outstanding technical services and developing capabilities. The results of these activities are collected in the report at hand. It is now the responsibility of the umbrella institutions, ETH Zurich and ETH Board, to secure adequate and continuous future funding for a sustainable development of the centre. Under such conditions, I strongly believe that the quality of the science that was enabled by CSCS during the last year together with the new organisation and direction that have been established, bode extremely well for what the centre will be able to achieve in the future.

Dr. Heinrich Rohrer Chairman of the 2003 CSCS working group

## 2. Word from the General Manager

2003 saw the preparation and acceptance of a major plan, aiming at positioning the CSCS as a key partner for supporting excellence in research and development of knowledge at the frontiers of science needing high performance IT capabilities. As a result of the recommendations made by the working group piloted by Dr. Heinrich Rohrer, the Centre started to reinforce its capacity to serve the national scientific community, to define and to implement the next generation of infrastructure both hardware and software- that will enable further scientific discovery, both on a national and international scale. As General Manager of the CSCS, I am very pleased to present you with an outlook on the scientific projects and on the work accomplished during this transition year. Based on this rich portfolio, and stimulated by the excellent experience with our present strategic partners the Computational Science Laboratory of ETH Zurich and Meteosuisse- close collaborations with scientific communities from the ETHs, the Universities and Universities of Applied Science, research institutions and partners from the private sector, will continue to develop, anchoring the CSCS in the ever evolving landscape for research and education, with specific skills and value added services. Since the beginning of 2004, the CSCS has become an autonomous unit of the ETH Zurich, working under global budget and performance mandate. The winter months of 2004 saw the indispensable changes take place that would make this new important step a reality: the CSCS Steering Board and Scientific Advisory Board were nominated, and a new internal structure was implemented at CSCS. This development necessitates investing both people competences and IT infrastructure, acting as stimulant for young talents. This exciting growth phase will be

accomplished in close synergy with our partners in the Italian speaking part of Switzerland, by contributing to a cluster of complementary competences.

Marie-Christine Sawley, General Manager

## 3. Partners and Projects

### 3.1 VA Tech Hydro Analysis of 3d Unsteady Free Surface Flows in Pelton Turbines:

Advanced Numerical and Experimental Investigations
The objective of this project is to develop an advanced method for flow simulation in Pelton turbines. Several water jets impinging the runner buckets ensure the motion of the impulse turbine, leading to complex characteristics of the flow,i.e. 3 D turbulent, 2 phases and unsteady. A newly developed CFD commercial code will be adapted and validated to perform such a flow simulation. An extensive experimental validation will be carried out through an innovative technique aimed to visualize the jet impingement and its complex interaction with the runner buckets. Furthermore, substantial work will be performed to develop modern tools for post processing CFD and experimental data. The result of the project will definitely allow the industrial partner to significantly improve the design process of Pelton turbines.

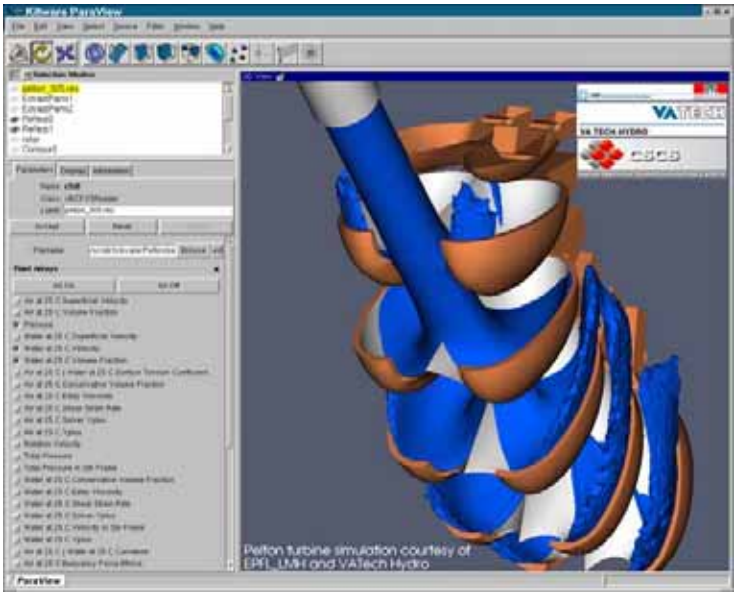


Figure 1: The water jet is shown leaving the injector, impinging the buckets at different angles and positions, and the water sheets being evacuated on the sides.

Project and Funding Partners includes: VA Tech Hydro SA; Ecole Polytechnique Federale de Lausanne, Laboratory for Hydraulic Machines; Swiss National Supercomputing Centre and the Innovation Promotion Agency (KTI/CTI) of the Swiss
Federal Office for Professional Education and Technology

Contact: J.M. Favre

### 3.2 CERN: High Energy Physics community

The Swiss Tier 2 of the CERN LCG Project The European High Energy Physics community is building the Large Hadron Collider (LHC) the worlds biggest accelerator at (CERN) in Geneva . Challenges to be faced by physicists are unprecedented: data collected by these experiments will allow for exploration of new frontiers of the fundamental laws of nature, like the Higgs mechanism with possible discovery of the Higgs boson. One of the greatest challenges of the LHC project will be the acquisition and analysis of the data. The equivalent data volume is between 100 MByte/sec and 1 GByte/sec. Each experiment is expected to collect 1 PByte of raw data per year. 2000 physicists per experiment contribute to the development of hardware and software and they expect to have almost instantaneous access to the data and to a set of up-to-date analysis tools. The goal of the LCG (LHC Computing Grid) project is to meet these unprecedented computing needs by deploying a worldwide computational grid service, integrating the capacity of scientific computing centres spread across Europe, America and Asia into a virtual computing organisation. Switzerland, as member state of CERN, actively participates in the LHC project as a whole. The CHIPP group reunites the University laboratories in Switzerland involved in scientific analysis and development of the data produced by the experiments of the LHC. The CSCS has teamed up with CHIPP since 2003 by establishing the first prototype of a LCG Tier-2 cluster.

Contact: G. Volpato

### 3.3 European Projects

EUROGRID

The main objective of EUROGRID was to build a European GRID infrastructure that gives users a seamless, secure access to High Performance Computing resources and that allows progress in computational science in Europe. In three years of activities this project has demonstrated the suitability of GRIDs for selected scientific and industrial communities, addressed the specific requirements for these communities, and highlighted the benefits of using GRIDs. CSCS contributed directly in the HPC Research GRID and in the Meteo-GRID work packages of the project. The first work package consiste in establishing a European GRID network of leading High Performance Computing centres from different European countries. The second work package's goal was to exploit the established GRID in order to deliver on-demand weather forecast services. Grid computing is emerging as an effective approach to solve large-scale problems that involve the cooperation between different entities and can require high-performance computing resources. The grid paradigm is particularly suitable for weather forecast applications that need observation data inputs from different sources and, depending on different parameters such as forecast time and resolution, demand a specific computing power. For this purpose, CSCS developed the LM plug-in application that extends the basic functionality of the standard EUROGRID software in order to provide an ASP solution for weather forecasts. This application allows the performance of high-resolution short-range weather forecasts with the relocatable non-hydrostatic Lokal-Modell (LM) of DWD in an UNICORE based grid.

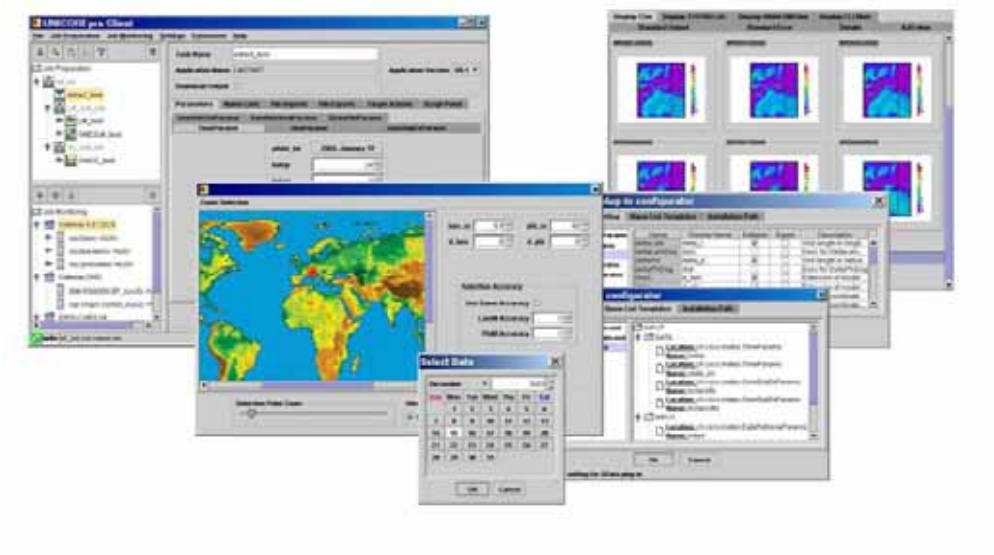

Figure 2: Overview of the graphical user interface of the LM plug-in.relocatable nonhydrostatic Lokal-Modell (LM) of DWD in an UNICORE based grid.

In particular, the LM plug-in is a Java application available as a UNICORE client plug-in that defines an abstract model for the weather forecast process and uses this model to build, configure and execute a job in an UNICORE grid. Performing a weather forecast with LM is a complex process that involves various activities such as derivation of the topographical data set for the selected geographical domain, extraction of initial and lateral boundary data sets for LM, interpolation with GME2LM, numerical weather prediction with LM, and final post processing and/or visualization of forecast products. Each activity has different requirements respect to software and hardware resources. For example the topographical data in the first step consist of high resolution information about orography, land fraction, soil type and vegetation that are derived from a large data set of about 7 GBs. This is not an expensive operation in terms of computing power but the availability of a global topographical data set has to be guaranteed. On the other hand the execution of LM is a computationally demanding task that requires high performance computing facilities in order to produce a weather prediction in a reasonable amount of time. Indicatively, a typical 48 hours forecast with LM for a domain of 300 x 300 grid points and 40 vertical layers needs up to 60 x $10^{12}$floating point operations. Therefore, the UNICORE paradigm is perfectly suitable for this kind of problem since it allows the selection of the most appropriate architecture for the specific task and uses heterogeneous resources in a collaborative way in order to produce the final results.

The final review meeting for the EUROGRID project was held on 22nd January 2004 in Paris. This was the occasion to show the results of three years of activities carried out by the project consortium. The project received very good comments from the reviewers, who particularly appreciated and underlined the technical value of development and improvements of the GRID middlewareand the latest development comments from the review the work done in the further development and improvement of the GRID middleware.

Contact: M. Ballabio

**ENACTS**

The ENACTS (European Network for Advanced Computing for Science) aims to evaluate future trends of the way in which computational science will be performed and the ensuing pan-European implications. The project activities were organized around 3 phases: a set of preliminary technology studies and surveys, a deployment of a grid testbed and users'need survey, and a final dissemination phase.

For the study phase different reports such as "GRID Service Requirements", "HPCTechnology Roadmap", "Data Management", "Distance Learning and Support" and "Software Efficiency and Re-usability" were produced . CSCS contributed to the preliminary study activities with the "Grid Enabling Technology" report written together with the Foundation for Research and TechnologyHellas (FORTH) in Greece. All the reports are now publicly available on the ENACTS web site.

During the 4th project meeting held in Prague on the 11-13 March 04, the ENACTS pan- European Metacentre was presented as applications demonstrator. In particular the work was based on QCDGrid (Quantum Chromodynamics) software, Globus middleware and XML technologies for meta-data representation and cataloguing. The demonstration testbed aimed to draw together the results from all of the technology studies and evaluate their practical consequences for operating a pan-European metacentre and constructing a best-practice model for collaborative working amongst individual facilities. The project has now entered its final phase and in the next year the users' needs survey will be produced and all dissemination activities will take place. In order to disseminate the project results, the ENACTS consortium will organize a workshop for users of molecular simulation techniques, one of the core user groups of computational science.

Contact: N. Nellari

**PRISM**

PRISM is a major EU-financed program for integrated earth system modeling with a goal to develop the pilot European climate modeling software infrastructure, enhance the efficiency of earth system modeling in Europe and pave the way for the establishment of a European Climate Computing Facility. The expected product will be a flexible, efficient, portable, and user friendly community infrastructure for earth system modelling and climate prediction. To reach this objective, PRISM will: -

-Create a European service and management infrastructure for developing, coordinating and executing a long-term programme of Europe-wide, multi-institutional climate and Earth System simulations

-Develop a European system of portable, efficient and user-friendly Earth System / climate community models and associated diagnostic/visualization software under standardised coding conventions that can be accessed by all European scientists.

As a result of the PRISM project, the scientific community involved in Earth system modelling in Europe will adopt a common software for model development, model diagnostics and visualization. This new approach will allow easy exchange of codes and easy execution of ensembles of climate simulations for different model configurations.

CSCS's contribution in the frame of this challenging project, was to assess the state, the trends, and the future of High Performance Computing (HPC) in relation to the development of PRISM components. This investigation is motivated by the need for early identification of the best suited programming languages and paradigms as well as parallelization strategies targeting the reduction of porting and maintenance efforts of the software product over different platforms, as well a good performance and scalability on leading edge HPC facilities over the years to come.

CSCS also substantially contributed to the definition of the PRISM Software Developer's Guide as the reference handbook describing the development practices, standards, and conventions recommended for the development of PRISM base software and components. The scope of this document includes any issue related to process, conventions, and standards in the design, implementation, and documentation of any software that will be developed in the frame of the PRISM project under the consideration of portability, sustained performance and ease of use .

Contact: A. Mangili

## 4. HPCN Technology and Resources

During this very important transition year the two major driving forces for the development of the CSCS High Performance Computing and Networking (HPCN) technologies and related services have been to continue delivering the high quality support to our national end-user community and to prepare for the major upcoming technology upgrades in 2004/2005 according to the new CSCS development plan. The permanently growing needs of our end-user communities, and a further reinforced emerging trend towards multi-physics and multi-scale application integration have driven our daily operational efforts in managing the very high and heterogeneous loads on both the parallel vector processing (PVP) NEC SX-5 and the massively parallel processing (MPP) IBM SP-4 supercomputers. Furthermore, the major upgrade projects of our data management services have been carried out. The data moving needs posed by HPC-systems have always required custom-enabled, supercomputing-specific data management enhancements (both for storage and networks) at the level of the architecture and software. Ever-higher data densities (for both disk and tape) and the permanently decreasing market cost of raw storage are however not being offset with corresponding data moving sustained performance improvements. This "divergence" issue, which is one of the biggest challenges for the mainstream market, is obviously even more critical for supercomputing centers. One of the major issues for the HPCN-centers within the time horizon of 2010 will be the integration of the heterogeneous supercomputers with the data management solutions and "hiding" the complexity introduced by the huge number of heterogeneous subcomponents. The CSCS data management upgrade project should set a base for future work of this kind and above all enable a smooth integration of the new CSCS supercomputing systems. In order to achieve its most important goal of making the most adequate HPCN-resources available (systems, networks, data management and storage) to the CSCS end-users community in a reliable, performing and easy-to-use fashion, the CSCS HPCN production environment has to be permanently developed and optimized based both on the continuous and pro active prospection and evaluation of new HPCN-technologies, as well as on the permanent assessment of the current and future users' requirements. To this end, a significant comprehensive analysis of the supercomputing technology and market trends has been initiated in the reporting year with the objective to provide the vision and strategic objectives that on a longer term will serve as a framework and fundament for the permanent detailed CSCS technology development planning process. The current "renaissance" of the

supercomputer architecture work both in the US and in Japan set a very positive and interesting environment for the CSCS upgrade projects in the nearest future.

Djordje Maric, CTO

**HPCN Resources**
In 2003, CSCS offered supercomputing services to the national
User community on the following architectures:

**Parallel Vector**
Processing (PVP), with a NEC SX-5 of 16 CPUs, totaling a theoretical peak performance of 128 GFlops and 64 Gbytes shared memory, running under Super-UX with NQS scheduler. The network connection is provided via GigabitEthernet, HiPPI and FastEthernet.

**Massively Parallel Processing (MPP),** with 8 IBM Regatta p-690 SMPs of 256 CPUs total, 768 GBytes of main memory, totaling a theoretical peak performance of 1.38 TFlops. The SP frames are tightly coupled and switched by a Double Colony system in order to provide a Parallel Environment with a Global Parallel File System of 4 TB. The overall system run on AIX with LoadLeveler job management system. The system is complemented by 2 Nighthawks (Power3 nodes, total of 32 CPUs and 32 GBytes main memory) with a peak performance of 48 GFlops.

Given the importance of the close integration of supercomputing with data management, CSCS has been offering its Users an application-oriented, integrated computing environment linked with very fast internal network connections.

The data management and archiving services are based on the SAM-FS Hierarchical Storage Management software, which handles an archived raw data volume currently in excess of 250 TB. A major upgrade of the CSCS Archive facility was started to allow Users to benefit from higher archive access performance and increased service availability. The core architecture of the high-performance production network is based on HiPPI and GigabitEthernet technologies with standard protocols. The deployment of the latest-available GigabitEthernet standard was launched during the reporting period, with the introduction of the routing equipment and two GigabitEthernet switches interconnecting the MPP, the PVP, the HP cluster, the Archive and the Front-end Environment. The CSCS local area network is integrated into the Swiss Academic and Research Network WAN (SWITCHlambda) ensuring the connection to CSCS's end-Users. The HPCN environment is constantly protected by a global security infrastructure that provides a suitable security service level for the national User community that comprises academia, federal government agencies and industry.

User Community The Swiss CSCS users community is widely distributed over the two Swiss Institutes of Technology and the Cantonal Universities (see also Fig. 3).

**HPCN Service Highlights**
In order to maintain and further develop the high quality of service provided to the broad and heterogeneous national User community, the HPCN Service Division has pursued a selected number of projects necessary to the future development of the Service (selected EU and KTI projects including GRID technologies evaluation). The focus of these development projects was twofold: (i)

further develop the key HPCN expertise to anticipate future service challenges, and (ii) in-house development of the methodologies and instruments not available on the market (tools for performance, scientific visualization, software engineering for large scientific applications and data basis) in order to provide new added value to users.

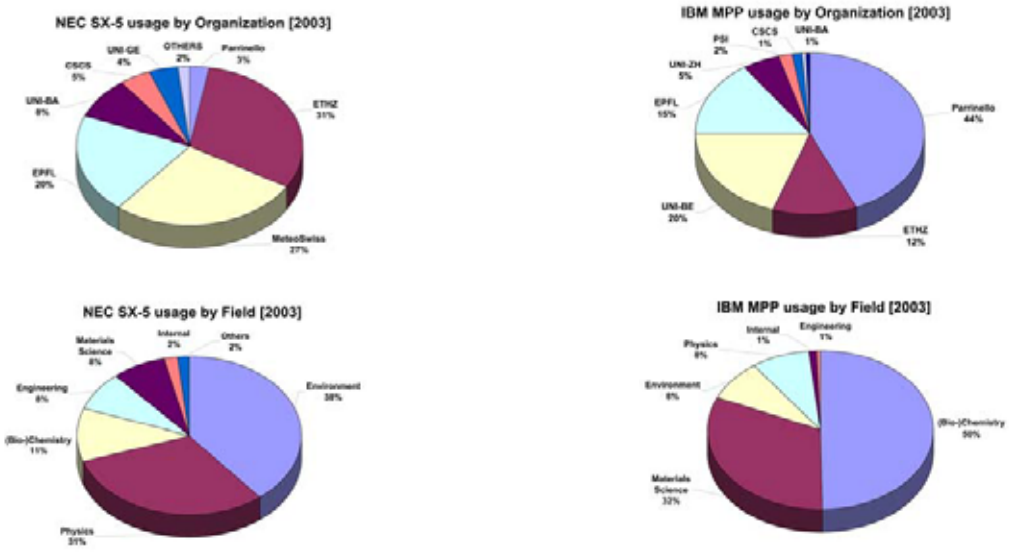


Figure 3: CSCS HPC resource usage statistics by fields and by organizations for 2003.

**HPC Systems Support**

A major success project started in 2003 was the upgrade of the CSCS data Archive facility, which involved both hardware and software upgrades as well as an architectural enhancement to the storage environment, along with the associated migration of the Archive service to the new upgraded environment. The CSCS data management system is designed to accommodate the permanently growing application requirements for total data storage, data movement and total data lifecycle management. The need for a sustainable and scalable annual growth in the range of +50% regarding both the capacity and the access bandwidth implies continuous and balanced extensions and migration towards higher density technology for disk, tape and data access paths, as well as major overall integration. The aim of the upgrade was to provide users with higher archive access performance and increased service availability, while still ensuring a seamless growth of the archive size. The major interventions and the new components that were integrated within the CSCS Archive production environment include: two new SUN SunFire V880 file and archive servers to increase I/O performance and availability of the file-serving system; Veritas Cluster Software to provide a high-availability solution in case of hardware and software failures as well as to provide absolutely minimum service downtime during periodic maintenance; integration of 6 TB raw of fast Disk Cache based on LSI Logic D280 to increase the cache size and performance, thus keeping a balanced architecture for optimal data moving performance; upgrade to the latest version of the HSM software and Filesystem (SAM-FS/QFS 4.0) to provide enhanced storage management capability and functionality; addition of a FiberChannel switch Brocade SilkWorm 3800 to load balance storage network traffic and eliminate single point of failures within the high-bandwidth FC network that interconnects the file servers with tape drives and disk cache; addition of a stand-by Automated Cartridge System Library Server to ensure redundancy of the tape library control

software. The whole upgrade has been planned to be implemented in steps, in order to minimize the service disturbance to all Users,with interventions scheduled at the times when critical production jobs were not impacted.

## 5. HPC Application Support

In the year 2003 much effort was spent in assisting the scientific community with the multiple facets of software engineering and those of application integration within the CSCS production environment. The aspects ranged from application porting, compilation and debugging, to high level algorithmic optimization, parallelization and vectorization. Solutions were implemented for data management and handling issues. We targeted the optimal integrated use of supercomputers, high speed networks and data management resources. These activities were mainly focused on the IBM MPP achitecture, which was into its first full year of production. Aiming at an efficient and effective use of the overall HPC facilities, the application support team continued the consolidation and the completion of the Computational Chemistry Framework, as well as the support and maintenance of Mathematical and Numerical Libraries. The available software portfolio now covers a wide spectrum of algorithms and methods, including specific architecture optimized libraries and development tools, along the most widely used Computational (Bio-)Chemistry application suites. Major achievements have also been made in the support of the NCCR-Climate community.

This community has important requirements not only related to efficient high-end computing, but also to data archiving and pre/post-processing. In this context the local establishment of the climatological ERA40 data base at CSCS represented a first important step towards allowing an integrated and user-friendly access to this data. Currently this dataset is widely used by a number of different research groups at ETH Zurich, MeteoSwiss, POW Davos and the University of Bern. In parallel we also provided support for the preparation of a new pre/post-processing Linux server that may now be used to access the archived ERA40 data, convert them to the required formats and prepare them for use in atmospheric and climate model simulations. Moreover, several new widely used climate applications where made available on the high-end computational facilities. The HPC Application Support group has also been involved in the European project PRISM , a pilot infrastructure project for the establishment of a EU climate research network. Our primary task was the definition of a set of recommendations and rules defining software engineering processing, coding rules and quality standards. This effort was included within the PRISM System Specification Handbook and proved to be a great opportunity for us to acquire and share new competencies on code portability and code quality standards across multiple platforms. Future involvements in this project will focus on execution and performance issues. Finally, a considerable effort was spent in processing incoming everyday User support requests as well as in consolidating and regularly updating the technical documentation made available under the CSCS User web portal.

**HPC Benchmarking and Development**

Major efforts have been invested in the further development of the "CSCS Performance Environment", essentially a collection of our own highly specialized system monitoring tools, with a particular focus on sustained performance aspects. Besides others, the performance environment consists of a set of client and server daemons permanently measuring runtime system, jobs and process performance. The currently supported platforms are the NEC SUPER-UX and IBM AIX based systems. Furthermore the server daemons are able to generate very compact process accounting files, that can be easily post-processed by a Java application we developed, reporting detailed accounting statistics at different levels (e.g. process, user, group, institute, application field, ...). Accounting data can be retrieved from databases (Oracle or MySQL) using JDBC API. Unlike other existing products, the tool allows the generation of global system usage statistics, as well as

detailed performance analysis of User codes. The investigation of emerging software technologies (Java, GRID, ..) has also been a key issue in extending the product spectrum that CSCS can offer its users. With the involvement in international projects such as EUROGRID and ENACTS it has been possible to explore GRID technologies. By using the acquired know-how it has been possible to develop a brand new product based on the LM regional weather forecast code able to deliver weather forecasts on demand in a GRID environment.

## 6. Advanced Scientific Visualization

The group provided visualization and media production to the overall CSCS user community and offered advanced prototyping and dedicated support in four activities: To further support our AVS/Express-based Molecular Sciences Visualization toolkit, with greater emphasis for crystallography (cf. Large User Project of Dr. Oganov, ETH-Z); To evaluate, prototype and implement several particle-based \ techniques for fluid flow visualization (cf. Large User Project of Prof. Kleiser, ETH-Z); to deploy the VTK/ParaView software enviroment on clusters with several interfaces for commercial flow solvers (CFX, TECPLOT, GAMBIT, MemCom) (cf. Institute of the Energy Sciences, EPF-L); and to develop a visualization environment for experimental and numerical data in turbo-machinery flow modelisation (cf. Industrial Project funded by the CTI: "Anaysis of 3D unsteady free surface flows in Pelton turbines" (see also Fig.1).

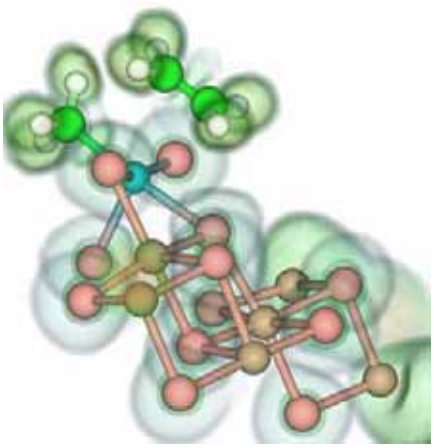

Figure 4: Data Visualization example: Structure of the pi-complex of an ethylene molecule with a Ti catalytic center in the chemical reaction leading to the formation of polyethylene. A parallel volume rendering of the electronic density around the molecule is performed with the VTK toolkit. A finite difference gradient estimator acts as a volume opacity multiplier to render homogeneous regions almost transparently. Model and Simulation by Mauro Boero (Dept. Of Physics, University of Tsukuba) and Michele Parrinello (CSCS), Data visualization by Jean M. Favre (CSCS)

## 7. MeteoSwiss

During the year under review, MeteoSwiss has carried out all its heavy computations at CSCS, as it has been doing for several years. The principal task outsourced to the CSCS is the computation of its numerical model simulating the atmospheric processes over a domain covering most of Western Europe. These simulations, starting from the state of the atmosphere at noon and midnight every day, serve primarily as guidelines for the weather forecasts issued by MeteoSwiss. But it is by far not the sole application. The results of these simulations also serve as input for follow-up models computing air particle trajectories and dispersion of pollutants for the National Emergency Operations Centre

(NEOC) located in Zurich as well as hydrological runoff forecasts at the Swiss National Hydrology Survey in Ittigen (BE). Model results are also sent operationally to the Swiss Federal Institute for Snow and Avalanche Research at Davos where they help to assess the risk of avalanches for the next three days. Next to these governmental institutions, model results are also disseminated to a large number of users like PhD students, researchers, firms and businesses in civil engineering, electricity production, agriculture, etc. Model development work is done on the computers of the CSCS, too. Model improvement is computationally intensive as any new scheme must be tested with a very large number of different weather situations in order to be certain that it will bring in average an improvement. As it has already been the case in the past years, the reliability of the CSCS for the production of our weather simulations was very high in 2003 and the support MeteoSwiss received from the CSCS specialists has been irreproachable both for the reaction time in case of problems during the production of the weather forecasts as well as for the improvement of the efficiency of our programme suite. Modern weather centres are large users of HPC facilities. They need them because their models become, like all the simulation models in science and engineering today, each year more complex, which means more computationally demanding. The supplementary requirement we have in meteorology is that our computations must be performed in a short lapse time; otherwise their operational utility drops dramatically. We are pleased to acknowledge that the CSCS has understood the national importance of the simulations of MeteoSwiss in Manno. It has also reacted very constructively and professionally to satisfy the time constrains under which our simulations must take place. For the future, it is of primary importance for MeteoSwiss that the CSCS keeps a very high HPC capability, first of all in computing power, but also in user support, without neglecting the needs for communication and archiving.

Jean Quiby Head, Modelling Group

## References


PRISM: PRogramme for Integrated earth System Modelling (http://prims.enes.org)

PRISM System Spec. Handbook
(http://prism.enes.org/Results/Documents/Handbook/handbook.v.1.0.3.pdf)

NCCR: National Centre of Competence in Climate Research
(http://www.nccr-climate.unibe.ch)

PRISM System Spec. Handbook
(http://prism.enes.org/Results/Documents/Handbook/handbook.v.1.0.3.pdf) PRISM

REDOC III.2 (http://www.cscs.ch/~amangili/papers/PRISM HPCtrends.pdf) PRISM

ARCDI II.5 (http://www.cscs.ch/~amangili/papers/PRISM SEguide.pdf)

CERN Large Hadron Collider (http://www.cern.ch/lcg)

EUROGRID: Application Testbed for European GRID computing
(http://www.eurogrid.org)

ENACTS: European Network for Advanced Computing Technology for Science
(http://www.enacts.org)

## 6.3 The Beowulf Clusters “Asgard” and “Hreidar”

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.

The 502-CPU Asgard Beowulf cluster built from 500 MHz Pentium-III CPUs, which was installed early in the year 2000 still works very well but is showing its age. The first stage of a replacement cluster, called Hreidar, was installed in summer of 2004 financed from startup funds of Prof. M. Troyer. This stage consists of 256 AMD Opteron CPUs clocked at 1.8 GHz, and each node has roughly eight times the compute power of an Asgard node.

The purchase of the second stage, consisting of additional 256 CPUs clocked at 2.2 GHz and connected by a very fast network is currently in progress. This stage is being financed from startup funds of Prof. Ralf Hiptmair (D-MATH), funds of the D-INFK as well as funds obtained by the Informatikdienste. A third stage is already being planned.

The contribution provided by the Informatikdienste will provide a large fraction of the computing power of the machine to all users of ETH. The Beowulf cluster is thus moving from a machine of the D-PHYS, D-MATH and D-MAVT to a central ETH resource, although substantial parts of the cluster remain dedicated to the departments financing the machine.

As regards the operating mode, the clusters are each 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 user projects the hardware, software, operating mode, account applications and user projects we refer to the Asgard web page at http://www.asgard.ethz.ch.

## 6.4 Information Technology Services

The following resources are available:

- Hewlett Packard Superdome Cluster consisting of
    - 1 HP Superdome (Stardust): 64 PA8600 CPUs (550 MHz), 64 GB Memory, 400 GB Disk, HP/UX Operating System
    - 1 HP Superdome (Pegasus): 32 Itanium2 CPUs (1500 MHz), 64 GB Memory, 400 GB Disk, HP/UX Operating System

  The cluster is used for parallel code taking advantage of the shared memory programming model offered by the cc-numa architecture of these systems. 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 cluster:

  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

- The Information Technology Services operate a Beowulf Cluster owned by the Departments Physics, Mathematics and Material Sciences. By the end of 2004 this cluster will be extended by 64 nodes for use as a central computing resource. The nodes will be Dual AMD Opteron 250 (2.4 GHz) systems with 8 GB memory and a Linux operating system. The cluster nodes will be connected by a high performance Quadrics QsNet II network.

# 7

# Outlook

This report documents the strength, scope and dynamics of CSE at ETH.

Computational research is stimulated in two directions, by creating the organisation and means to foster interdisciplinary research on an ETH wide basis, and by strengthening in each field the research which uses computation as a major tool. In both directions we expect to see further development.

In the various departments of ETH researchers in various fields of computation have been hired and we expect this trend to continue in the future.

In the coming year, the Master program in CSE will be finalized and approved so that our first set of Bachelors, which will finish in the fall of 2005, can directly enter the Master program. We shall see that more courses will be established which are directly tailored to the needs of students in CSE and this trend will continue in the years to come. In addition, more and more courses will be taught in English. As there is at the moment no strong organization in place for the handling of many applicants from outside of ETH, we shall currently not heavily advertise the new Master program. However this is definitely intended in the future.

In the summer of 2006 we are planning on a small, more workshop like, conference with our first group of Master students and with scientists involved in CSE and its teaching in order to assess the Bachelor and the Master program. This will give us the necessary feedback to optimize our programs.

We are of course looking forward to organize the International congress on Industrial and Applied Mathematics, ICIAM 2007, which will be held in Zürich. A considerable part of this congress will cover also the CSE domain.

Overall, we look optimistically into the future and are already looking forward to see the next annual report to find out about new exciting research happening at ETH.

Zürich, October 22, 2004
Rolf Jeltsch

# 8

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