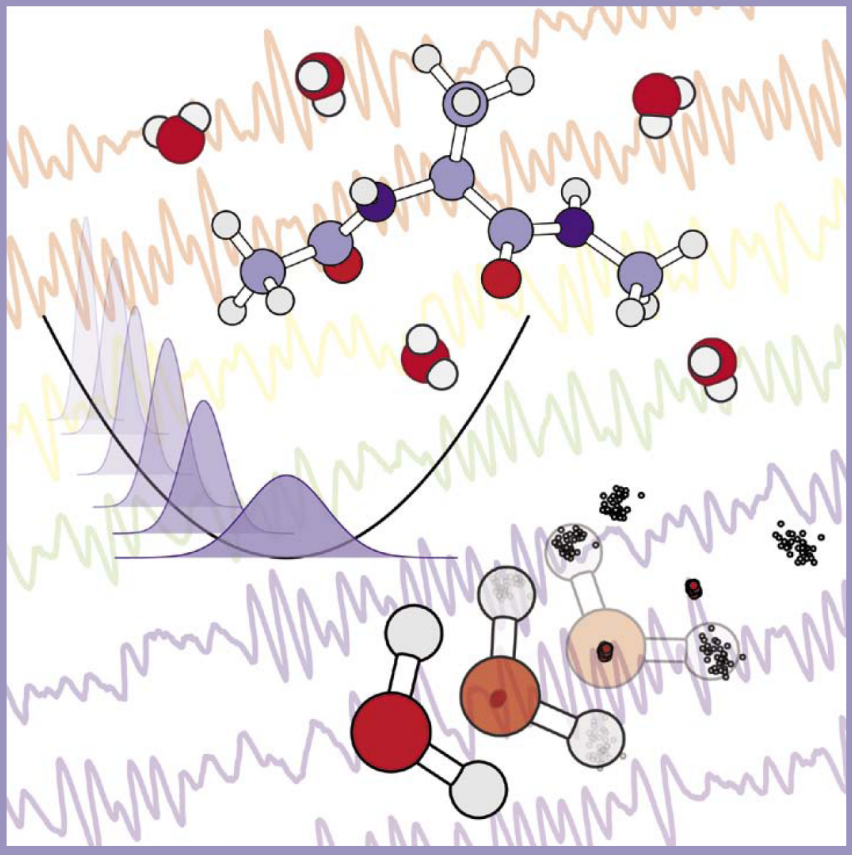
Annual Report 2010 / 2011

[C⁴]

Competence Center for Computational Chemistry



IBM

University of Zurich[UZH]

ETH Eidgenössische Technische Hochschule Zürich

Annual Report

[C4]

Competence Center
for Computational Chemistry

July 2010 to June 2011

Impressum

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C^4 on the Internet:
www.c4.ethz.ch

Cover figure provided by Michele Ceriotti, winner of the IBM Research Forschungspreis 2010. Caption:

A colored(correlated)-noise Langevin equation can be tuned based on analytical estimates in the harmonic limit. When used as a thermostat for molecular dynamics, it then allows both to sample efficiently the canonical ensemble and to model the quantum nature of lighter ions, substituting or complementing path integral methods.

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Contents

1 About C^4

The Competence Center for Computational Chemistry [C^4] is a network of computational chemists of the IBM Zürich Research Laboratory, the University of Zürich, and the ETH Zürich. The goal of C^4 is to seek new frontiers and opportunities in molecular modeling and simulation, to cater to the flow of know-how within this community, and to serve as a platform for the interaction with partners from other areas of science or from outside academia. C^4 was launched twenty years ago as a scientific collaboration between the IBM Research Laboratory and ETH Zürich, and has grown considerably since. Today, the C^4 network covers a much broader spectrum of research activities, and its output in terms of scientific results and achievements is still on the increase.

The Steering Committee consists of Prof. Alessandro Curioni, head of computational sciences at IBM Zürich Research, Profs. Jürg Hutter (University of Zürich), Wilfred F. van Gunsteren, and PD Dr. Hans P. Lüthi (both ETH Zürich). C^4 does not know formal membership. A "member" defines itself by the involvement in the activities of C^4.

This is the 18th Annual Report of the Competence Center for Computational Chemistry [C^4] reporting on its activities between July 2010 and June 2011. We also encourage you to visit our website, www.c4.ethz.ch .

2 The Year in Review

You may have noticed a change in the format of this year's Report. With the Zürich computational chemistry having grown substantially, it became increasingly difficult to present the full scope of the research activities in this report. This Annual Report therefore has changed its appearance. For the first time we do no longer publish research abstracts, an information which can easily be found using on-line sources such as the Web of Science. Instead, we granted each research group one page to list its research interests and to direct the interested audience to its home page. Still, we hope that this report will serve as the "yellow pages" of "computational chemistry made in Zürich".

We also have a change of editor. Halua Pinto de Magalhães, PhD student in the group of H.P. Lüthi, is the new editor of the Annual Report. He succeeds Peter Limacher, who is now a post-doctoral fellow at McMaster University in Ontario (Canada).

C4 Seminar

The actual "backbone" of C^4 is its Seminar Program. During the 2010 Fall- and 2011 Spring-Term the C^4 Seminar Program covered 14 lectures, again some of them presented by leaders in the field of computational chemistry. The seminar, which takes place every second Thursday during the semester, enjoys remarkable popularity. The complete seminar program is listed in the respective section of this report.

C4 Workshop

On January 13, the 2011 C^4 Workshop entitled "Advancing the Frontiers of Modeling and Simulation in Chemistry and Materials Science" was hosted by the IBM Research Laboratory in Rüschlikon. There were forty scientific presentations given (33 posters, 7 lectures), and there was the opportunity to visit the Nanotech Center shortly before its inauguration in May 2011. This was the fourth time a C^4 Workshop was held jointly with another institution, and the second time the event was held out-of-town.

Compute Resource

The C^4 compute-cluster Obélix, a 32 node IBM Opteron cluster operated by the ETH Informatikdienste was decommissioned in July of 2011 after five years of nearly uninterrupted service. At the same time the existing C^4 Brutus share was extended by 10 standard and 5 fat nodes, i.e. a total of 720 cores, based on an infrastructure-grant of ETH and a financial contribution of the ETH Department of Chemistry and Applied Biosciences.

Many of the members of the C^4 community are also users of the resources of the Centro Svizzero die Calcolo Scientifico (CSCS), i.e. were awarded computing time

based on proposals they had submitted. These three resources respond to a specific demand, and the results and achievements reported in this report typically involve "machine cycles" drawn from more than just one of these resources.

The IBM Research Award

In 2007, the ETH Schulleitung approved the "IBM Research Forschungspreis", an award for outstanding MSc and PhD theses sponsored by the IBM Zürich Research Laboratory. This year, the prize was awarded to Michele Ceriotti (Group of Prof. M. Parrinello) for his thesis entitled "A novel framework for enhanced molecular dynamics based on the generalized Langevin equation" *(see also Feature Article in this report)*.

The 2010 Award Ceremony, for the first time, took place at the ETH Tag with the Rector, Prof. Heidi Wunderli-Allenspach, handing out the award to the winner. Michele Ceriotti also presented his research at the occasion of a regular C^4 Seminar held at the IBM Research Laboratory in Rüschlikon. For more detail please refer to the respective section in this report.

Outlook

The C^4 Steering Committee would like to thank the community for its active participation in its program and activities. Also in the next year we will make sure that C^4 remains a valuable platform for the Zürich computational chemistry community.

Hans P. Lüthi, Leiter C^4
October 27, 2011

3 The C^4 Network & Areas of Research

The C^4 Network involves researchers from different participating institutions. The ETH Zürich is represented by the Departments of Chemistry and Applied Biosciences, Physics and Materials Science. Further, there are the Institute of Physical Chemistry and the Institute of Organic Chemistry at the University of Zürich as well as the IBM Zürich Research Laboratory.

Note that only a relatively small fraction of the research reported in this document was performed using C^4 compute resources; its capacity would be much to small to generate the scientific output listed here. The main idea behind this document is to have a compilation of the research in computational chemistry "made in Zürich", and to offer a listing of competencies and skills available.

The C^4 community

Research Group	*Institute*
Prof. K. Baldridge	Organic Chemistry UNI ZH
Prof. P. Chen*	Organic Chemistry ETH
Prof. C. Copéret**	Inorganic Chemistry ETH
Prof. A. Curioni	IBM Zürich Research Laboratory
Prof. W. F. van Gunsteren	Physical Chemistry ETH
Prof. A. Gusev*	Polymers ETH
Prof. I. Hermans	Chemical and Bioengineering
Prof. P. Hünenberger	Physical Chemistry ETH

Research Group	*Institute*
Prof. J. Hutter	Physical Chemistry UNI ZH
PD Dr. H.P. Lüthi	Physical Chemistry ETH
Prof. R. Nesper	Inorganic Chemistry ETH
Prof. M. Parrinello	Physical Chemistry ETH
Prof. M. Quack	Physical Chemistry ETH
Prof. M. Reiher	Physical Chemistry ETH
Prof. G. Schneider	Pharmaceutical Sciences ETH
Prof. F. Schoenebeck	Organic Chemistry ETH
Prof. N. Spaldin**	Materials Theory ETH
Prof. M. Troyer	Theoretical Physics ETH
Prof. V. Vogel	Biologically Oriented Materials ETH
Prof. P. Werner	Theoretical Physics ETH

*) No contributions for this year's report
**) Newly appointed

4 C4 Activities in 2010/2011

C4 Seminar

The C4 Seminar Program of the 2010 Fall- and 2011 Spring Term covered a total of 14 lectures, some of them presented by leaders in the field of computational chemistry and physics. The seminar again enjoyed remarkable popularity bringing together thirty to fifty (or more) students and researchers each time. One C^4 seminar was hosted by the IBM Research Laboratory, and two seminars were held jointly with the ETH Physical Chemistry Colloquium, and the Seminar for Theory, Spectroscopy and Dynamics, respectively.

C4 Tutorials

With CECAM being established in Switzerland, the offering for tutorials and workshops has increased considerably, both, in number and in the spectrum of topics covered. The CECAM Zurich node is lead by our colleague Prof. Matthias Troyer of the Institute of Theoretical Physics. C^4 did not offer its own tutorials. However, in order to respond to the demand of the local community, C^4 will offer tutorials again.

C4 Workshop

Two years after the Workshop with the Novartis Institute of Biomedical Research in Basel, the C^4 went out-of-town again. The 2011 C^4 Workshop was hosted by the IBM Research Laboratory in Rüschlikon. The lectures given by members of both teams, i.e. host and guest teams, along with the more than thirty posters presented by young C^4 scientists and IBM representatives allowed for an intense exchange between industrial and academic researchers. The workshop program is listed on the next page. An article on the event published in the IBM Research on-line newsletter can be found via the C^4 Web pages.

On the following pages you will find the C^4 Seminar Programms along with the Call for Participation for the C^4 Workshop.

ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

COMPETENCE CENTER FOR COMPUTATIONAL CHEMISTRY C4
ETH Zürich / University of Zürich / IBM Research

Seminar Programm Herbstsemester 2010

Auditorium HCI J6, ETH Hönggerberg
13:00-14:00

23. 09. 2010
Prof. Chantal Daniel, Université de Strasbourg, Strasbourg (France)
Photophysics of Photoisomerisable Rhenium(I) Complexes:
a Theoretical Analysis

07. 10. 2010
Prof. Christof Haettig, Ruhr-Universität Bochum, Bochum (Germany)
Coupled Cluster Methods for Ground and Excited States and Properties
of Small and Large Molecules

21. 10. 2010
Prof. Gisbert Schneider, ETH Zürich
Computer-assisted Drug Design: Exploring Virtual Chemical Space

26 .10 2010 (HCI J3 at 16:45)
Prof. Attila G. Császár, Eötvös University, Budapest (Hungary)
Computational Molecular Spectroscopy
(with the Kolloquium für Physikalische Chemie and the Swiss Chemical Society)

18. 11. 2010
Prof. Ken Houk, UCLA Los Angeles (California, USA)
Reactivity, Selectivity and Dynamics of Cycloadditions

02. 12. 2010
Prof. Angela K. Wilson, University of North Texas, Denton (Texas, USA)
Strategies for Quantitative Computational Modeling Across the Periodic Table

16. 12. 2010
Prof. Jürgen Gauss, Johannes Gutenberg Universität, Mainz (Germany)
Cost-Effective Methods for the Treatment of Relativistic Effects
in Quantum Chemistry

13.01. 2011
C4 WORKSHOP at IBM Research Laboratory, Rüschlikon
See separate announcement

www.c4.ethz.ch

ETH

Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

COMPETENCE CENTER FOR COMPUTATIONAL CHEMISTRY C4
ETH Zürich / University of Zürich / IBM Research

Seminar Programm Frühjahrssemester 2011

Auditorium HCI J7, ETH Hönggerberg
13:00-14:00
(unless otherwise noted)

24. 02.2011, Jointly with the IBM Research Seminar Program *
IBM Research Forschungspreis Award Lecture
Dr. Michele Ceriotti, Oxford University (Oxford, United Kingdom)
The Generalized Langevin Equations and Molecular Dynamics: From Enhanced Sampling to Nuclear Quantum Effects

03. 03. 2011
Prof. Hendrik Zipse, Ludwig-Maximilians-Universität München (Germany)
Computational Catalysis Research

18. 03. 2011, Jointly with the ETH Seminar for Theory, Spectroscopy and Dynamics*
Prof. John Stanton, University of Texas at Austin (Texas, USA)
High Accuracy Quantum-chemical Methods and Vibronic Coupling: Quantatively Accurate Spectral Predictions for Difficult Problems

31. 03. 2011
Prof. Gisbert Schneider, ETH Zürich
Computer-assisted Drug Design: Exploring Virtual Chemical Space

14. 04. 2011
Prof. Rodney J. Bartlett, University of Florida, Gainesville (Florida, USA)
How and Why Coupled-cluster Theory Became the Reference Method in Quantum Chemistry

28. 04. 2011 **Easter Break** (no seminar)

12. 05. 2011
Prof. Gerhard Stock, Universität Freiburg (Germany)
How Complex is the Dynamics of Protein Folding?

26. 05. 2011
Prof. Cherif Matta, Mount Saint Vincent University, Halifax (Nova Scotia, Canada)
Hydrogen-Hydrogen Bonding: A Weak Interaction in Molecules and Crystals

*) see separate announcement for time and location

www.c4.ethz.ch

ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

University of Zurich[UZH]

IBM

C4 WORKSHOP

Advancing the Frontiers of Modeling and Simulation in Chemistry and Materials Science

13. JANUARY 2011
IBM RESEARCH LABORATORY
RUESCHLIKON

CALL FOR PARTICIPATION

THE WORKSHOP

The goal of the Workshop, hosted by the Computational Sciences Group of the IBM Research Laboratory in Rüschlikon, is to promote the scientific exchange between IBM Research and its partners of the C4 community.

The Program contains **Oral Presentations** given by scientists of IBM Research as well as by C4 delegates, an extended **Poster Session**, which will give ample opportunity for the scientific exchange between participants, and a **Guided Tour** of part of the laboratory, including the newly built Nanotechnology Center. The event will start at 9:00 and is scheduled to end at 17:30.

PARTICIPATION

Those interested in participating in the workshop are kindly requested to submit Title and Abstract of their scientific contribution to c4@phys.chem.ethz.ch. Contributions from all areas of computational chemistry are welcome. The program committee will select the oral presentations from the submissions received. The C4 delegation will be limited to 40 participants. Each participant should either contribute a presentation, or should be a (co-) author of a poster.

DEADLINES

- Suggestions for presentations need to be received by Friday, December 3, 2010.
- December 16, 2010: Notification of participants and publication of the Program

ORGANIZERS

A. Curioni (IBM Research) and H.P. Lüthi (C4)

5 IBM Research Forschungspreis

The Prize and the Prize Winners

At the end of the 2007 Summer Term, the ETH Schulleitung approved the "IBM Research Forschungspreis", an award for outstanding MS and PhD theses sponsored by our partner, the IBM Zurich Research Laboratory.

2007 Sandra Luber (Group of Prof. M. Reiher)
Towards the Calculation of Raman Optical Activity Spectra of Large Molecules

2008 Daan Geerke (Group of Prof. W.F. van Gunsteren)
Classical Hamiltonians in Molecular Simulation: Force-Field Development and Explicit Inclusion of Electronic Polarization and Quantum Effects

2009 Sereina Riniker (Group of Prof. W.F. van Gunsteren)
Free Energies of Binding of Benzene Derivatives to Alpha-Cyclodextrin: Sensitivity of the Free-Energy Components to Temperature and to the Restraining of Molecular Motion

In 2010, the prize in the amount of CHF 4'000 was awarded to Michele Ceriotti (Group of Prof. M. Parrinello) for his PhD thesis *"A novel framework for enhanced molecular dynamics based on the generalized Langevin equation"* (see Feature Article in the next section).

The Award Jury, consisting of Profs. Alessandro Curioni, U.W. Suter and PD Dr. H.P. Lüthi awarded Dr. Michele Ceriotti the IBM Research Forschungspreis for his innovative use of the inherent non-Markovian features of Generalized Langevin Equations to craft an excellent and promising tool for simulations with well-defined uncertainties and trade-offs, as well as his applications of these methods to complex atomistic modeling problems.

The Call for Nominations for the 2011 IBM Research Forschungspreis was issued at the end of the Spring Term. It is for MSc theses submitted during the past two years.

Generalized Langevin Equation Thermostats

Michele Ceriotti
Physical and Theoretical Chemistry Laboratory, Universityof Oxford, South Parks Road, Oxford OX1 3QZ, UK and Computational Science, Department of Chemistry and Applied Biosciences, ETH Zürich, USI Campus, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland

Michele Parrinello
Computational Science, Department of Chemistry and Applied Biosciences, ETH Zürich, USI Campus, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland

Molecular dynamics is a precious tool that can help us to interpret experimental results and to predict the properties of new compounds. From simulations one can access dynamical information on the behaviors of chemical, biological and condensed phase system at the atomic scale as well as atomic configurations that are consistent with the experimental conditions. From these configurations one can compute thermal averages of macroscopic quantities and thereby compare the results from simulations with those from experiments. To do this properly one must modify Hamilton's equations and incorporate an interaction with a heat reservoir so that the canonical ensemble, which corresponds to the experimental constant temperature conditions, is sampled.

Many different approaches – typically referred to as *thermostats* – have been proposed for sampling the constant-temperature ensemble via continuous dynamics, and the various methods can be classified according to whether they are deterministic[1, 2] or based on stochastic dynamics[3, 4, 5, 6]. The prototypical example of this second category is the Langevin equation, which was initially introduced as a model for Brownian motion[7], and has been used for a long time in molecular dynamics (MD) as a convenient and efficient tool for obtaining trajectories which sample from the canonical ensemble[4, 8]. In its original form, the Langevin equation

$$\ddot{q} + \gamma\dot{q} - \xi = 0 \tag{1}$$

is based on the assumption of instantaneous system-bath interaction. Here γ is a damping coefficient related to viscous drag, and ξ corresponds to an uncorrelated random force term ($\langle\xi(t)\xi(0)\rangle = \delta(t)$) which models collisions with the bath particles.

A non-Markovian, generalized version of the Langevin equation arises in the context of Mori-Zwanzig theory[9, 10, 11]. When one integrates out part of the dynamical variables from a Hamiltonian system, a non-Markovian stochastic equation for the remaining degrees of freedom arises, which contains finite-memory friction and noise. A simple example of these history-dependent stochastic equations, in the

absence of an external potential, is

$$\ddot{q} + \int_{-\infty}^{t} K(t-s)\,\dot{q}(s)\,s - \zeta = 0, \tag{2}$$

where $K(t)$ is a positive real function which describes the friction, and $\zeta(t)$ is a Gaussian process, with time correlation function $H(t) = \langle \zeta(t)\,\zeta(0)\rangle$. The fluctuation-dissipation theorem, which ensures that configurations visited along the trajectory are distributed according to canonical statistics, requires that $H(t) = k_B T\,K(t)$. Within this formalism the conventional Langevin equation is recovered as an approximation, in the limit of a clear separation between the characteristic time-scales of the system's dynamics and of the system-bath interaction.

This class of non-Markovian stochastic differential equations has been extensively exploited to model the dynamics of open systems interacting with physically-relevant baths (see e.g. Refs. [12, 13, 14]). In many cases, however, one is mostly interested in equilibrium properties. The trajectory of the system is therefore irrelevant – the only thing that matters is that configurations are sampled from the appropriate statistical ensemble. This leads one to question: could non-Markovian Langevin dynamics be used as a tool rather than a physical model? In other words, could an appropriate coloured-noise, stochastic dynamics be used to design more efficient thermostats and could these thermostats extend the number of physical observables accessible within molecular dynamics?

This line of reasoning was the basis for the development of a framework for generalized Langevin equation (GLE) thermostatting[15, 16], which proved to be exceptionally flexible. It has been used to successfully provide efficient canonical sampling in a variety of contexts and to construct non-equilibrium dynamics that better describe the quantum nature of light nuclei with negligible overhead with respect to classical dynamics.

The generalized Langevin equation as a thermostat

A good thermostat should be both simple and flexible. However, more importantly, it it should be possible to predict the effect of changes in the parameters, so that expensive benchmarks can be avoided. To achieve these goals, we first exploited the fact that the non-Markovian dynamics (2) can be cast into a Markovian form by supplementing the physical momentum p with a set of n additional momenta $\{s_i\}$:

$$\begin{aligned} \dot{q} =& p \\ \begin{pmatrix} \dot{p} \\ \dot{\mathbf{s}} \end{pmatrix} =& \begin{pmatrix} -V'(q) \\ \mathbf{0} \end{pmatrix} - \begin{pmatrix} a_{pp} & \mathbf{a}_p^T \\ \bar{\mathbf{a}}_p & \mathbf{A} \end{pmatrix} \begin{pmatrix} p \\ \mathbf{s} \end{pmatrix} + \begin{pmatrix} b_{pp} & \mathbf{b}_p^T \\ \bar{\mathbf{b}}_p & \mathbf{B} \end{pmatrix} \begin{pmatrix} \boldsymbol{\xi} \end{pmatrix}, \end{aligned} \tag{3}$$

where $\boldsymbol{\xi}$ is a vector of $n+1$ uncorrelated, Gaussian variates. Eq. (3) is equivalent to a non-Markovian dynamics for the physical coordinates only. The friction memory kernel can then be of the form $K(t) = 2a_{pp}\delta(t) - \mathbf{a}_p^T e^{-|t|\mathbf{A}} \bar{\mathbf{a}}_p$, and the

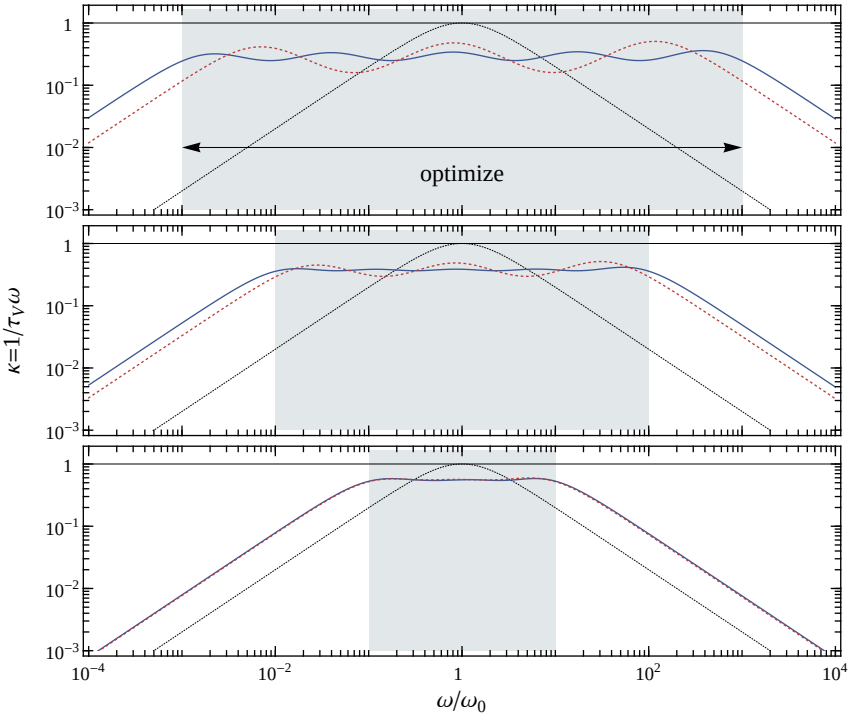

Figure 1: Sampling efficiency for the potential energy of a harmonic oscillator, plotted as a function of the frequency ω. The $\kappa(\omega)$ curve for a white-noise Langevin thermostat optimized for $\omega = \omega_0$ (black, dotted lines) is contrasted with those for a set of optimized GLE thermostats. The panels, from bottom to top, contain the results fitted over frequency ranges spanning two, four and six orders of magnitude around $\omega = 1$ respectively. Blue, continuous lines correspond to matrices with $n = 4$ additional degrees of freedom s_i, while the red, dashed lines are for $n = 2$.

reader is referred to [15, 16] for a more detailed discussion of the derivation, and for the practical issues involved in the implementation of this generalized Langevin dynamics.

Since the dynamics is determined by the entries of two $(n+1) \times (n+1)$ matrices, eq. (3) bestows a great deal of flexibility. However, because there are now so many parameters, having an *a-priory* strategy for parameter selection is of paramount importance - one can no longer rely on using benchmarks to explore the parameter space. With this in mind it is useful to observe that, for a harmonic potential, the force term $V'(q)$ is linear. This means that the whole set of equations for $(q, p, \mathbf{s})$ is a linear, Markovian set of stochastic differential equations so their statistical and dynamical properties can be obtained analytically[17]. Moreover, in a

multi-dimensional harmonic system, the properties of the dynamics are invariant under unitary transformations of the coordinates. Therefore, applying a set of independent GLE's to the Cartesian coordinates is equivalent to applying them to the normal modes representation.

Using these two observations we can tackle the problem of predictability. For any set of GLE parameters it is possible to calculate an analytical estimate of the sampling properties over a range of frequencies that encompasses all the time scales for the problem. This allows one to quickly and cheaply tune the parameters using an automated fitting procedure[18]. The resulting, optimized parameters can be easily transferred from one system to another, which makes it possible to cover most practical cases by means of a small library of parameters[16].

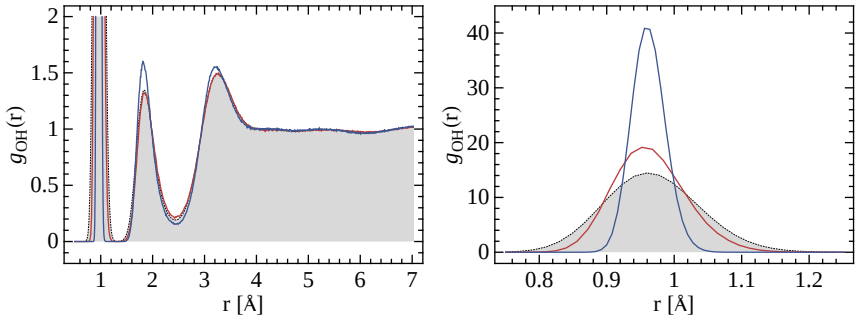

Figure 2: Oxygen-hydrogen radial distribution function for a molecular dynamics simulation of a water model[19], at 298 K and experimental density. The shaded curve corresponds to a reference PIMD simulation, the blue curve to a purely classical dynamics, and the red curve has been obtained with a GLE quantum thermostat. The rightmost panel shows the intramolecular peak in detail.

GLE for canonical sampling

In order to sample the canonical ensemble at temperature T, a fluctuation-dissipation relation $H(t) = k_B T K(T)$ must hold between the friction kernel and the noise memory function. This corresponds to a simple constraint on the matrices entering the Markovian form (3). This constraint completely determines the statistical ensemble sampled by the stochastic dynamics. However, even with this constraint in place, there is still considerable flexibility available in the manner in which the dynamical properties are manipulated. For instance, one can quantitatively gauge the efficiency of sampling by computing the correlation time of the potential energy V for a harmonic oscillator of frequency ω, normalized by the intrinsic time scale of the oscillations

$$\kappa_V^{-1} = \omega\tau_V = \frac{\omega \int_0^\infty \langle (V(t) - \langle V \rangle)(V(0) - \langle V \rangle) \rangle \, \mathrm{d}t}{\langle V^2 \rangle - \langle V \rangle^2}. \tag{4}$$

One can then easily verify that for a white-noise Langevin equation with friction γ this indicator of sampling efficiency reads $\kappa_V(\omega) = (\omega/2\gamma + \gamma/2\omega)^{-1}$ – a curve which is peaked for $\omega = \gamma$ and which decays to zero for lower and higher frequencies. This implies that, when using a white-noise Langevin thermostat, only the observables which are related to molecular motions with a time scale close to $2\pi/\gamma$ will be sampled with optimal efficiency.

In contrast when a GLE thermostat is used it is possible to fit the parameters such that the $\kappa(\omega)$ curve is nearly constant over a broad range of frequencies (see figure 1), that encompasses all the relevant time scales[18]. This ensures that all of the observables will be sampled in an efficient manner and, what is more important, no expensive benchmarks for the thermostat parameters are required prior to the production calculations. We have tested this idea with a thorough comparison agains other thermostatting techniques in the challenging case of path integral (PI) molecular dynamics[20]. "Optimal sampling" GLE had performances comparable to the best results obtained by the other methods, including also the approaches which exploit information of some of the vibrational modes to perform a targeted thermostatting.

The GLE is flexible enough to also enforce *inefficient* sampling of sections of the vibrational spectrum. This is precisely what is needed to maintain adiabatic decoupling in Car-Parrinello-like dynamics[21], and to preserve long-time dynamics while coupling strongly to fast vibrational modes, which is required to stabilize multiple time step MD without affecting the efficiency of sampling[22].

Non-equilibrium GLE

When the fluctuation dissipation theorem is assumed, the generalized Langevin equation framework that has been introduced provides a powerful set of tools for performing canonical sampling. However, the formalism is also useful when this constraint is removed – when there is no relation between the two matrices which enter equation (3) – as, in the harmonic limit, the resulting non-equilibrium GLE will thermalize different normal modes at different temperature. Hence, one can for instance design a "δ-thermostat" which sets the normal modes within a narrow frequency window at a finite temperature, while freezing all the other modes at a much lower effective temperature[23]. Once applied to a realistic simulation, this GLE dynamics would selectively excite a few normal modes, in a completely automatic manner.

This frequency-dependent thermalization can be put to good use when one remembers that the configurational probability distribution for a collection of quantum harmonic oscillators at the physical temperature T matches exactly that of purely classical oscillators *provided that they are sampled at a frequency-dependent effective temperature* $T^\star(\omega) = (\hbar\omega/2k_B)\coth(\hbar\omega/2k_BT)$. Hence, we have designed a set of GLE parameters that enforce this effective temperature curve. This result-

ing "quantum thermostat" allows one to model nuclear quantum effects (zero-point energy and non-constant specific heat in particular) in weakly anharmonic problems, with the same computational cost as a simulation based on classical MD[24]. By carefully tuning the strength of coupling it is also possible to model qualitatively very anharmonic systems such as liquid water[18, 15] (figure 2). This method is of particular interest when used in conjunction with ab-initio molecular dynamics, as the cost of calculating energies and forces in these simulations makes it almost impossible to converge simulations which treat nuclear quantum effects using path integral methods.[25]. An interesting feature of the quantum thermostat is that it allows one to compute the momentum distribution for the atoms – which can be measured by inelastic neutron scattering and which contains useful information on the chemical environment of light nuclei – in a completely transparent way[25].

Quantum thermostat simulations make it possible to gauge the importance of nuclear quantum effects inexpensively, but do not allow for systematic convergence, which can be problematic when quantitative results are required. To overcome this difficulty, we combined a non-equilibrium GLEs with path integral dynamics[26]. Systematic convergence is obtained by increasing the number of path integral replicas, while a carefully designed GLE ensures that convergence is achieved very rapidly. Typically, for a given level of accuracy one can reduce the number of replicas by a factor of 5 to 10 (figure 3). It is interesting to note that this stochastic approach yields better performances than high order path integral techniques[27, 28, 29], which are considerably more complex and which are plagued by statistical inefficiency problems[30].

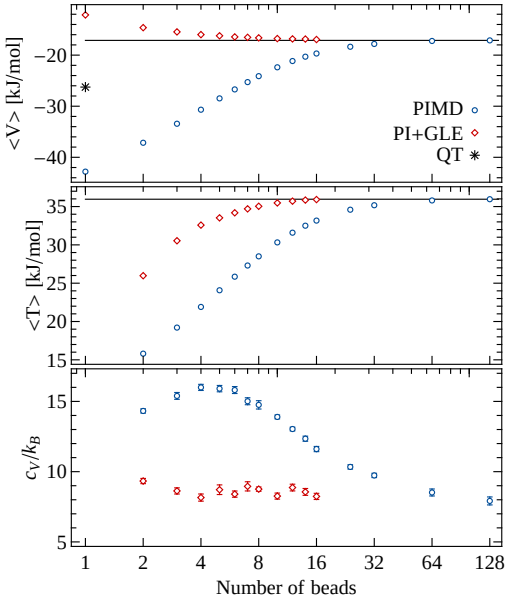

Figure 3: The average value of the potential energy, the virial kinetic energy estimator and the constant-volume specific heat for a simulation of flexible water[19] at $T = 298$ K are plotted as a function of the number of beads. Results with conventional PI and with with an approach combining PI with non-equilibrium colored-noise dynamics[26] are compared, and the value of $\langle V \rangle$ obtained with the quantum thermostat (QT) is also reported.

Conclusions

The generalized Langevin equation thermostat we have presented provides a consistent framework which can be adapted to assist molecular dynamics simulations in many different ways. Thanks to on an *a-priori* optimization of the thermostat parameters, based on analytical predictions in the harmonic limit, one does not need to perform expensive benchmarks to choose the parameters of the thermostat. Furthermore, one can tune the thermostat and thereby minimize the disturbance on selected vibrational modes. One can also, by releasing the constraints which correspond to the canonical fluctuation-dissipation relations, generate a class of non-equilibrium dynamics, whose steady state can be designed so as to model the quantum behaviour of light nuclei. This approach can be brought to systematic convergence by combining an appropriate coloured noise with path integral molecular dynamics, in an approach that gives accurate results for only a fraction of the cost incurred in conventional techniques. The variety of applications that we have developed in a short time frame suggests that this generalized Langevin framework may find soon other uses in molecular dynamics, and in related simulation techniques.

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6 Operation of the C4 Compute Resources

The C4 Shareholder Part of the Brutus Cluster

Ten Sun Fire X4440 with 4 Quad-Core AMD Opteron Processors 8380, 128 GB ECC RAM, and a local scratch space of 2.7 TB per node. The local scratch space is built of attached SAS storage. Five StorageTek 2530 arrays with 12 x 900 GB disks each provide the local scratch space for two attached Sun Fires. There is some additional storage for mid-term data storage. The equivalent of 30 Sun x6440 blades core is also a part of the share.

The C4 share is part of the 640 CPU share on Brutus of Profs. Wilfred van Gunsteren and Markus Reiher.

IBM Cluster e1350 "Obélix"

The Obélix cluster was decommissioned on 30th July 2011 after an uninterrupted uptime of 1'846 days of the fileserver, the most essential part of the cluster. By this date, an era reached its end. The Obélix cluster served more than 100 users over more than 6 years as a reliable computing facility. The management team of Obelix wishes to thank all the users as well as the members of the steering committee for their confidence and the fruitful collaboration.

Outlook

Based on a proposal of C4 and the Department of Chemistry and Applied Biosciences, an extension of the active share on Brutus by another ten standard- and five fat-nodes was approved by the Vice President Research in July 2011. The new nodes are currently in the beta-test phase and will be made available to the community soon.

Eric Müller, HPC Group, Informatikdienste ETH Zürich,
November 2011

7 Presentations of the Groups & their Publications in 2010/2011

Overview

Group of Kim K. Baldridge
Organic Chemistry Institute
UZH Zurich

Areas of Research:
Electronic Structure Theory Development and Applications, Computational Science and Grid Technologies

Keywords:
Quantum Chemistry, Chemical Structure, Electronic Transport, Optical Properties, Chemical reactivity, Dispersion Enabled DFT, Data Analysis

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Chem. Comm., **2011**,*in revision*.

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Areas of Research:
Material, Molecular and Surface chemistry, Catalysis, Imaging and Electronics, NMR spectroscopy

Keywords:
Computation chemistry, Periodic calculations, NMR, vibrational spectroscopy, C-H activation, C1-chemistry, alkene metathesis, alkane chemistry, metal oxides, nanoparticles, hybrid materials

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Chem. Commun., *47*, 490 (**2011**).

Group of Alessandro Curioni
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Zurich Research Laboratory

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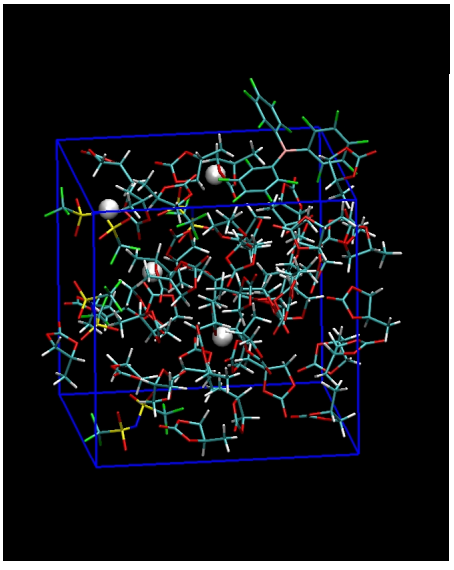
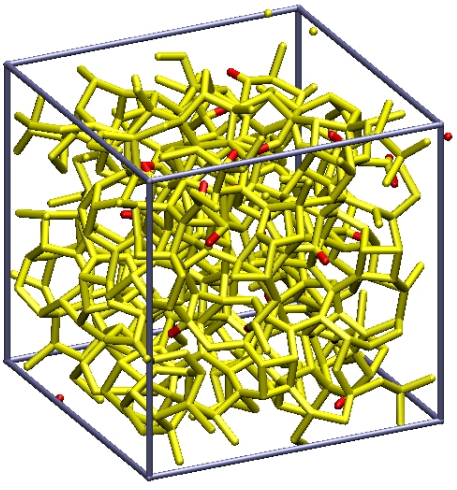
Areas of Research:
Simulation of complex systems in material sciences and biochemistry, parallel computing

Keywords:
Computational sciences, multiscale simulations, density functional theory and applications, algorithms re-engineering for massively parallel computers, simulations for energy storage and conversion.



(a) Simulation of propylene carbonatestability for Li/Air Batteries



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Areas of Research:

- Development of algorithms for efficient search of configuration space
- Simulation of long-time scale events
- esting and improvement of molecular models and force fields by comparison of of simulation results to experimental data
- Simplification of force fields
- Methods for calculating free energy and entropy differences in molecular systems
- Representation of electrostatic interactions in molecular simulations
- Role of electrostatic interactions in (bio-)molecular systems
- Determination of spatial molecular structure on the basis of NMR data
- Determination of spatial molecular structure on the basis of X-ray diffraction data
- Quantum mechanical simulation of biochemical phenomena
- Development of simulation software
- Application of simulation techniques to dynamically or functionally interesting systems or phenomena

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J. Phys. Chem. (**2011**)*in press*

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The GROMOS++ software for the analysis of biomolecular simulation trajectories
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J. Phys. Chem. (**2011**) *in press*

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J. Chem. Theory. Comp. (**2011**) submitted, incl. supp. mat.

A.P.E. Kunz, Z. Lin, W.F. van Gunsteren
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Mol. Phys. (**2011**) submitted

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Biochemistry (**2011**) submitted, incl. supp. mat.

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J. Comput. Chem. (**2011**)*in press*

A.P. Eichenberger, L.J. Smith, W.F. van Gunsteren
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FEBS (**2011**) submitted, incl. supp. mat.

D.A. Niggli, M.O. Ebert, Z. Lin, D. Seebach, W.F. van Gunsteren
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Chem. Eur. J. (**2011**) accepted, incl. supp. mat.

D. Steiner, W.F. van Gunsteren
An improved structural characterisation of reduced french bean plastocyanin based on NMR data and local-elevation molecular dynamics simulatio
J. Biomolecular NMR (**2011**) submitted, incl. supp. mat.

A. Choutko, W.F. van Gunsteren, P.H. Hünenberger
Preferential affinity of the components of liquid mixtures at a rigid non-polar surface: Enthalpic and entropic driving forces
ChemPhysChem (**2011**) submitted

N. Hansen, P. Kraus, H. Sassmannshausen, T. Timmerscheidt, W.F. van Gunsteren
An effective force field for molecular dynamics simulations of dimethyl sulfone
Mol. Phys. (**2011**) in press

J.R. Allison, S. Riniker, W.F. van Gunsteren
Coarse-grained models for the solvents dimethyl sulfoxide, chloroform and methanol
J. Chem. Phys. (**2011**) submitted, incl. supp. mat.

Z. Lin, H. Liu, S. Riniker, W.F. van Gunsteren
On the use of enveloping distribution sampling (EDS) to compute free enthalpy differences between different conformational states of molecules: application to 310-, α, and π helices
J. Chem. Theory. Comp. (**2011**) submitted, incl. supp. mat.

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J. Comput. Chem. (**2011**) submitted, incl. supp. mat.

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Areas of Research:
Sustainable chemistry and reaction engineering

Keywords:
Selective Oxidations, peroxide activation, catalysis, free radical chemistry, theoretical kinetics, transition state theory

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ChemSusChem, DOI: 10.1002/cssc.201100266 **2011**, *published online*.

Group of Philippe H. Hünenberger
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Areas of Research:
Computer simulation of molecular systems

Keywords:
Computer simulation, molecular dynamics, method development, force field, electrostatics, boundary conditions, conformational sampling, free-energy calculations, ionic systems, (bio)molecular systems

Main research topics:
The research of our group focuses on the development and application of methods for the *classical computer simulation of molecular systems*, namely in terms of *method development*:

- Treatment of electrostatic interactions
- Force-field parametrization (GROMOS)
- Thermodynamic boundary conditions
- Enhanced conformational sampling
- Extended-system methods
- Free-energy calculations
- Development of simulation algorithms
- Development of trajectory analysis methods

and in terms of *applications*:

- Single-ion solvation (book: http://www.csms.ethz.ch/single_ion_solvation)
- Properties of ionic systems (electrolyte solutions, crystals)
- Simulation of biomolecular systems (with a main focus on carbohydrates and lipids)
- Role of electrostatic interactions (hydrogen bonding, salt bridges) in (bio)molecular systems

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New functionalities in the GROMOS biomolecular simulation software.
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Calculation of relative free energies for ligand-protein binding, solvation and conformational transitions using the GROMOS software.
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B.A.C. Horta, Z. Lin, W.F. van Gunsteren and P.H. Hünenberger
Reoptimized interaction parameters for the peptide-backbone model compound N-methylacetamide in the GROMOS force field: Influence on the folding properties of two betapeptides.
J. Chem. Theory Comput., submitted (**2011**).

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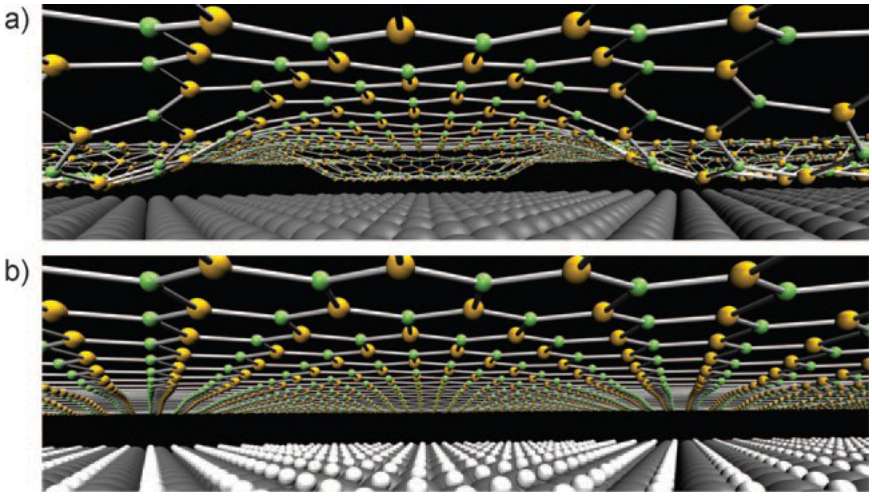
Areas of Research:
Method development and applications of ab initio molecular dynamics, molecules at interfaces (solid/liquid, liquid/vapor), chemical reactions in solution

Keywords:
Electronic structure theory, molelcular dynamics, density functional theory, condesned phase, interfaces, liquids, solutions, chemical reactions



3D representation of the results from the structure optimizations with DFT. a) Pristine h-BN/Rh(111). b) h-BN/Rh(111) with one H atom per Rh unit intercalated between the h-BN and the topmost Rh(111) layer. The corrugation amplitude of the h-BN layer is enhanced by a factor of two in the pictures. Rh gray, B orange, N green, H white. Atom sizes are not to scale.
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Jan Philipp Hofmann, Stefan Zweidinger, Marcus Knapp, Ari Paavo Seitsonen, Karina Schulte, Jesper N. Andersen, Edvin Lundgren and Herbert Over
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Journal of Physical Chemistry C 114, 10901-10909 (**2010**)

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Areas of Research:
Electronic Structure Theory and Applications, Computational Science

Keywords:
Quantum chemistry, chemical bonding, quantitative structure-property relationships (QSPR), chemical reactivity; wave function theory, density functional theory, data processing, data analysis

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J. Phys. Chem. A, 114, 2221-2229 (**2010**)

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Endocyclic Cleavage in Glycosides with 2,3-trans Cyclic Protecting Groups, *J. Am. Chem. Soc.*, 133, 5610-5619 (**2011**)

P.A. Limacher and H.P. Lüthi
Cross Conjugation
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P.A. Limacher, Q. Li, H.P. Lüthi, On the Effect of Electron Correlation on the Second Hyperpolarizability of Extended Conjugated Oligomer Chains, *J. Chem. Phys.*, 135 014111-4 (**2011**)

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D-CHAB, Lab Inorganic Chemistry
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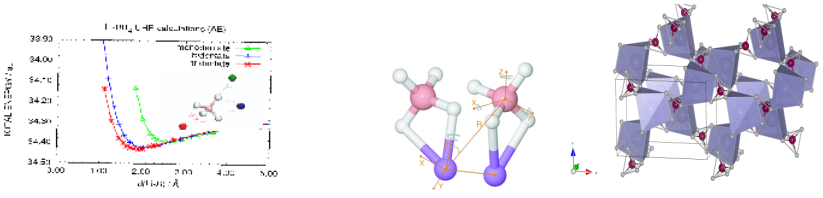
Areas of Research:
Computational chemistry, inorganic crystal structure modelling, structure prediction, phase stability.

Keywords:
Quantum chemistry calculations, DFT, structure stability, metal borides, lithium-containing metal oxides, hydrogen sorption.

Ab-initio crystal structure prediction is still one of the most challenging and interesting issues in condensed matter science. The first difficult task is the determination of the irreducible descriptors required to search for the global minima among different conformational geometries, a molecular system can adopt when visiting the many local minima of the potential energy surface. The ab-initio computational methodology of crystal structure prediction combines cluster modeling, via global minimization techniques, in particular, the Simulated Annealing method, and periodic lattice calculations, based on Density Functional Theory and quantum chemistry calculations. Whereas known experimental structures are available, the comparison with them helps to validate the predictability power of the computational approach and provides a molecular insight of stable and metastable structures of the particular system under study. After the identification of possible low energy structures, the necessary step is the thermodynamics of those particular phases. Furthermore, the structure stability is ascertained by performing the lattice dynamics, via phonon calculations. The compounds investigated up to now are selected complex borohydrides, metal borides, metal borocarbides and transition metal oxides of interest in materials science for energy applications as possible candidate hydrogen storage materials and substrate for the lithiation process. An example of the computational methodology applied to the ground-state determination of $LiBH_4$ is reported in the figure below.



Cluster model (UHF) $\xrightarrow[\text{SA}]{}$ Periodic lattice calculations

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Area of Research:
Computer Simulations of Materials and Biomolecules

Keywords:
Ab-initio molecular dynamics, enhanced sampling methods, collective variables, nucleation, phase change materials, hydrogen bonded systems, ligand protein interaction, large motions in proteins and RNA.

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J. of Comput. Chem., 32 (12), 2627-2637, (**2011**)

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Areas of Research:
Molecular Kinetics and Spectroscopy

Keywords:
Molecular Kinetics, Spectroscopy, Parity Violation, Chiral Molecules, Quantum Dynamics, Fundamental Symmetries, Quantum Chemical Kinetics, Tunneling, Infrared Spectroscopy, Terahertz Spectroscopy, Atmospheric Spectroscopy, Methane, Astrophysical Spectroscopy.

The group "Molecular Kinetics and Spectroscopy" of Martin Quack at ETH has as main research theme the understanding of fundamental, physical-chemical molecular primary processes. The basic research question concerns the fully quantum mechanical molecular motion, which is at the origin of all chemical reactions. An essential aspect of the research is the systematic combination of experimental and theoretical studies. The experimental studies concentrate on high resolution infrared spectroscopy, infrared multiphoton excitation and time resolved kinetic spectroscopy. While most of the experiments address fundamental questions, some practical applications relate to atmospheric and astrophysical spectroscopy and to isotope separation. The theory covers full-dimensional quantum dynamics by discrete variable representation techniques, finite basis set representation as well as diffusion quantum Monte Carlo methods. Approximate theories are developed and tested in relation to exact theories (an example is the quasiadiabatic channel reaction path hamiltonian theory for tunneling reactions). Another focus of theory is the time dependent quantum dynamics in intramolecular energy flow and vibrational redistribution, coherent infrared multiphoton excitation and laser chemistry as well as time dependent quantum statistical mechanical approaches to these processes. Finally, the group studies fundamental symmetry principles in molecular processes and molecular chirality in relation to parity violation. Our theoretical developments have led to large increases in the predicted parity violating energy differences between enantiomers, making these now a realistic goal for our current experiments.

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Synopsis:
Our research concentrates on theory in chemistry with a special emphasis on so-called first-principles methods, which are deeply rooted in quantum mechanics.

Areas of Research:
Relativistic Quantum Chemistry and Atomic Physics, Electron-Electron Interaction — DMRG and DFT, Theoretical Bio-Inorganic Chemistry and Coordination Chemistry, Quantum Chemical Analysis of Novel Compounds, Vibrational Spectroscopy of Large Molecules

Keywords:
Relativistic Quantum Chemistry and Atomic Physics, Electron-Electron Interaction — DMRG and DFT, Theoretical Bio-Inorganic Chemistry and Coordination Chemistry, Quantum Chemical Analysis of Novel Compounds, Vibrational Spectroscopy of Large Molecules

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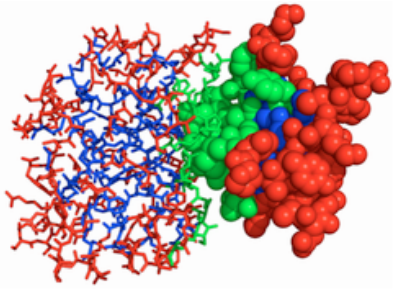
Areas of Research:
Machine learning in drug discovery, modeling of structure-activity landscapes, virtual screening, De novo design

Keywords:
Drug discovery, molecular design, neural networks, kernel-based machine learning, evolutionary optimization, ant colony systems, visualization

Our research activities concentrate on method development for virtual screening, molecular de novo design, and adaptive autonomous systems in drug discovery. We combine computer-based pattern recognition and machine learning with compound synthesis and biochemical activity determination. Our research activities include algorithm and software development for drug design, as well as practical applications in hit and lead finding.



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Group of Franziska Schoenebeck
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Areas of Research:

Physical organic chemistry, computational and experimental chemistry

Research interests in the Schoenebeck group are in the area of physical organic chemistry. The emphasis is on understanding reactivity and mechanisms, ultimately seeking the design of new catalysts and the development of novel applications in organic, bioorganic and materials chemistry.

Keywords:

Reactivity, Design, Mechanisms, QM

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Areas of Research:
Computational condesned matter physics and high performance computing

Keywords:
Computational physics, strongly correlated fermions, ultracold quantum gases, Bose Einstein condensation, quantum devices, quantum Monte Carlo methods, tensor network methods, computational provenance

Special highlights:
One highlight of the previous year was that our paper on the validation of a quantum simulator [Trotzky et al., Nature Physics (2011)] was chosen by Science magazine as one of the key papers in one of their breakthroughs of the year 2010.

Another highlight was the publication of a review [Gull et al, Rev. Mod. Phys. (2011)] on a new class of quantum Monte Carlo methods developed by our group that substantially speeds up simulations within the framework of dynamical mean field theory.

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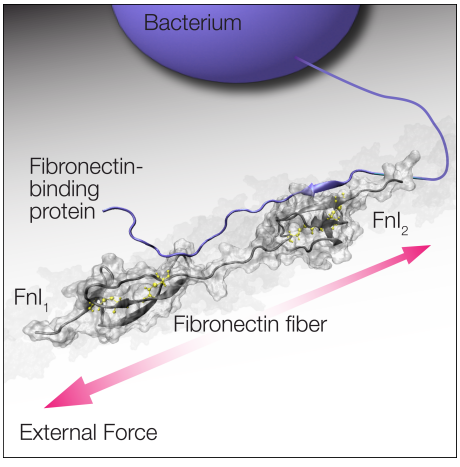
Areas of Research:
Extracellular matrix proteins, cell adhesion proteins & mechanotransduction

Keywords:
Cell adhesion, extracellular matrix, cytoskeleton, fibronectin, integrin, filamin, plectin, mechanosensing, bacterial adhesion, steered molecular dynamics, computational biology



Bacteria can adhere to Fibronectin fibres in connective tissues by using their adhesion proteins (purple) to bind to certain recognition sites in the fibre (FnI_1 and FnI_2, grey). Steered molecular dynamics simulations show how mechanical stretching of the Fibronectin (pink arrows) caused by cells leads to a partial detachment of the bacterial protein (illustration not to scale).

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8 Acknowledgements

The C^4 Steering Committee wishes to acknowledge the excellent collaboration with the High Performance Computing Group of the ETH Informatikdienste. Special thanks go to Eric Müller for the great job he did running Obélix and the Boars.

We would like to thank the VP Research of ETH, Prof. R.Y. Siegwart, for granting an additional share of C^4 nodes on the Brutus server. This acquisition was supported also by the ETH Department of Chemistry and Applied Biosciences.

It was a great pleasure for the C^4 delegates of ETH and the University of Zurich to participate in the C^4 Workshop hosted by our partner, the IBM Research Laboratory in Rüschlikon. Special thanks go to Prof. Alessandro Curioni and his team of the IBM Industrial Solutions Laboratory (ISL) who made this event possible.

After four years of doing an excellent job as editor of the C^4 Annual Report, Peter Limacher is now a post-doc at McMaster University in Hamilton (Ontario, Canada).

Finally, we wish to thank the C^4 community for its active participation in our programs.