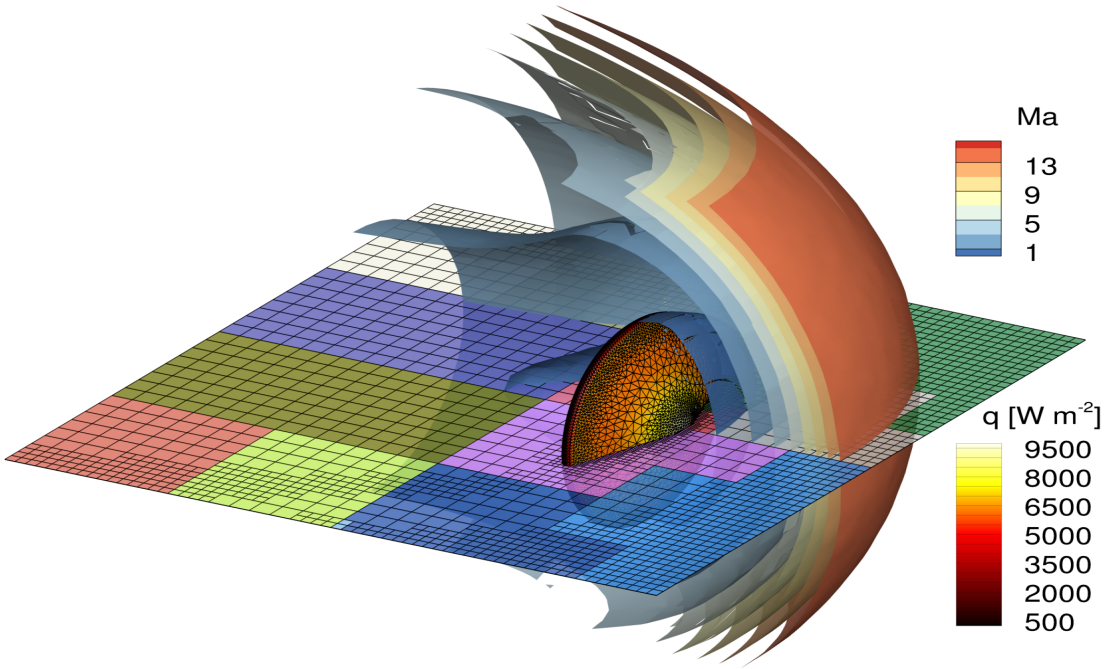
ETH zürich



Computational Science and Engineering (CSE)

Annual Report 2016/2017

CSE

Computational Science and Engineering

Annual Report 2016 / 2017

July 2016 to July 2017

Impressum:

ETH Zürich

Editors:

Vasile Gradinaru, Ralf Hiptmair, Markus Reiher
ETH Zürich

PDF files of this report are available from:

Dr. Vasile Gradinaru
Seminar for Applied Mathematics
Tel.: 41 44 632 3448
E-mail: vasile.gradinaru@math.ethz.ch

or may be downloaded from:

www.rw.ethz.ch

CSE curricula at ETH Zürich on the internet:

www.rw.ethz.ch *or* www.cse.ethz.ch

Cover:

Simulation of the hypersonic flow around a planetary probe geometry shown together with its surface mesh and colored by surface heat flux (see chapter 4).

Groups having contributed to this report

Research Group	Institute	Projects	Publs.
P. Arbenz	Computer Science	34	82
K. Boulouchos	Engines and Combustion Laboratory	35	83
C. Coperet	Inorganic Chemistry	40	84
R. Hiptmair	Seminar for Applied Mathematics	41	86
P. Hora	Virtual Manufacturing	46	
P. Hünenberger	Physical Chemistry	48	88
P. Jenny	Fluid Dynamics	49	89
A. Jentzen	Seminar for Applied Mathematics		91
M. Kröger	Polymer Physics	50	93
M. Luisier	Integrated Systems Laboratory	51	95
S. Mishra	Seminar for Applied Mathematics	52	97
R. Müller	Biomechanics	53	98
M. Parrinello	Computational Science & USI	54	99
M. Quack	Physical Chemistry	62	100
M. Reiher	Physical Chemistry	63	102
J. Richardson	Physical Chemistry	64	104
S. Riniker	Physikal Chemistry	65	105
C. Schär	Atmospheric and Climate Science	66	106
C. Schwab	Seminar for Applied Mathematics	67	109
P. Tackley	Geophysics	72	112
W. van Gunsteren	Physical Chemistry	73	114

Table of Contents

1	Introduction	9
2	Education	13
3	CSE Case Studies Seminar	21
4	Computational Highlight	25
5	CSE Research Projects	33
6	High Performance Hardware	77
7	Publications in 2016/2017	81

1

Introduction

CSE Report 2017: Editorial

R. Hiptmair*

A fashion, a trend, the dawn of a new age? Down to earth, let me start with reporting that during this years' meetings with students in the CSE study programs, I repeatedly found myself confronted with questions about the eligibility and relevance of courses about "**machine learning**" and "**deep learning**" and inquiries whether these subjects would be promoted to a central role in the CSE curriculum in the near future. Had I missed some important development? I was high time to learn about their significance for CSE from two ETH-based experts, Prof. J. Buhmann and Prof. T. Hofmann.

J. Buhmann, D-INFK

Joachim Buhmann is a physicist by training and received his PhD in physics from TU München in 1988. After a few years in the US, he was a professor for practical computer science at the University of Bonn from 1992 to 2003 before he joined D-INFK of ETH Zurich in 2003 as a full Professor of Computer Science.
His research interests cover the area of pattern recognition and data analysis, i.e., machine learning, statistical learning theory and applied statistics. The application areas range from computer vision and image analysis, remote sensing to medical informatics. He regularly teaches courses on "Statistical learning theory" and "Machine learning".

T. Hofmann, D-INFK

Thomas Hofmann did a PhD in Computer Science at the University of Bonn in 1997 and then worked in the Artificial Intelligence Laboratory at MIT, the International Computer Science Institute of the University of California, Berkeley, and in 1999 he joined Brown University as an assistant professor. In 2004 he became director of the Institute for Integrated Publication and Information Systems at the Fraunhofer Institute and Professor of Computer Science at the Technical University of Darmstadt, Germany.

From 2006 he served as Director of Engineering of the research department of Google Switzerland in Zurich and in 2014 he was appointed full professor of Data Analytics at D-INFK of ETH Zurich. His research focus is machine learning, specifically in problems that involve learning algorithms as well as statistical models and their architectures, such as deep neural networks. He offers the course "Deep learning".

*SAM, ETH Zürich, CH-8092 Zürich, hiptmair@sam.math.ethz.ch

He is also co-founder and CTO of the start-up company 1plusX and co-director of the Max Planck-ETH Center for Learning Systems.

I would like to thank the two colleagues for taking the time to meet me. I have extracted main points addressed in our conversation, which was in German, of course, and I am going to present them in the form of a fictitious interview:

1. What is machine learning?
   JB: The data-driven and stochastic generation of extremely high-dimensional implicit models encoded in algorithms. It represents a new paradigm in modeling, completely different from the traditional approach of capturing the behavior of a system "by a few simple equations" after careful analysis.

2. What are the foundations of machine learning?
   TH: It is based on (stochastic) approximation (theory) and continuous optimization, which, in turn, draw heavily on tools from linear algebra. Stochastic differential equations and gradient flows also come into play.

   JB: In light of data complexity a rigorous theory of machine learning may always remain elusive. Observing the behavior of the algorithms rather than analyzing them will drive research in the field.

3. Is machine learning really new?
   JB: Fundamental ideas and algorithms date back to the 1980s and 1990s, but their potential could not be realized before the arrival of sufficient and widely available computing power.

4. Does there exist a connection between machine learning and high-performance computing (HPC)?
   TH: Vectorization, parallelization, GPU-based acceleration, smart memory management, and other techniques from HPC are essential to meet the computational demands of machine learning algorithms when processing huge data sets, in particular in the training phase.

5. What is the role of (black-box) software?
   TH: Software libraries is indispensable due to the need for extreme performance. For instance, my group uses Google's open source TensorFlow library, which provides advanced HPC capabilities. However, using such tools as "black box" without proper understanding of the algorithms is not advisable.

6. Is machine learning important for CSE?
   JB: Absolutely, no question whatsoever! Machine learning algorithms can be regarded as a new class of tools for numerical simulations: Training and learning replaces mathematical modeling and model design by human experts.

Zürich, December 22, 2017

Ralf Hiptmair,

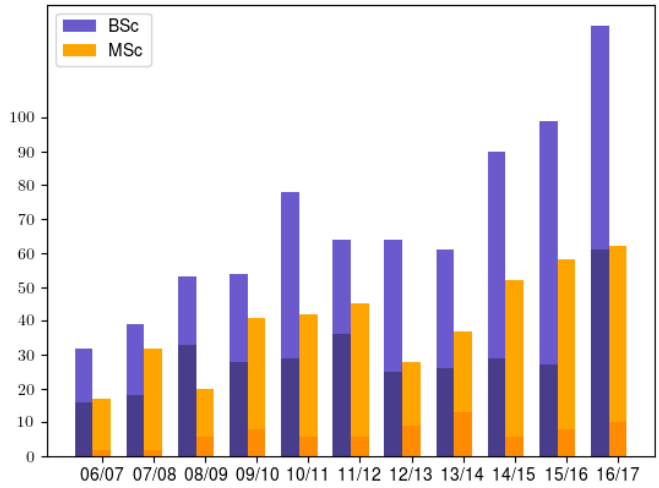
Director of Studies CSE, member of the CSE Committee

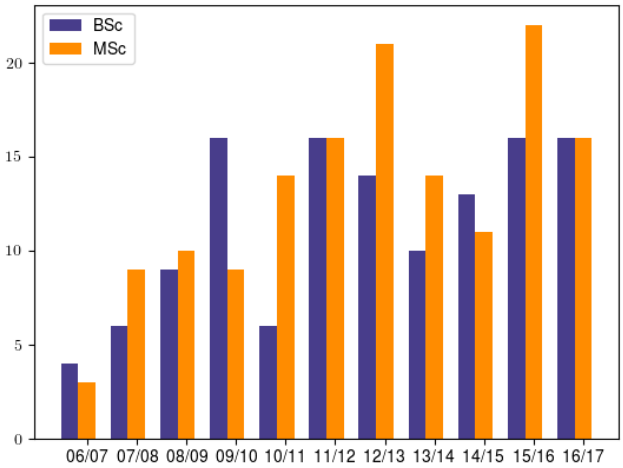
2

Education

In September 2016, 67 new students started their CSE Bachelor studies, 61 in the first semester and 6 in the third semester. From outside ETH 10 students entered the CSE Master curriculum.
The total number of CSE students enrolled at 14th December 2016 was 189 (headcount: 127 in the BSc program and 62 in the MSc program).

In the past academic year 32 students have successfully finished a CSE curriculum, 16 Bachelor students and 16 Master students, and have received a CSE degree, some with very good scores. In the following list we give the name of the student, the title of the Bachelor/Master thesis and the name and the department of the advisor.
The Willi Studer Preis 2017 for the best CSE Master Diploma in the past academic year was awarded to Thijs Vogels.





Number of CSE students in the curriculum; dark = number of new students
Number of CSE graduates

Bachelor Theses

Christian Baumann
Dirichlet Boundary Value Problems on Deformed Domains
(Ralf Hiptmair, D-MATH)

Till Ehrengruber
Implementation of Efficient Finite Element Solvers in Dynamic Programming Languages (JULIA)
(Ralf Hiptmair, D-MATH)

Florian Frei
Serialization of Hagedorn wavepackets in C++ with HDF5 Interface
(Vasile Gradinaru, D-MATH)

Fabian Keller
Application of QMC Rules to Partial Differential Equations with Uncertain Coefficient
(Christoph Schwab, D-MATH)

Fabian Hillebrand
Extended DOF-Handler for BETL2
(Ralf Hiptmair, D-MATH)

Ramona Hohl
Segmentation of 3D Scans of Garments Exploiting UV Mapping
(Olga Sorkine-Hornung, D-INFK)

Mara Ana Iosif
The valuation of financial options using models with stochastic volatility and jumps
(Walter Farkas, UZH)

Pascal Iselin
Strang Spliting for the TDSE and HDF5 Serialization
(Vasile Gradinaru, D-MATH)

Franziska Krummenacher
Bayesian optimal experimental design for detecting vortex wakes
(Petros Koumoutsakos, D-MAVT)

Cedric Münger
Algebraic Multigrid for Regularized Magnetostatics
(Ralf Hiptmair, D-MATH)

David Schmidig
Accelerating Graph Computations with Approximation Techniques based on Linear Algebra
(Torsen Hoefler, D-INFK)

Lukas Schwander
NoSQL Data Management
(Gustavo Alonso, D-INFK)

Fabian Schwarz
Scars and the likelihood of being trapped in a random potential
(Hans Herrmann, D-PHYS)

Eric Sinner
Multi-Grid Random Field Generator
(Patrick Jenny, D-MAVT)

Raphael Suter
Belief Propagation for Inference in Dynamical Systems
(Joachim Buhmann, D-INFK)

Matthias Untergassmair
Time Propagation of Hagedorn Wavepackets - an Efficient Implementation in C++
(Vasile Gradinaru, D-MATH)

Master Theses

Gabriele Abbati
Feature Selection in Medical IT: Surgery Prediction for Lumbar Spine Stenosis
(Joahim Buhmann, D-INFK)

Mark Ballandies
Dynamic Network Analysis in a Real Time Environment
(Dirk Helbing, D-GESS)

Sumitkumar Govindkumar Chouhan
Algorithms for Collateral Optimization
(Erich Walter, D-MATH)

Matthias Frey
Matched Distributions in Cyclotrons with Higher Order Moments of the Charge Distributions
(Andreas Adelmann, PSI)

Xiaolin Guo
Feasibility Study for Achieving Performance Portable Global Weather and Climate Models on Icosahedral Grids using DSL Libraries
(Christoph Schär, D-USYS)

Prashanth Kanduri
An Enriched Discontinuous Galerkin Method for Resolving Boundary Layers of the Eddy Current Problem on Curved Surfaces
(Ralf Hiptmair, D-MATH)

Marc Maetz
Central Schemes for the Induction Equation
(Siddhartha Mishra, D-MATH)

Raphael Stadler
Algorithmus eines automatischen Justageprozesses einer Wägezelle
(Konrad Wegener, D-MAVT)

Fabio Rossetto
Wireless Sensor Network Localization using Time of Flight measurements
(Raffaello D'Andrea, D-MAVT)

Felix Thaler
Multi-GPU Two-Component Fluid Mixtures with the Lattice Boltzmann Method
(Ilya Karlin, D-MAVT)

Alexander Xandeep Varghese
Towards Detection and Tracking of Featureless Object by Semantic Segmentation
(Margarita Chli, D-MAVT)

Benedek Vartok
Integration of Animation Input Device in Blender and Pose Space Interpolation with Dynamics
(Olga Sorkine-Hornung, D-INFK)

Thijs Vogels
Kernel-predicting convolutional neural networks for denoising Monte Carlo renderings
(Andreas Krause, D-INFK)

Kevin Wallimann
Syntactic Dependencies in Sequence-to-Sequence Learning for Machine Translation
(Thomas Hofmann, D-INFK)

Daniel Wälchli
Higher order proposal schemes for Transitional Markov Chain Monte Carlo, an Application to Hierarchical Bayesian methods
(Petros Koumutsakos, D-MAVT)

Alessio Zanchettin
Autonomous Quadrotor Landing on a Moving Platform with only Onboard Sensing and Computing
(Davide Scaramuzza, UZH)

Listed below are term papers written by the CSE Master students in the past two semesters.

Term Papers

Giuseppe Accaputo
A Comparison of Algorithms Related to Trace Minimization to Compute a Small Number of Eigenvalues of a Real Symmetric Matrix
(Peter Arbenz, D-INFK)

Stefan Beyeler
Novel Features for Visual Place Recognition
(Roland Siegwart, D-MAVT)

Lars Blatny
2-D FEM Poisson Solver for Ion Flow Problems
(Jasmin Smajic, D-ITET)

Temmy Bounedjar
Structured Modeling of Indoor Environments
(Roland Siegwart, D-MAVT)

Michaja Bösch
Gazebo-based Simulations for Formation Control Algorithms
(John Lygeros, D-ITET)

Michel Breyer
A Design Tool for 3D-Printable Push Puppets
(Markus Gross, D-INFK)

Carlo Del Don
Developing a Geometry Processing Toolbox for Garment Virtualization
(Olga Sorkine-Hornung, D-INFK)

Thomas Denoreaz
Pose Estimation and Correspondence using Locally Invariant Shape Features
(Anton Gunzinger,D-ITET)

Prashanth Kanduri
Low-Latency Classification of Poker-Card Suites using a Neuromorphic Co-Processor and a Dynamic Vision Sensor
(Giacomo Indiveri, D-ITET)

Jernej Fink
Extending LGen with New Types and Algorithms
(Markus Püschel, D-INFK)

Florian Frei
Interaction of a "cold plume" with a subduction zone
(Taras Gerya, D-ERDW)

Thomas Graf
Runge-Kutta discontinuous Galerkin schemes for the induction equation using multidimensional Riemann solvers
(Roger Käppeli, D-MATH)

Linus Groner
To Push or to Pull: On Reducing Communication and Synchronization for SSSP, BC and MST
(Torsten Hoefler, D-INFK)

Sarah Jetzer
Deep structured features for semantic segmentation
(Luca Benini, D-ITET)

Leyla Kern
Automatic topology creation and parameterization of haloalkanes
(Philippe Hüneberger, D-CHAB)

Samuel Keusch
Where is this Webcam located?
(Luc Van Gool, D-ITET)

Fabio Luchsinger
2D Numerical Modeling of Pebble Accretion Influence on Planetesimal Evolution
(Taras Gerya, D-ERDW)

Mojimir Mutny
Stochastic Second-Order Optimization via von Neumann Series
(Nicolai Meinshausen, D-MATH)

Donjan Rodic
FEM-MMP Coupling for EM Calculation over Multilayer Geometries
(Christian Hafner, D-ITET)

Lukas Strebel
Turbulence with OpenACC
(Oliver Fuhrer, MeteoSwiss)

Isabelle Tan
Traffic Light Control Optimisation with Q-learning
(Monica Menendez, D-BAUG)

Fabian Thüring
Implementing the Dynamical Core of COSMO in GridTools
(Oliver Fuhrer, Meteo-Swiss)

Hantian Zhang
Electro-Positron Collision to 3 Jets at NNLO
Thomas Gehrmann, D-PHYS

Tobias Wicky
Minimizing Communication in Forward Substitution via Inversion of Triangular Submatrices
(Torsten Hoefler, D-INFK)

Zürich, November 1, 2017
Vasile Gradinaru,
Advisor of Student Studies CSE and member of the CSE Committee
(Fachberater RW und Mitglied des Ausschusses Rechnergestützte Wissenschaften)

For detailed information on the RW/CSE curricula at ETH Zürich see:
www.rw.ethz.ch *or* 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 HS16

22.09.16	George Haller, Nonlinear Dynamics What Are Fluid Vortices and How Do We Identify them in Turbulence?
29.09.16	Habib Ammari, Seminar for Applied Mathematics (SAM) Bio-Inspired Imaging
03.11.16	Klaas Enno Stephan, Biomedical Engineering UZH and ETH Translational Neuromodeling
10.11.16	Kristina Shea, Engineering Design and Computing Laboratory Computational Design and Digital Fabrication
24.11.16	Romain Teyssier, Computational Astrophysics, UZH Computing the Universe: Modern Challenges for Computational Astrophysics
01.12.16	Daniel Meyer, Fluiddynamik Quantifying Uncertainty in Subsurface Flows
15.12.16	Marcelo Buffoni, Bernardo Galletti, ABB Switzerland Numerical Simulations of Electric Arcs for High-Voltage Gas Circuit Breakers

Case Studies Seminar FS17

02.03.17	Rima Alaifari, Seminar for Applied Mathematics (SAM) Stable Phase Retrieval
06.04.17	Eleni Chatzi, Structural Engineering On the Use of Metamodels for Simulation and Diagnostics of Dynamical Systems
04.05.17	Jeremy Richardson, Theoretical Molecular Quantum Dynamics Path-Integral Quantum Dynamics in Complex Molecular Systems
11.05.17	Daniel Leuenberger, MeteoSwiss Forecasting the Weather with Supercomputers
18.05.17	Jonathan Home, Quantum Electronics Pursuing High Fidelities in Trapped-Ion Quantum Computing

4

Computational Highlight

Computational Highlight: Parallel Simulation of Rarefied Gas Flows in Complex Domains at Arbitrary Knudsen Number

Stephan Küchlin Patrick Jenny

December 6, 2017

1 Introduction

Fluid-flows covering a wide range of Knudsen numbers (Kn)—where Kn is defined as the ratio of molecular mean-free path to a relevant flow length scale—occur in many situations, such as space vehicle thruster nozzle flow, reentry flows and expansion flows in physics experiments. These flows are challenging to simulate numerically, since the Navier-Stokes-Fourier description of gas flow is no longer valid. The adequate mathematical model for these situations is the Boltzmann equation, an evolution equation for the fluid density in a high dimensional phase-space under the influence of binary molecular collisions. The established numerical technique for stochastic computer simulations of the Boltzmann equation is the Direct Simulation Monte Carlo (DSMC) method pioneered by Bird [2]. Here, the particle density is treated in the point-mass approximation—it is represented by an ensemble of computational particles. DSMC delivers accurate results irrespective of Kn. However, its computational cost becomes prohibitively large in the near continuum range (where Kn is small). This is due to the fact that binary collisions are treated explicitly. The Fokker-Planck (FP) based particle Monte Carlo scheme introduced by Jenny et al. [3, 6] mitigates this problem. Here, the particle evolution is assumed to follow a continuous stochastic process. FP simulations are efficient for low to moderate Kn flows, but become inaccurate for very large Kn. Because both DSMC and FP are particle methods that differ only in the treatment of the collision operator, they may be seamlessly coupled to form the FP-DSMC method [4], which allows for efficient and accurate simulations of rarefied gas flows at all Kn.

Recent developments at the Institute of Fluid Dynamics at ETH have focused on the efficient parallel implementation of the FP-DSMC algorithm to allow for the simulation of practically relevant flow situations in complex domains.

2 Stochastic Simulation of the Boltzmann Equation

The fundamental equation solved in the study of rarefied gas dynamics is the Boltzmann equation

$$\frac{Df(\boldsymbol{x},\boldsymbol{c};t)}{Dt} = \frac{1}{m}\int_{\mathbb{R}^3}\int_0^{4\pi} \left(f(\boldsymbol{x},\boldsymbol{c}^*;t)f(\boldsymbol{x},\boldsymbol{c}_1^*;t) - f(\boldsymbol{x},\boldsymbol{c};t)f(\boldsymbol{x},\boldsymbol{c}_1;t)\right)|\boldsymbol{g}|\sigma(\theta,\boldsymbol{g})\mathrm{d}\theta\mathrm{d}\boldsymbol{c}_1, \quad (1)$$

which describes the evolution of the phase density $f(\boldsymbol{x}, \boldsymbol{c}; t)$ of the gas, which in turn is defined such that

$$N(\boldsymbol{x}, \boldsymbol{c}; t) = \frac{1}{m} f(\boldsymbol{x}, \boldsymbol{c}; t)\, \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{c} \tag{2}$$

is the number of molecules with position and velocity vectors in the differential element of phase space with volume $\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{c}$, located at point $\{\boldsymbol{x}, \boldsymbol{c}\}$. In Equation (1), $\boldsymbol{g}$ is the relative velocity vector between two colliding molecules with pre-collision velocities $(\boldsymbol{c}, \boldsymbol{c}_1)$ and post-collision velocities $(\boldsymbol{c}^*, \boldsymbol{c}_1^*)$, σ is the collision cross-section and m is the molecular mass. The explicit time dependence of f is dropped in the following for notational convenience.

The phase density may be factored into the gas density $\rho(\boldsymbol{x})$ and the normalized conditional velocity probability density $f_\zeta\left(\boldsymbol{c}; \boldsymbol{x}\right)$, i.e.,

$$f(\boldsymbol{x}, \boldsymbol{c}) = \rho(\boldsymbol{x}) f_\zeta\left(\boldsymbol{c}; \boldsymbol{x}\right). \tag{3}$$

The velocity PDF must fulfill $\int_{\mathbb{R}} f_\zeta\left(\boldsymbol{c}; \boldsymbol{x}\right) \mathrm{d}\boldsymbol{c} \equiv 1$. The total mass is given by

$$\mathcal{M} = \iint_{\mathbb{R}^6} f(\boldsymbol{x}, \boldsymbol{c}) \mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{c} = \int_{\mathbb{R}^3} \rho(\boldsymbol{x}) \mathrm{d}\boldsymbol{x}. \tag{4}$$

2.1 Computational Model

Instead of discretizing Equation (1) on a 6-dimensional grid, relevant practical flows are almost exclusively solved by means of a Monte Carlo approach, in which f is represented by an ensemble of computational particles in the point-mass limit and the particle positions and velocities are evolved in a Lagrangian framework. The solution quantities are macroscopic values such as mean velocity, density and pressure, which may be computed in terms of means of the particle ensemble. Different algorithms may now be formulated by the treatment of the right hand side of Equation (1)—the collision operator—with regards to the particle ensemble.

2.2 Direct Simulation Monte Carlo (DSMC)

As mentioned above, DSMC is the most popular algorithm. Here, an appropriate number of pairs of computational particles within the same grid cell is selected for collision at each time step. The relative velocity vector $\boldsymbol{g}$ is evaluated for each pair, and, with probability $\sim |\boldsymbol{g}|$, the particle velocities are updated by computing a collision with random plane angle. The position update ("streaming") follows as a separate step.

2.3 Fokker-Planck Method

In the Fokker-Planck method, the evolution of the particle position and velocity vectors $(\boldsymbol{x}, \boldsymbol{c})$ is assumed to follow a continuous stochastic drift and diffusion process rather than a jump process, viz.

$$\begin{aligned} \mathrm{d}c_i &= A_i(\boldsymbol{c})\, \mathrm{d}t + D(\boldsymbol{c})\, \mathrm{d}W_i, \\ \text{and} \quad \mathrm{d}x_i &= c_i \mathrm{d}t, \end{aligned} \tag{5}$$

with vector of drift coefficients $\boldsymbol{A}$ and diffusion coefficent D and where $\mathrm{d}W_i(t)$ is an increment of a Wiener process satisfying $\overline{\mathrm{d}W_i} \equiv 0$ and $\overline{\mathrm{d}W_i \mathrm{d}W_j} \equiv \delta_{ij}\mathrm{d}t$ [6]. Under these assumptions, the evolution of the phase density becomes a Fokker-Plack equation

$$\frac{Df\left(\boldsymbol{x}, \boldsymbol{c}\right)}{Dt} = -\frac{\partial}{\partial c_i}\left(A_i(\boldsymbol{c}) f\left(\boldsymbol{x}, \boldsymbol{c}\right)\right) + \frac{1}{2}\frac{\partial^2}{\partial c_i \partial c_i}\left(D(\boldsymbol{c}) f\left(\boldsymbol{x}, \boldsymbol{c}\right)\right). \tag{6}$$

The specific forms of $\boldsymbol{A}$ and D are chosen such that—under the condition that momentum and energy are conserved—certain moments of the phase density relax to their equilibrium values at the same rate as dictated by the full Boltzmann collision operator. For example, choosing $\boldsymbol{A}$ as a cubic polynomial in velocity, correct relaxation of moments up to heat fluxes may be ensured, i.e. the simulation will reproduce the correct Pradtl number [5]. The crucial difference to DSMC is that the system (5) may be integrated accurately with large time-steps that can be substantially larger than the mean collision time, which needs to be resolved in DSMC.

2.4 Fokker-Planck-DSMC Algorithm

For high Kn, the approximation (6) is no longer accurate and the discontinuous nature of individual particle collisions must be taken into account. In this regime, DSMC is efficient. For smaller Kn, however, FP achieves very good agreement with full DSMC calculations with substantial savings in computational cost. It is therefore natural to combine the two algorithms. The resulting FP-DSMC scheme to advance the simulation for one time step reads as follows [4]:

1. **streaming:** advance particle positions, enforce boundary conditions (equivalent to DSMC)
2. **sampling:** compute ensemble moments and macroscopic values in each grid cell from the particles (equivalent to DSMC)
3. **collision operator selection:** in each grid cell, evaluate the ratio of the number of computational particles in the given cell to the number of collision pairs that would be considered in a DSMC step, $\frac{N_C}{N_C^{\text{coll}}} =: a$.

   if $a < 1$ choose FP

   else choose DSMC
4. **velocity update:** in each cell, apply the selected collision operator to the particles in the given cell

3 Implementation

In the following, we describe some key features of our parallel implementation of the simulation algorithm given above (c.f. Section 2.4). The sections below are adapted from References [8] and [7].

3.1 Particle and Mesh Data Structures Ordered by Space-Filing Curve

Adapted from [7]: A (discrete approximation to a) space-filling curve (SFC) assings a unique integer index I to any d-dimensional discrete coordinate, and vice versa. Since computer memory is adressed sequentially, storing data partaining to a physical spatial position in memory must always rely on a given ordering of the physical coordinates. For example, a common choice for the index of cells on a regular, 3D Cartesian mesh with n_i, n_j and n_k cells in x, y and z directions is $I = i + n_i j + n_i n_j k$. It turns out that there exist better choices, which furthermore allow for an elegant implementation of local mesh refinement and parallel load balancing, as well as easy treatment of particle movement through an arbitrarily refined and parallely distributed mesh. Specifically, we use various 3D Hilbert curves, which allow for a purely local construction of I as a function of any

discretized spatial coordinate, without input of a specific mesh structure. These curves also have a recursive property, meaning that all coordinates within a given orthant of the discretized space map to a compact set in index space. In other words, a Hilbert curve defines a unique ordering of the cells in an arbitrary quad/octree.

3.1.1 Mesh Data

Our mesh data structure is thus simply a list of cells, augmented and sorted by the respective index of each cell on the SFC [7]. If a cell is refined during the simulation, it is simply replaced in the list by the 2^d sub-cells. All other cells—the rest of the cell list—remain unchanged. Due to the properties of the SFC, the cell list does not need to be resorted. Local mesh refinement is thus also a "local" operation in terms of mesh data. In particular, in the parallel domain-decomposition framework, refinement on the grid of one process need never to be communicated to other processes.

The choice of which cells to refine is automated: at present, we evaluate the local equilibrium mean free path length in each cell at given time intervals, and if a cell's diameter exceeds the obtained value by a given threshold, the cell is refined.

3.1.2 Particle Data

Like the mesh data, particle data are stored contiguously, sorted by the SFC index corresponding to the position of each particle. The sorting is done each time step using a parallel integer sorting algorithm with linear runtime. Due to the recursive nature of the SFC, it is sufficient to store for each cell the index of the first particle with key greater or equal to the cell's key but smaller than the key of the next cell. Independent of the specific layout of the mesh, there is no need to explicitly trace the particles and no recursive cell lookup procedure, since the calculation of the particle SFC index is mesh-independent [7, 8].

3.2 Complex Geometry Handling via Ray Tracing

Adapted rom [8]: Boundary conditions are enforced by detecting intersections of particle trajectories with boundaries and modifying them appropriately, e.g. via specular reflection, re-sampling of the velocity according to a given wall kernel, or deletion of the particle at a stream or outflow boundary. The computationally expensive step here is detecting the boundary intersection. To allow for arbitrarily complex geometry while maintaining performance, we use Intel's open source ray-tracing library Embree [9] for intersection queries. The geometry is in no direct relation to the mesh. This immersed boundary approach is very flexible, so that geometry can be input to the simulation via standard surface triangulation file-formats "nastran" or "stl".

3.3 Parallelization

Adapted from [8]: We exploit both coarse and fine grained parallelism in our implementation. The overall flow domain is desomposed and solved on multiple processes that communicate particles via message passing (MPI). On each process, the individual simulation tasks (c.f. Algorithm (2.4)) are performed in parallel by multiple threads using OpenMP. In particluar, the particle streaming step is parallel on the individual particle level, the sampling and velocity update is parallel on the individual cell level, and the sorting of the particle data is also accomplished in parallel. For solution file output, each process writes its part of the mesh into a simultaneously accessed file using MPI file I/O

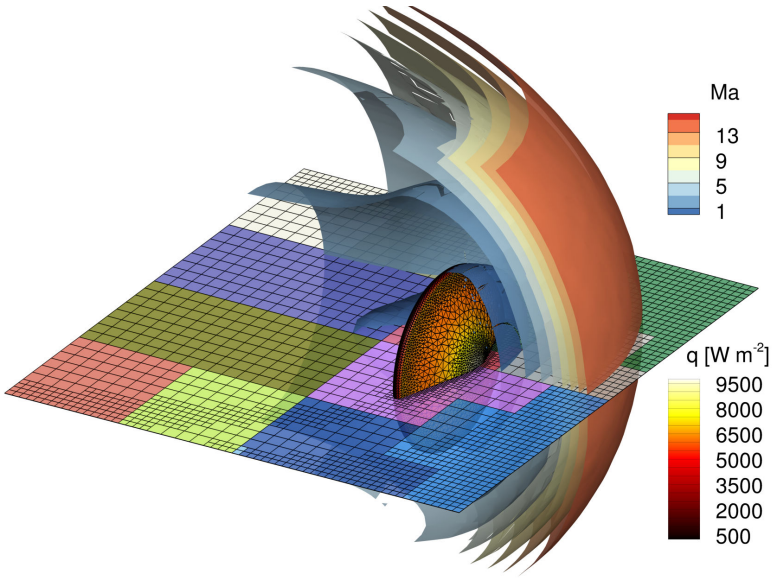


Figure 1: Results from the simulation of hypersonic flow around a planetary probe geometry shown together with its surface mesh and colored by surface heat flux. Also shown are Mach iso-surfaces. The slice plane shows the automatically refined volume mesh and the colors show the decomposition of the domain for parallel processing.

routines. The only remaining serial part of the algorithm is particle communication between processes at each time step.

4 Numerical Application

Adapted from [7]: We simulate hypersonic reentry flow over a generic planetary probe geometry (70 degree blunted cone flow, as studied experimentally by Allegre et al. [1]). The simulation is run in parallel on 48 nodes of the Euler III cluster, each using 4 cores (8 threads). The mesh is automatically refined at multiple time-instances at run time according to an estimate of the local equilibrium Knudsen number. The simulation is performed both using pure DSMC and using FP-DSMC, with the latter resulting in over 10 times faster simulations with excellent agreement to the DSMC reference runs. Figure 1 shows a typical simulation result in terms of Mach number iso surfaces and surface heat flux to the geometry (shown together with the surface triangulation).

5 Conclusion

We are continuing the development of a parallel, high-performance rarefied gas dynamics solver capable of simulating relevant practical flow problems. Our current implementation is able to handle complex geometry and simulate dilute gas flow at arbitrary Knudsen number. We have implemented local mesh refinement and parallel load balancing to tackle problems featuring large density contrasts. Current efforts are focused on criteria for the automated refinement process, as well as implementing local time stepping.

References

[1] J. Allègre, D. Bisch, and J.C. Lengrand. "Experimental Rarefied Density Flowfields at Hypersonic Conditions over 70-Degree Blunted Cone". In: *Journal of Spacecraft and Rockets* 34.6 (Nov. 1997), pp. 714–718.

[2] G.A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Oxford University Press, 1994.

[3] M. Hossein Gorji and Patrick Jenny. "An efficient particle Fokker-Planck algorithm for rarefied gas flows". In: *Journal of Computational Physics* 262.0 (2014), pp. 325–343.

[4] M. Hossein Gorji and Patrick Jenny. "Fokker-Planck-DSMC algorithm for simulations of rarefied gas flows". In: *Journal of Computational Physics* 287.0 (2015), pp. 110–129.

[5] M.H. Gorji, M. Torrilhon, and P. Jenny. "Fokker-Planck model for computational studies of monatomic rarefied gas flows". In: *Journal of Fluid Mechanics* 680 (Aug. 2011), pp. 574–601.

[6] Patrick Jenny, Manuel Torrilhon, and Stefan Heinz. "A solution algorithm for the fluid dynamic equations based on a stochastic model for molecular motion". In: *Journal of Computational Physics* 229.4 (2010), pp. 1077–1098.

[7] Stephan Küchlin and Patrick Jenny. "Automatic mesh refinement and parallel load balancing for Fokker-Planck-DSMC algorithm". Manuscript submitted for publication. 2017.

[8] Stephan Küchlin and Patrick Jenny. "Parallel Fokker-Planck-DSMC algorithm for rarefied gas flow simulation in complex domains at all Knudsen numbers". In: *Journal of Computational Physics* 328 (2017), pp. 258–277.

[9] Ingo Wald et al. "Embree: A Kernel Framework for Efficient CPU Ray Tracing". In: *ACM Trans. Graph.* 33.4 (July 2014), 143:1–143:8.

5

CSE Research Projects

Title: **Parallelization of the time integration for time-periodic flow problems**

Researchers: Peter Arbenz[⋆]
Daniel Hupp[⋆]
Dominik Obrist[†]

Institute/ Group: [⋆]Computer Science Department, ETH Zürich
[†]ARTORG Center, University of Bern

Description:
We investigate parallel algorithms for the solution of flow problems that are periodic in time. Finite difference approximations on a mesh in space-time are used. For periodic solutions, the discretized problem can be written as a large non-linear system of equations. This system of equations is solved by a Newton-Krylov method, using a preconditioned GMRES solver. The parallel performance of this algorithm is illustrated by a number of numerical experiments in one and two space dimensions.

References:

P. Arbenz, D. Hupp, and D. Obrist. *Comparison of parallel time-periodic Navier–Stokes solvers.* Accepted for publication in the proceedings of PPAM 2011, Lublin, Poland, September 10-13, 2017.

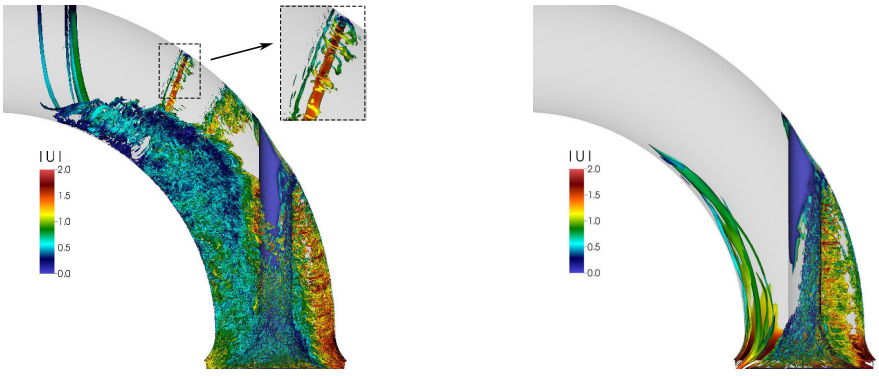
D. Hupp, P. Arbenz, and D. Obrist. *A parallel Navier–Stokes solver using spectral discretization in time.* Int. J. Comput. Fluid Dyn., 30 (7-10): 489-494 (2016) doi: 10.1080/10618562.2016.1242725.

P. Benedusi, D. Hupp, P. Arbenz, R. Krause: *A parallel multigrid solver for time-periodic incompressible Navier–Stokes equations in 3D.* In: Numerical Mathematics and Advanced Applications - ENUMATH 2015. B. Karasözen, M. Manguoglu, M. Tezer–Sezgin, S. Göktepe, Ö. Ugur (eds.). Lecture Notes in Computational Science and Engineering 112. Springer, 2016. pp. 265-273. doi:10.1007/978-3-319-39929-4_26.

D. Hupp, D. Obrist, P. Arbenz: *Multigrid preconditioning for time-periodic Navier–Stokes problems.* Proc. Appl. Math. Mech. (PAMM) 15, 595–596 (2015).

Title:	Direct numerical simulation of the flow in the intake pipe of an internal combustion engine
Institute/ Group:	G.K. Giannakopoulos[1], C.E. Frouzakis[1], K. Boulouchos[1], P.F. Fischer[2,3], A.G. Tomboulides[4] [1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ [2] Department of Computer Science, University of Illinois, Urbana-Champaign, IL, U.S.A. [3]Mathematics and Computer Science Division, Argonne National Laboratory, Chicago, IL, U.S.A. [4] Department of Mechanical Engineering, Aristotle University of Thessaloniki, Greece

The incompressible flow in the intake pipe of a laboratory-scale internal combustion engine at Reynolds numbers corresponding to realistic operating conditions was studied with the help of direct numerical simulations. The mass flow through the curved pipe remained constant and the valve was held fixed at its halfway-open position, as is typically done in steady flow engine test bench experiments for the optimization of the intake manifold. The flow features were identified as the flow evolves in the curved intake pipe and interacts with the cylindrical valve stem. The sensitivity of the flow development on the velocity profile imposed at the inflow boundary was assessed. It was found that the flow can become turbulent very quickly depending on the inflow profile imposed at the pipe inlet, even though no additional noise was added to mimic turbulent velocity fluctuations. The transition to turbulence results from competing and interacting instability mechanisms both at the inner curved part of the intake pipe and at the valve stem wake. Azimuthal variations in the local mass flow exiting the intake pipe were identified, in agreement with previously reported measurement results, which are known to play an important role in the charging motion inside the cylinder of an internal combustion engine.



(a) (b)

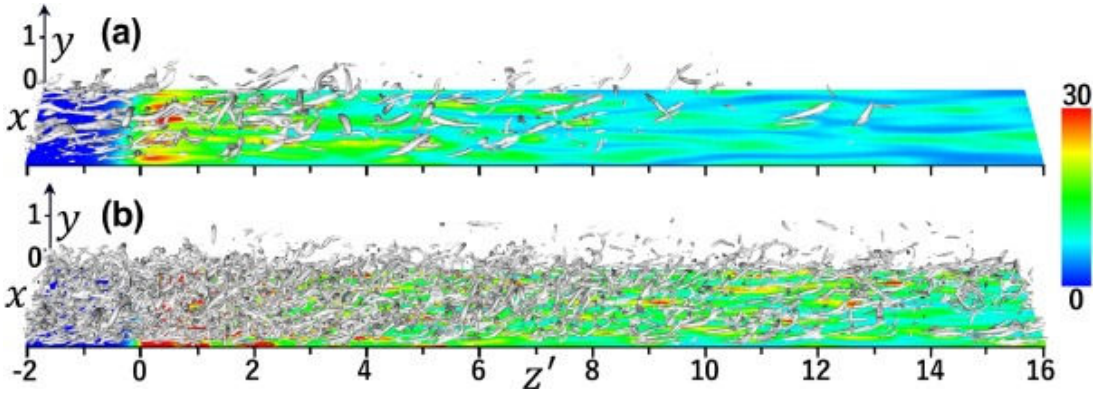
Vortical structures visualized as $\lambda_2 = 15$ isosurfaces on the symmetry plane colored with the flow velocity magnitude for simulations with ((a) parabolic and (b) power-law inflow velocity profile ($Re = 33,000$). Hairpin-like vortices around the primary vortex ring can be seen in the inset in (b).

References:

K. Giannakopoulos, C.E. Frouzakis, K. Boulouchos, P.F. Fischer, A.G. Tomboulides, Direct numerical simulation of the flow in the intake pipe of an internal combustion engine, *Int. J. Heat Fluid Flow*, 68, 2017, 257-268.

Title:	Direct numerical simulation of turbulent channel-flow catalytic combustion: Effects of Reynolds number and catalytic reactivity
Institute/ Group:	B.O. Arani[1], C.E. Frouzakis[1], J. Mantzaras[2], F. Luzzi[1], K. Boulouchos[1] [1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ [2]Combustion Fundamentals Group, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

Three-dimensional direct numerical simulations of fuel-lean hydrogen/air turbulent catalytic combustion were carried out in a platinum-coated planar channel with isothermal walls and an incoming fully-developed turbulent flow, at two inlet bulk Reynolds numbers ($Re_H = 5,700$ and 12,360 based on the channel height) and four global catalytic reaction rates. The turbulent flow laminarization due to heat transfer from the hot catalytic walls was appreciable, with turbulent intensities dropping by 37% and 25% at the channel outlet for the low and high Re_H, respectively. The ratio of the local average turbulent hydrogen conversion rate to the corresponding local laminar conversion rate was found to be a monotonically increasing function of streamwise distance, Reynolds number Re_H, and catalytic reactivity. Despite the turbulent flow laminarization, ratios at the channel outlet reached values up to 170% for the highest $Re_H = 12,360$ and for infinitely-fast catalytic chemistry. A correlation was further established for the ratio of the turbulent hydrogen conversion rate at finite-rate chemistry to the corresponding turbulent conversion rate at infinitely-fast chemistry. The instantaneous local catalytic reaction rates exhibited large fluctuations, which were up to 300% and 500% for the low and high Re_H, respectively. Fourier analysis indicated that a diminishing catalytic reactivity acted as a low-pass frequency filter for the overlying fluctuations of the turbulent flow.



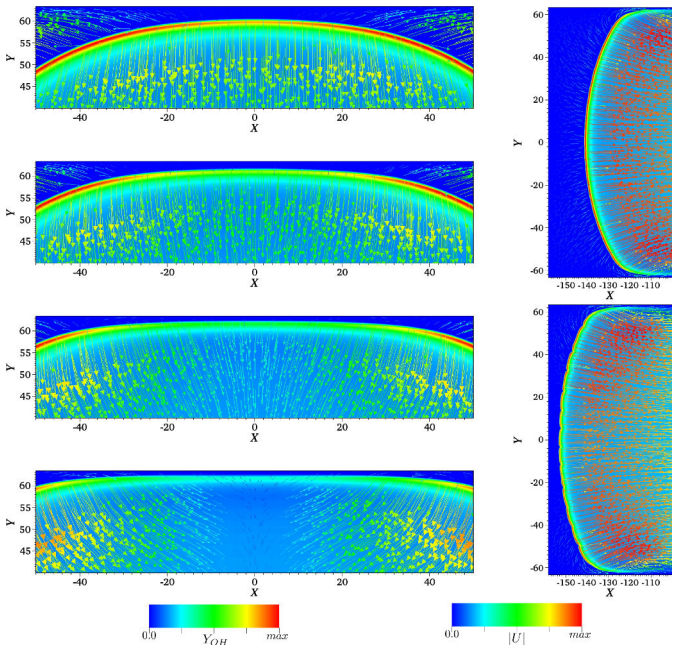
Snapshot of vortical structures (gray isosurfaces of $\lambda_2 = -1$) over the lower-half channel domain superposed on the non-dimensional temperature gradient on the lower wall at (a) low and (b) high Re_H. The catalytic wall is at $z' \geq 0$.

References:

• B.O. Arani, C.E. Frouzakis, J. Mantzaras, F. Lucci, K. Boulouchos, Direct numerical simulation of turbulent channel-flow catalytic combustion: Effects of Reynolds number and catalytic reactivity, *Combust. Flame*, 187, 2018, 52-66.

Title:	Laminar syngasair premixed flames in a closed rectangular domain: DNS of flame propagation and flame/wall interactions
Institute/ Group:	M. Jafargholi, G.K. Giannakopoulos C.E. Frouzakis, K. Boulouchos Aerothermochemistry and Combustion Systems Laboratory, ETHZ

The propagation of a lean laminar premixed syngasair flame is investigated numerically in a confined rectangular domain with isothermal walls at a temperature that is lower than that of the unburned mixture. Initiated by a hot kernel, the flame propagates towards the cold walls, setting in motion the initially quiescent mixture and compressing the gases, so that propagation proceeds under varying flow and thermodynamic conditions. The complex flow field changes structure and its effect on the local propagation characteristics is quantified by following the local displacement speed together with the local flow velocity and stretch rate. The flame first quenches head-on at the horizontal walls and then propagates towards the lateral walls affected by side-wall quenching. During the final stage, thermodiffusive instabilities are triggered along the front whose thickness has become half of the initial mainly because of the increased pressure. The temporal evolution of the quenching distances, the wall heat flux distribution and the heat transfer to the cold walls are quantified during the whole process. Except for the stages of the initial flame kernel growth and the final consumption of the fuel in the near-wall region, the fuel is consumed at an almost constant rate.



Left column: Distribution of hydroxyl mass fraction superimposed on the velocity vectors during flame propagation towards (left column) the upper wall and (right column) the left wall showing the cellular structures that form along the front. Vectors are colored by the velocity magnitude.

References:

M. Jafargholi, G. K. Giannakopoulos, C. E. Frouzakis, K. Boulouchos, Laminar syngasair premixed flames in a closed rectangular domain: DNS of flame propagation and flame/wall interactions, *Combust. Flame*, 188, 2018, 453-468.

Title:	Fundamental Aspects of Jet Ignition for Natural Gas Engines
Institute/ Group:	E. Mastorakos[1], P. Alison[1], A. Giusti[1], P. Oliveira[1], S. Benekos[2], C.E. Frouzakis[2], Y.M. Wright[2], K. Boulouchos[1] [1]Mechanical Eng. Dept., University of Cambridge, [2]Aerothermochemistry and Combustion Systems Laboratory, ETHZ

Large-bore natural gas engines may use pre-chamber ignition. Despite extensive research in engine environments, the exact nature of the jet, as it exits the pre-chamber orifice, is not thoroughly understood and this leads to uncertainty in the design of such systems. In this work, a specially-designed rig comprising a quartz pre-chamber fit with an orifice and a turbulent flowing mixture outside the pre-chamber was used to study the pre-chamber flame, the jet, and the subsequent premixed flame initiation mechanism by OH* and CH* chemiluminescence. Ethylene and methane were used. The experimental results are supplemented by LES and 0D modelling, providing insights into the mass flow rate evolution at the orifice and into the nature of the fluid there. Both LES and experiment suggest that for large orifice diameters, the flow that exits the orifice is composed of a column of hot products surrounded by an annulus of unburnt pre-chamber fluid. At the interface between these layers, a cylindrical reaction zone is formed that propagates in the main chamber in the axial direction assisted by convection in the jet, but with limited propagation in the cross-stream direction. For small orifice diameters, this cylinder is too thin, and the stretch rates are too high, for a vigorous reaction zone to escape the pre-chamber, making the subsequent ignition more difficult. The methane jet flame is much weaker than the one from ethylene, consistent with the lower flame speed of methane that suggests curvature-induced quenching at the nozzle and by turbulent stretch further downstream. The velocity of the jet is too high for the ambient turbulence to influence the jet, although the latter will affect the probability of initiating the main premixed flame. The experimental and modelling results are consistent with ongoing Direct Numerical Simulations at ETH Zurich.

References:

E. Mastorakos, P. Allison, A. Giusti, P. De Oliveira, S. Benekos, Y. Wright, C. Frouzakis, K. Boulouchos, Fundamental Aspects of Jet Ignition for Natural Gas Engines, *SAE Int. J. Eng.*, 10(5), 2429-2438, 2017.

Title: A LES-CMC formulation for premixed flames including differential diffusion

Institute/ Group: D. Farrace[1], K. Chung[1], M. Bolla[1], Y. M Wright[1], K. Boulouchos[1], E, Mastorakos[2]

[1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ

[2] Department of Engineering, University of Cambridge, Cambridge, U.K.

A finite volume Large Eddy Simulation-Conditional Moment Closure (LES-CMC) numerical framework for premixed combustion developed in a previous study, is extended to account for differential diffusion. The non-unity Lewis number CMC transport equation has an additional convective term in sample space proportional to the conditional diffusion of the progress variable, that in turn accounts for diffusion normal to the flame front and curvature-induced effects. Planar laminar simulations are first performed using a spatially-homogeneous non-unity Lewis number CMC formulation and validated against physical-space fully-resolved reference solutions. The same CMC formulation is subsequently used to numerically investigate the effects of curvature for laminar flames having different effective Lewis numbers: a lean methane-air flame with hydrogen-air flame with $Le_{eff} = 0.99$ and a lean $Le_{eff} = 0.33$. Results suggest that curvature does not affect the conditional heat release if the effective Lewis number tends to unity, so that curvature-induced transport may be neglected. Finally, the effect of turbulence on the flame structure is qualitatively analysed using LES-CMC simulations with and without differential diffusion for a turbulent premixed bluff body methane-air flame exhibiting local extinction behaviour. Overall, both the unity and the non-unity computations predict the characteristic "M-shaped flame observed experimentally, although some minor differences are identified. The findings suggest that for the high Karlovitz number (up to 10) flame considered, turbulent mixing within the flame weakens the differential transport contribution by reducing the conditional scalar dissipation rate and accordingly the conditional diffusion of the progress variable.

References:

• D. Farrace, K. Chung, M. Bolla, Y.M. Wright, K. Boulouchos, E. Mastorakos, A LES-CMC formulation for premixed flames including differential diffusion, *Combust. Theory Model.*, (in press).

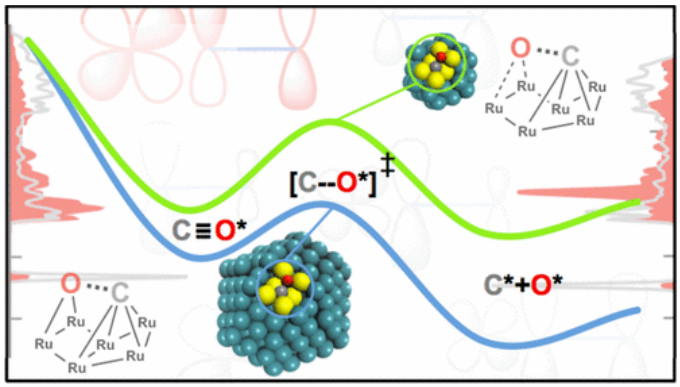
CSE group research description

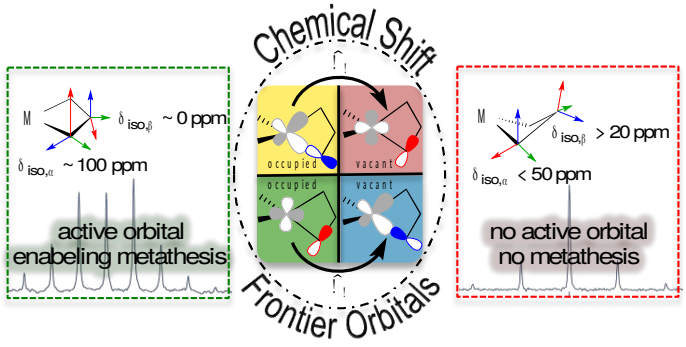
Institute/Group: Department of Chemistry and Applied Biosciences, Laboratory of Inorganic Chemistry. Comas-Vives and Copéret Groups.

Researchers: Lucas Foppa, C. Gordon, E. Lam, K. Larmier, Aleix Comas-Vives and Christophe Copéret

Description:

Our research activities in the field of computational chemistry aim at providing key information in order to understand at molecular level how heterogeneous catalysts work. One intensive area of research is the use of *ab initio* calculations in combination with spectroscopic techniques, in particular IR and NMR, in order to assign the active sites of heterogeneous catalysts. We study by means of first principles the reactivity of catalytic processes taking place on the surface of metal oxides, on single site catalysts oxides, single-site catalysts and of metallic nanoparticles supported on oxides. We combine different techniques adapted to the system of interest and the time-scale: static calculations, *ab initio* molecular dynamics (including metadynamics) and microkinetic modeling.





Group of Prof. Ralf Hiptmair
(Seminar for Applied Mathematics, D-MATH)

❶ HYDI – A C++ Finite Element Framework

From 2013 through 2016 a modern, highly modular, general, 3D finite element code has been developed as part of the CTI-funded project "Simulation of Arc-Extinction in Switching Chambers" jointly with ABB corporate research in Baden-Dättwil. Lead developers were R. Casagrande and Ch. Winkelmann. This code adheres to object-oriented and generic-programming software design paradigms and has the following features:

- Can handle unstructured 3D hybrid meshes comprising tetrahedra, hexahedra, prisms, and pyramids.
- Complies with the DUNE mesh interface specification.
- Implements hierarchic Lagrangian (nodal), edge, and face finite elements of arbitrary polynomial degree.
- Accommodates non-matching meshes across interfaces.
- Offers full support for Discontinuous Galerkin (DG) methods.
- Provides shared-memory parallelization.

Comprehensive unit tests and a thorough and current documentation are supplied.

The HYDI code is the software platform for an ongoing SNF-funded project on "Coupling of Finite Elements and Multiple Multipoles for Computational Electromagnetism". This project explores ways to combine local mesh-based discretization by means of finite elements with Trefftz methods (using auxiliary multipole sources). The latter numerical technology was successfully employed in the software OpenMaxwell developed in the group of Ch. Hafner at D-ITET, ETH Zürich. Coupling policies under investigation are

- to link Trefftz methods and variational formulations by means of Dirichlet-to-Neuann operators.
- a least squares approach leading to a PDE-constrained optimization problem,
- mortar-type coupling by means of Lagrange multipliers leading to a three-field formulation.

These activities are pursued by D. Casati in his PhD project and implementation in HYDI has already been completed.

The development of HYDI was supported by CTI grant 15183.1 and ABB Schweiz AG, Corporate Research. The integration of Trefftz methods is funded by SFN grant 2000021_165674/1.

❷ BETL – A C++ Boundary Element Template Library

BETL is a header-only template library mainly intended for the Galerkin boundary element discretization of 3D boundary integral operators as they arise in various physical and engineering applications. Prominent examples are, e.g., electrostatic or thermal models as well as the scattering of acoustic and electromagnetic waves. Fully continuous, tangentially continuous, and discontinuous boundary element functions are supported, but extension to other approximation spaces is easy. BETL relies on transformation-based adaptive quadrature to deal with singular integral kernels. Integration of 3rd party libraries for local low-rank matrix compression is available. BETL also offers comprehensive support for low-order polynomial Galerkin finite element methods (nodal and edge finite elements).

BETL has been developed by Dr. Lars Kielhorn as part of the project "Edyson 2020: Entwicklung eines effizienten C++ Simulationscodes zur Berechnung elektromagnetischer Felder auf der Grundlage von FEM-BEM Kopplung" jointly with Robert-Bosch GmbH, Germany. It is used for eddy current and electromechanical simulations at Bosch Corporate Research.

BETL is also used for teaching in the courses "Numerical Method for Partial Differential Equations" and "Advanced Numerical Methods for CSE" as well as for BSc thesis projects.

BETL's development was funded by Robert Bosch GmbH as part of the project "Edyson 2010: Entwicklung eines effizienten C++ Simulationscodes zur Berechnung elektromagnetischer Felder auf der Grundlage von FEM-BEM Kopplung".

❸ Second-Kind Boundary Integral Equation Methods for Scattering at Composite Objects

We target frequency-domain acoustic and electromagnetic scattering of incident waves at objects that consist of several homogeneous, isotropic materials. The behavior of the fields can be modelled using boundary integral equations (BIE) for unknown traces on the interfaces between material domains. The BIE are amenable to Galerkin discretization by means of boundary element methods (BEM).

In this project we investigate so-called 2nd-kind boundary integral equations, which arise from new multi-potential representation formulas. These BIE are set in L^2-type spaces and, thus, no continuity constraints have to be imposed on the boundary elements. in addition, natural choices for local basis functions will lead to well-conditioned linear system, for which iterative solvers converge fast.

The new formulations have been implemented both in 2D and 3D and their excellent performance has been demonstrated in numerical tests. The 3D implementation was based on the finite element template library BETL.

This research was supported by SNF under grant 200021_137873/1 "Well-conditioned Boundary Integral Formulations for Scattering"

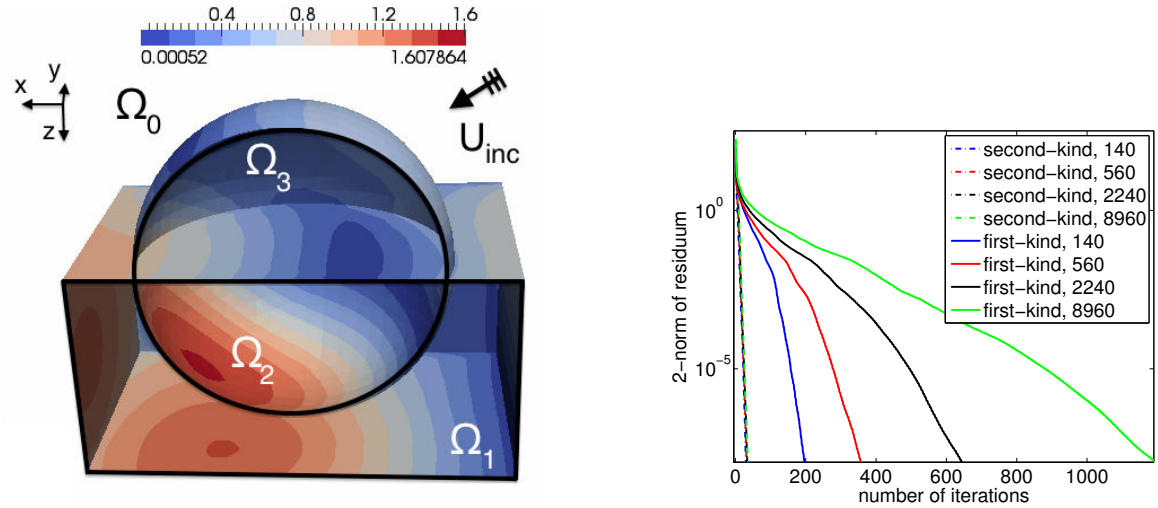


Figure 1: 2nd-kind BIE/BEM for EM scattering at compisite object: trace of electric field (left) and convergence history of GMRES

❹ Multi-Trace Boundary Integral Equations

We consider scalar or vectorial 2nd-order diffusion or scattering transmission problems in the exterior of a bounded domain $\Omega_Z \subset \mathbb{R}^d$. The coefficients are assumed to be piecewise constant with respect to a partition of $\mathbb{R}^d \setminus \overline{\Omega}_Z$ into subdomains. Dirichlet boundary conditions are imposed on $\partial\Omega_Z$.

In the spirit of domain decomposition, we recast the transmission problems into two novel well-posed *multi-trace boundary integral equations*. Their unknowns are functions on the product of subdomain boundaries. Compared to conventional single-trace formulations they offer the big benefit of being amenable to operator preconditioning. We could achieve a comprehensive numerical analysis of the new formulations. Moreover, numerical tests have confirmed the efficacy of operator preconditioning.

This project was funded by Thales SA, France, with grant "Preconditioned Boundary Element Methods for Electromagnetic Scattering at Dielectric Objects"

❺ Shape Sensitivity and Shape Optimization

For a functional F that depend on the solution u of a boundary value problem on a domain Ω we study the impact of small perturbations of Ω on $f(u)$. This can be quantified by the directional shape gradient, the "derivative" of $F(u)$ in a "direction of deformation" of Ω. For second order elliptic boundary value problems formulas for shape gradients involve both the solution of the boundary value problem (state problem) and the solution of a related adjoint boundary value problem. Equivalent formulas based either on integration over Ω or its boundary $\partial\Omega$ can be derived. However, in the case of finite element approximation of both state and adjoint problem the volume formulas provide significantly more accurate approximations of shape gradients. We could give a rigorous justification for this observation.

Shape gradients are a key building block for descent methods for shape optimization. The

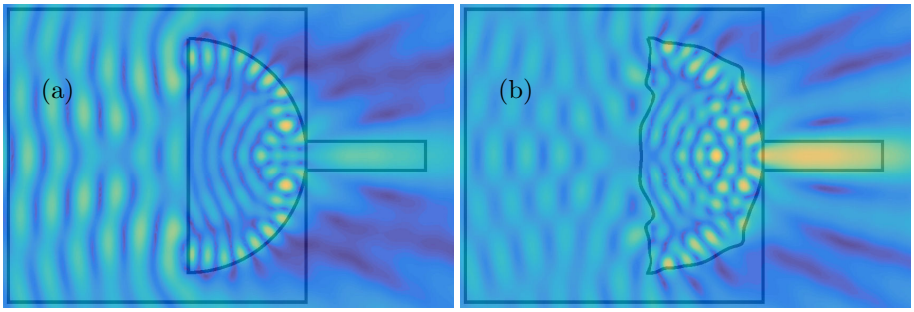


Figure 2: Shape optimization of microlenses (Paganini et al. 2015): An incoming plane wave hits (from the left) a cylindrical lens with semi-circular cross section (a). The shape of the lens is optimized to maximize the focused light in the thing rectangle on the backside of the lens (b).

other is a suitable representation of shape deformations. We use a volume based encoding of shape distortions by means of tensor product splines. In this space we express the shape gradient through its H^1-representative. Line search along this direction is used for the iterative minimization of the objective functional. This techniques has successfully been employed for shape optimization of nano-lenses, see Figure 2.

The project "Computational Nano-Optics: Shape Calculus and Inverse Problems" was funded by ETH Zurich under CHIRP grant CH1-02 11-1.

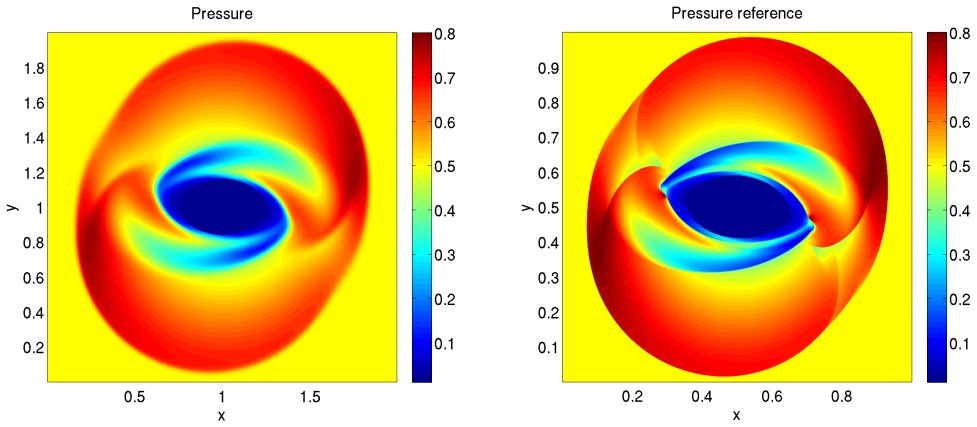


Figure 3: Ad ❻: Rotor problem, (Hiptmair and Pagliantini 2017, Sect. 4.3.4). Numerical solution on a 1600×1600 Cartesian mesh obtained with the lowest order FV-FEEC scheme and Heun timestepping with CFL-number 0.4. Finite volume scheme for the extended Euler equations based on an HLL approximate Riemann solver. The color map of the pressure plot is scaled to the extrema of the "reference" solution on a 3200×3200 mesh, shown on the right side.

❻ Splitting-Based Structure Preserving Discretizations for Magnetohydrodynamics

This topic is joint work with S. Mishra and was investigated by C. Pagliantini in her PhD

project. In contrast to the widely used finite volume (FV) methods she pursued a radically different approach comprising the following key elements:

1. The MHD equations are split into so-called extended Euler equations modeling fluid motion taking into account the Lorenz force, and Maxwell's equations in their magneto-quasistatic form for the electromagnetic fields.
2. The magnetic vector potential is used a primary electromagnetic quantity so that the divergence-free condition for the magnetic induction is automatically satisfied.
3. The discretization of the magnetic advection-diffusion equation takes the cue from Finite Element Exterior Calculus (FEEC) using a Galerkin approach and discrete differential forms, here incarnated through families of $\mathbf{curl}$-conforming finite elements.
4. A stabilized mesh-based Eulerian discretization of magnetic transport using upwinding by extrusion contraction discretization of the Lie derivative of differential forms.
5. A first-order finite volume spatial discretization of the extended Euler system of conservation laws.

The resulting method has proved to be remarkably stable for a range of challenging test problems. Unfortunately, extension to high-order FV treatment of the extended Euler system has not yet been accomplished.

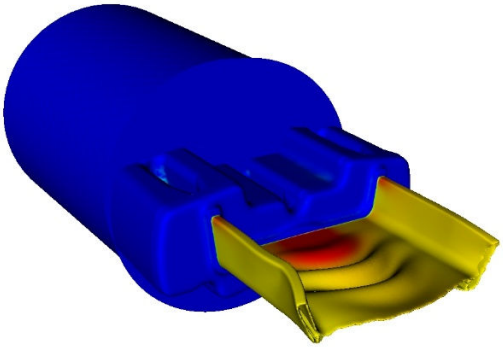
Group: Institute of Virtual Manufacturing

Researchers: Dr. Niko Manopulo, David Hora, Michele Crosio, Prof. Dr. Pavel Hora

Description:

1. *GPU accelerated simulation of complex extrusion processes*

Metal profiles with complex cross-sections are often manufactured by extrusion. The process consists in pressing a voluminous billet through an opening in the die with the desired cross-sectional shape. Given the high temperatures and deformation rates as well as the extreme hydrostatic pressures, the computational modeling of the process is highly challenging. In addition to an ALE formulation, which prevents mesh distortion, a mixed pressure displacement FE formulation is employed, to tackle the sensitive pressure computation under uncompressible material flow. The complex shape of the profiles, which often feature very slender geometries (~0.1mm) require a very fine meshing especially around and after the die opening. This in combination with the complex FEM framework employed leads to very high computational costs. In the scope of the project, the symmQMR linear equation solver has been implemented to run on the GPU (nVidia Tesla P100). For a geometry initially meshed with 3 million tetrahedral elements, this resulted in a net speedup of 200% with respect to computations made with the PARDISO solver on 14 Intel Xeon E5-2697 CPU cores.



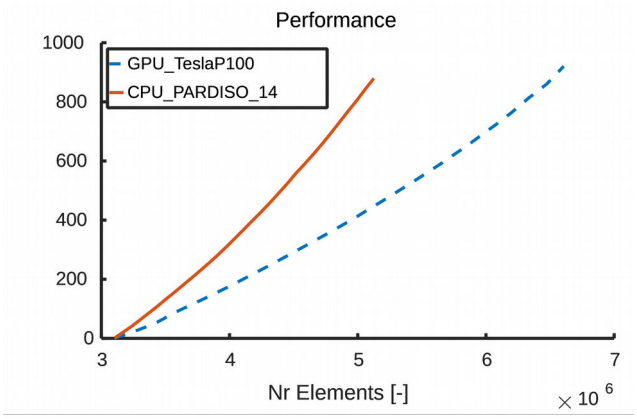


Figure 1. Simulation of the extrusion process (left) and performance gain on GPU (right)

2. *A particle tracking algorithm for the efficient determination of longitudinal weld lines in extruded profiles*

The material interface between two subsequent billets during a continuous extrusion process is inhomogeneous due to the welding of the two workpieces. These so-called welding lines persist in the extruded profile and remain visible, thus leading to scrap. The accurate prediction and minimization of visible welding lines is therefore of utmost cost relevance. A particle tracking algorithm has been implemented in this project for the recognition of material points originating in the billet interface, within the extruded profile. The relative area of the marked material, which trespasses a given cross-section of the profile is used to determine the final length of the longitudinal weld line.

References:

The summarized activities have not yet been published

Group: Prof P.H. Hünenberger - Computer Simulation of Molecular Systems (CSMS)

Researchers: Prof P.H. Hünenberger / Pavel Oborský / David Hahn / Marina Pereira / Alzbeta Kubincová

Description: 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: www.csms.ethz.ch/publications/book)
- 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

Institute of Fluid Dynamics / Computational Fluid Dynamics and Multi-Scale Modeling

Researchers: Prof. Dr. Patrick Jenny, Nemanja Andric, Oliver Brenner, Dr. Davide Cortinovis, Rajdeep Deb, Robert Epp, Valentin Giddey, Dr. Karim Khayrat, Thomas Kummer, Stephan Küchlin, Dr. Adrien Lücker, PD Dr. Daniel W. Meyer, Arthur Moncorgé*, Daniel Oberle, Dr. Franca Schmid, Dr. Ran Sui*, Philipp Weiss *) external

Description:
Most of our current research projects are grouped into the following four major directions:

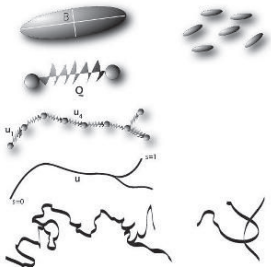
(1) Flow and transport in porous and fractured media: This is a collaborative research effort with researchers from Chevron, Total, and Stanford University. Subsurface flows of water or oil are determined by the permeability distribution K(**x**), which is typically a very heterogeneous quantity. For fast flow and transport simulations with K(**x**) given, we have been generalizing our multiscale finite-volume method (MSFV). Moreover, with K(**x**) being a highly uncertain quantity, we are developing numerical methods that translate given statistics for K(**x**) to flow and transport statistics. In the context of geothermal energy production, we are developing numerical solution methods for the coupled flow/geomechanics problem. Lastly, we have been working on models for single- and multi-phase transport that enable a simplified representation of pore-scale effects at larger scales.

(2) Fluid dynamics in biomedical systems: We are collaborating with researchers from the Universities of Arizona, Berlin, Bern, San Diego, and Zürich. In a first research area, we have been devising a computational modeling framework that sheds light on the rheological influence of red blood cells (RBCs) on cerebral blood flow in capillary networks. Moreover, we have been developing a numerical model for oxygen transport from capillaries to tissue. These models allow us to investigate the heterogeneity of capillary transit times of RBCs or the so-called neurovascular coupling linking neuronal activity to cerebral blood flow. Our second focus deals with the development of a numerical model of the human hearth that accounts for electrophysiology as well as structure mechanics. We intend to use this model for the investigation of novel heart assist device concepts.

(3) Turbulence modeling and turbulent reactive flow: The combustion of fuel sprays is central in aircraft turbines and Diesel engines. We are conducting direct numerical simulation (DNS) studies to investigate the dynamics of evaporating fuel droplets in turbulent flows. Our DNS results provide valuable data that guide an ongoing model development effort in the context of statistical turbulence modeling or more precisely one-dimensional turbulence.

(4) Rarefied gas dynamics: This research area is relevant for the simulation of flows in, e.g., nano-scale devices, during re-entry of a space vehicle, or of plasma. In a first subproject, we have been developing a general-purpose algorithm that encompasses all Knudsen number (Kn) regimes and that is applicable for practically relevant geometries (Kn characterizes the degree of gas rarefaction). This approach is based on our inexpensive Fokker-Planck collision operator for small and intermediate Kn. A second subproject deals with the study of gas-surface and gas-gas interactions for species separation at high Knudsen numbers. This work benefits from detailed molecular dynamics simulations of gas molecules interacting with solid walls.

Group: Computational Polymer Physics, D-MATL, ETH Zurich



Researchers: Prof. Martin Kröger [1]
Prof. Ying Li [2]
Prof. Avraham Halperin [3]
Prof. Andreas Bausch [4]
Prof. Nigel Clarke [5]

Affiliations: [1] Polymer Physics, D-MATL, ETH Zürich
[2] University of Connecticut, USA
[3] CEA Grenoble, France
[4] TU Munich, Germany
[5] University of Sheffield, United Kingdom

Description:

Computational Polymer Physics @ ETH recently focused its attention on viscoelasticity and permeability of carbon buckypaper [1], self-assembled core-polyethylene glycol-lipid shell nanoparticles subjected to flow [2], integrators for molecular and particle simulation [3], tumbling-snake dynamics [4], molecular dynamics simulations of polymer crystallization under confinement [5], the effect of boundaries on the contraction of active gels [6], and the modeling of polymer structure and conformations in polymer nanocomposites [7]. Details available at www.complexfluids.ethz.ch

[1] Z. Shen, M. Röding, M. Kröger, Y. Li, *Polymers* **9** (2017) 115.
[2] Z. Shen, H. Ye, M. Kröger, Y. Li, *Phys. Chem. Chem. Phys.* **19** (2017) 13294-13306.; *Nanoscale* **8** (2017) 14821-14835.
[3] X. Shang, M. Kröger, B. Leimkuhler, *Soft Matter* **13** (2017) 8565-8578.
[4] P.S. Stephanou, T. Schweizer, M. Kröger, *J. Chem. Phys.* **146** (2017) 161101.; *J. Chem. Phys.* **144** (2017) 124905.
[5] C. Luo, M. Kröger, J.-U. Sommer, *Polymer* **109** (2017) 71-84.
[6] M. Schuppler, F.C. Keber, M. Kröger, A.R. Bausch, *Nat. Commun.* **7** (2017) 13120.
[7] A. Karatrantos, N. Clarke, M. Kröger, *Polym. Rev.* **56** (2017) 385-428.

Title: *Ab-initio* simulations of the electrostatics in CBRAM cells

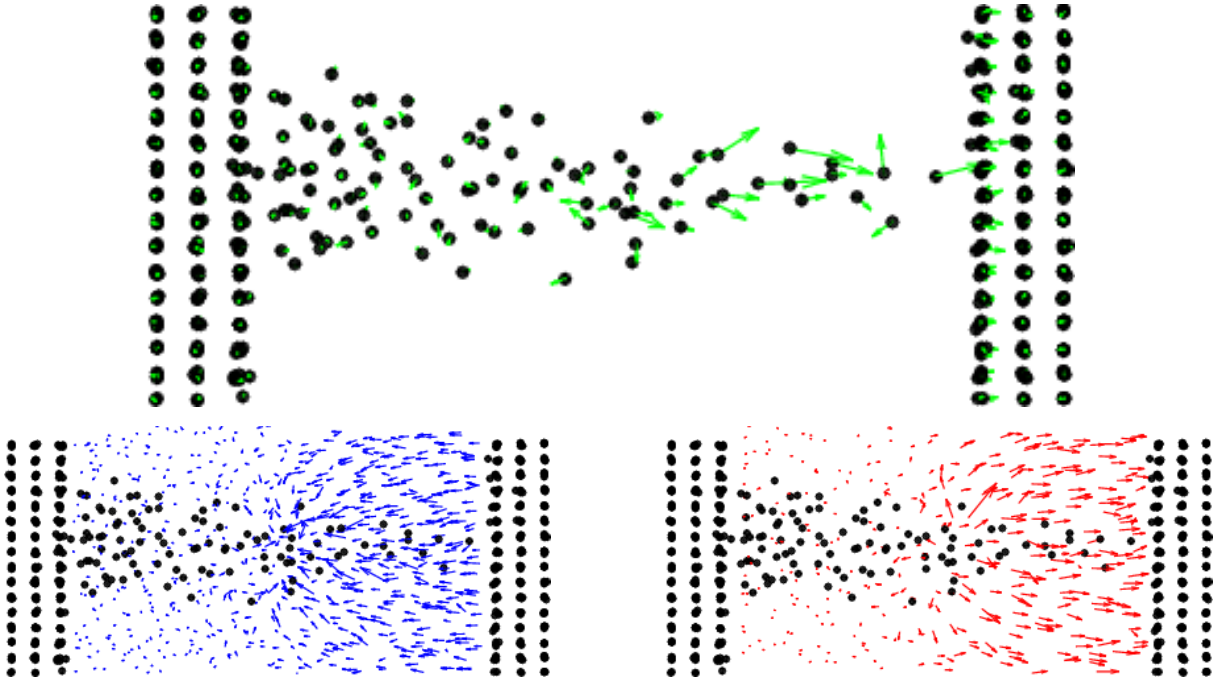
Researchers: Samuel Andermatt
Fabian Ducry
Mathieu Luisier

Institute/ Group: Integrated Systems Laboratory/
Nano-TCAD Group

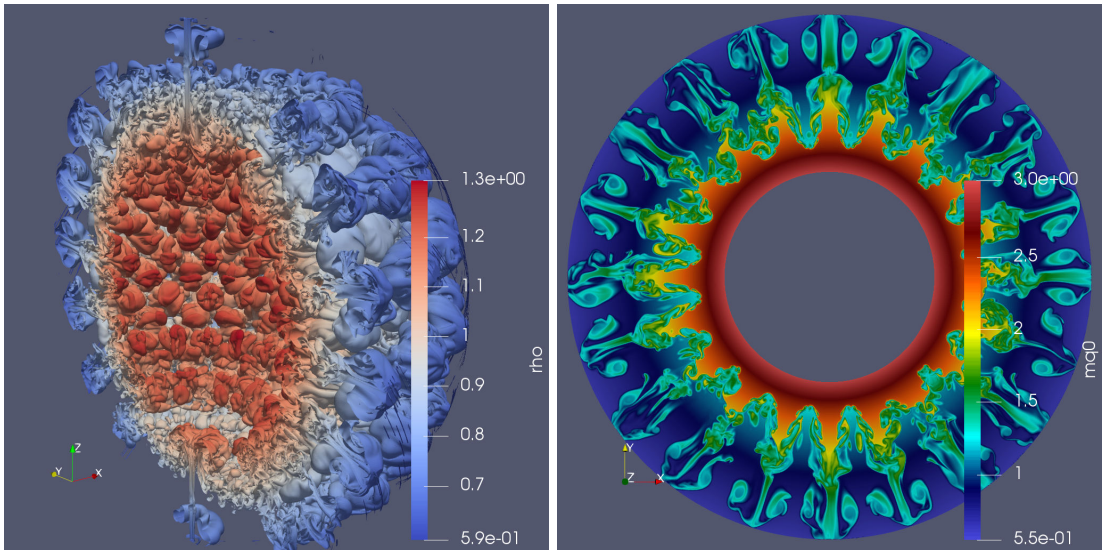
Description:

The electrostatic and switching properties of conductive bridging random access memories (CBRAM) strongly depend on the atomic properties and configuration of the underlying nano-filaments that form between two metallic plates through a dielectric layer. Due to the extremely narrow dimensions of these filaments, high electric field intensities are expected. To design better performing CBRAM cells it is therefore essential to precisely understand the interplay between the atomic positions and the electric field resulting from an externally applied bias.

We used a method called Ehrenfest molecular dynamics (EMD) at the density functional theory (DFT) level of accuracy to calculate the electrostatic forces inside a CBRAM cell. A potential difference was applied at the boundaries of the system. The simulations were performed in the simulation package CP2K with an MPI parallel approach, where on each node a hybrid CPU/GPU approach was employed with OpenMP threading on the CPU and the GPU code implemented in cuda. Collaborations with experimentalists have been established to shed light on fabricated devices and to guide future experiments.



Electrostatic forces in a CBRAM cell. The black dots represent copper atoms, while the surrounding silicon and oxygen atoms are not depicted. (Top) Forces acting on the copper atoms. They concentrate at the tip of the filament, where the charges are maximal and the field the strongest. (Bottom) Forces inside the amorphous silicon dioxide matrix that surrounds the copper filament. The atoms themselves are not visualized. The forces on the oxygen (blue) and silicon (red) atoms follow the plotted electronic field lines.



Insitute: Research group of S. Mishra, SAM, ETH Zurich.

Researchers: S. Mishra, F. Leonardi, K. Lye, C. Pares Pulido, S. Gurjar, L. Grosheintz Laval.

Description: Research in the group of S. Mishra is focussed on the design, analysis and implementation of efficient numerical methods for nonlinear hyperbolic and convection-dominated partial differential equations and their application in fluid dynamics and astrophysics. In 2017, one of the major research projects in the group has been the continuing development of a novel solution concept, that of statistical solutions, for compressible as well as incompressible Euler equations of fluid dynamics. This solution concept is promising in terms of the possibility of proving global well-posedness. It also appears to be a natural paradigm for uncertainty quantification in turbulent fluid flows. Statistical sampling techniques such as Monte Carlo are combined with efficient arbitrary high-order finite volume, DG and spectral (viscosity) methods to compute the (multi-point) statistics for turbulent flows.

Among other projects pursued in the group in 2017, notable examples include the design of well-balanced schemes for simulating astrophysical flows, arbitrary high-order schemes for simulating anelastic flows and the simulation of powder cloud avalanches using multiphase flows.

Institute/Group: Institute for Biomechanics / Laboratory for Bone Biomechanics

Researchers: Nicholas Ohs
Gianna Marano
Duncan Betts
Patrik Christen
Peter Arbenz (collaborator at the Computer Science Department)
Ralph Müller

Description:

The Laboratory for Bone Biomechanics aims at providing a bridge between biologists, who have brought molecular and cellular components within the realm of engineering, and engineers, who have brought the methods of measurement, analysis, synthesis, and control within the realm of molecular and cell biology. More specifically, new developments in biomechanical research are aimed at the quantification and modelling of bone at the molecular, cellular, and organ level incorporating novel principles and techniques of mechanics, imaging, and computational modelling applied to the areas of tissue engineering and regeneration, systems mechanobiology and personalized medicine.

We have started to build up a computational framework that integrates the group's image processing as well as mechanobiological computer simulation at the molecular, cellular, and organ level. The framework is implemented in Python using unit tests and git versioning. It includes helper modules such as reading/writing specialized image formats as well as SI unit handling with the Python package pint. The framework abstracts CSCS usage and thus any program within the framework can be run on the supercomputer without any modifications. Image processing, image segmentation, and multiresolution image registration methods and a solver for advection and diffusion equations for remodelling simulations have been integrated.

One of our published computational modelling contributions is the simulation of load-adaptive bone remodelling in osteoporosis. Osteoporosis is a major medical burden and its impact is expected to increase in our aging society. The bone remodelling algorithm is implemented with an advection equation and a mechanical feedback loop where the micro-finite element solver ParOSol was used on the Cray XC30 system at CSCS. The predicted bone loss revealed realistic changes on the organ level and on biomechanical competence. One limitation of this study is that high-resolution micro-CT images were used that cannot be obtained in vivo in patients. We therefore currently investigate whether the lower image resolution systems used in the clinic would also provide adequate images for our simulations. It would potentially allow the prognosis of aging and diseases such as osteoporosis directly in an individual patient and thus in a personalized manner. Our framework is used for this purpose on CSCS's Cray XC40 system.

A good example for possible MSc and BSc theses in computational science and engineering in our group is a current MSc thesis on the optimisation of iteratively running finite element analyses. The bone remodelling simulation require a finite element calculation in each simulation time step. Since only small changes in the element values are expected within one time step, the solution from one iteration might be used as an initial guess for the start vector of the next iteration to achieve faster convergence. Tests on human bone are encouraging already indicating that this indeed is the case.

Title: Communication: Role of explicit water models in the helix folding/unfolding processes

Researchers: F. Palazzesi[1]
M. Salvalaglio[2]
A. Barducci[3]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera italiana, 6900 Lugano, Switzerland
[2] Department of Chemical Engineering, University College London, London WC1E 7JE, United Kingdom
[3]Universite de Montpellier, CNRS, UMR 5048, Centre de Biochimie Structurale, Montpellier, France

Description:

In the last years, it has become evident that computer simulations can assume a relevant role in modelling protein dynamical motions for their ability to provide a full atomistic image of the processes under investigation. The ability of the current protein force-fields in reproducing the correct thermodynamics and kinetics systems behaviour is thus an essential ingredient to improve our understanding of many relevant biological functionalities. In this work, employing the last developments of the metadynamics framework, we compare the ability of state-of-the-art all-atom empirical functions and water models to consistently reproduce the folding and unfolding of a helix turn motif in a model peptide. This theoretical study puts in evidence that the choice of the water models can influence the thermodynamic and the kinetics of the system under investigation, and for this reason cannot be considered trivial.

References: *J. Chem. Phys* 145, 2016, 121101
DOI: 10.1063/1.4963340

Title: Overcoming time scale and finite size limitations to compute nucleation rates from small scale well tempered metadynamics simulations

Researchers: M. Salvalaglio[1]
P. Tiwary[2]
G. M. Maggioni[3]
M. Mazzotti[3]
M. Parrinello[4]

Institute/Group: [1]Department of Chemical Engineering, University College London, London WC1E 7JE, United Kingdom
[2]Department of Chemistry, Columbia University, New York, New York 10027, USA
[3]Institute of Process Engineering, ETH Zurich, CH-8092 Zurich, Switzerland
[4]Department of Chemistry and Applied Biosciences, ETH Zurich, CH-8092 Zurich, Switzerland and Facolta di informatica, Istituto di Scienze Computazionali, Universita della Svizzera Italiana,6900 Lugano, Switzerland

Description:

Condensation of a liquid droplet from a supersaturated vapour phase is initiated by a prototypical nucleation event. As such, it is challenging to compute its rate from atomistic molecular dynamics simulations. In fact, at realistic supersaturation conditions condensation occurs on time scales that far exceed what can be reached with conventional molecular dynamics methods. Another known problem in this context is the distortion of the free energy profile associated to nucleation due to the small, finite size of typical simulation boxes. In this work the problem of time scale is addressed with a recently developed enhanced sampling method while contextually correcting for finite size effects. We demonstrate our approach by studying the condensation of argon, and showing that characteristic nucleation times of the order of magnitude of hours can be reliably calculated. Nucleation rates spanning a range of 10 orders of magnitude are computed at moderate supersaturation levels, thus bridging the gap between what standard molecular dynamics simulations can do and real physical systems. Published by
the calculation of nucleation rates from first principles still

References: *J. Chem. Phys.* 145, 2016, 211925
DOI: 10.1063/1.4966265

Title: A variational conformational dynamics approach to the selection of collective variables in metadynamics

Researchers: J. McCarty[1]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zurich and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera italiana, 6900 Lugano, Switzerland

Description:

In this paper we combine two powerful computational techniques, well-tempered metadynamics and time lagged independent component analysis. The aim is to develop a new tool for studying rare events and exploring complex free energy landscapes. Metadynamics is a well-established and widely used enhanced sampling method whose efficiency depends on an appropriate choice of collective variables. Often the initial choice is not optimal leading to slow convergence. However, by analyzing the dynamics generated in one such a run with a time-lagged independent component analysis and the techniques recently developed in the area of conformational dynamics, we obtain much more efficient collective variables, that are also better capable of illuminating the physics of the system. We demonstrate the power of this approach in two paradigmatic examples.

References: *Cond-mat-stat-mech. arXiv:* 2017, 1703.08777vl

Title: Conformational Entropy as Collective Variable for Proteins

Researchers: F. Palazzesi[1]
O. Valsson[1,2]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, ETH Zurich, and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera italiana, 6900 Lugano, Switzerland
[2] National Center for Computational Design and Discovery of Novel Materials MARVEL, Università della Svizzera italiana, 6900, Lugano, Switzerland

Description:

Many enhanced sampling methods, such as Umbrella Sampling, Metadynamics or Variationally Enhanced Sampling, rely on the identification of appropriate collective variables. For proteins, even small ones, finding appropriate collective variables has proven challenging. Here we suggest that the NMR S^2 order parameter can be used to this effect. We trace the validity of this statement to the suggested relation between S^2 and entropy. Using the S^2 order parameter and a surrogate for the protein enthalpy in conjunction with Metadynamics or Variationally Enhanced Sampling we are able to reversibly fold and unfold a small protein and draw its free energy at a fraction of the time that is needed in unbiased simulations. From a more conceptual point of view this implies describing folding as a resulting from a trade off between entropy and enthalpy. We also use S^2 in combination with the free energy flooding method to compute the unfolding rate of this peptide. We repeat this calculation at different temperatures to obtain the unfolding activation energy.

References: *Phys-chem-ph, arXiv:* 2017, 1704.03344vl

Title: Unbinding Kinetics of a p38 MAP Kinase Type II Inhibitor from Metadynamics

Researchers: R. Casasnovas[1]
V. Limongelli[2,3]
P. Tiwary[4]
P. Carloni[1]
M. Parrinello[5]

Institute/Group: [1]Computational Biomedicine (IAS-5/INM-9), Forschungszentrum Jülich, Jülich 52425, Germany
[2]Università della Svizzera Italiana (USI), Faculty of Informatics, Institute of Computational Science - Center for Computational Medicine in Cardiology, via G. Buffi 13, CH-6900, Lugano, Switzerland
[3]Department of Pharmacy, University of Naples "Federico II", via D. Montesano 49, Naples I-80131, Italy
[4]Dept. of Chemistry, Columbia University, New York, 10027, USA
[5]Dept. of Chemistry and Applied Biosciences, ETH Zurich, and Faculty of Informatics, Institute of Computational Science, Università della Svizzera Italiana, via G. Buffi 13, Lugano 6900, Switzerland

Description:

Understanding the structural and energetic requisites of ligand binding toward its molecular target is of paramount relevance in drug design. In recent years, atomistic free energy calculations have proven to be a valid tool to complement experiments in characterizing the thermodynamic and kinetic properties of protein/ligand interaction. Here, we investigate, through a recently developed metadynamics-based protocol, the unbinding mechanism of an inhibitor of the pharmacologically relevant target p38 MAP kinase. We provide a thorough description of the ligand unbinding pathway identifying the most stable binding mode and other thermodynamically relevant poses. From our simulations, we estimated the unbinding rate as koff = 0.020 ± 0.011 s−1. This is in good agreement with the experimental value (koff = 0.14 s−1). Next, we developed a Markov state model that allowed identifying the rate-limiting step of the ligand unbinding process. Our calculations further show that the solvation of the ligand and that of the active site play crucial roles in the unbinding process. This study paves the way to investigations on the unbinding dynamics of more complex p38 inhibitors and other pharmacologically relevant inhibitors in general, demonstrating that metadynamics can be a powerful tool in designing new drugs with engineered binding/unbinding kinetics.

References: *J. Am. Chem. Soc.,* 139, 2017, 4780-4788
DOI: 10.1021/jacs.6b12950

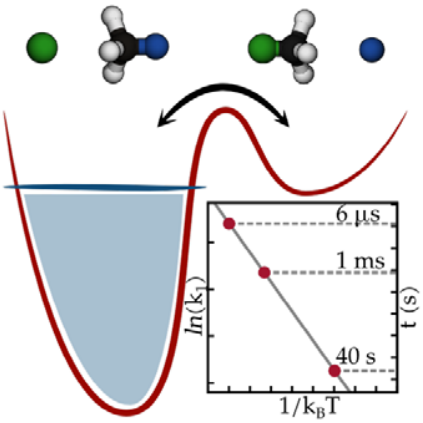
Title: Variational Flooding Study of a S_N2 Reaction

Researchers: C. M. Piccini[1]
J. Mc. Carty[2]
O. Valsson
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zurich, 8093 Zurich, Switzerland and
Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera italiana, 6900 Lugano, Switzerland

Description:

We have studied the reaction dynamics of a prototypical organic reaction using a variationally optimized truncated bias to accelerate transitions between educt and product reactant states. The asymmetric SN2 nucleophilic substitution reaction of fluoromethane and chloromethane CH3F + Cl− ⇌ CH3Cl + F− is considered, and many independent biased molecular dynamics simulations have been performed at 600, 900, and 1200 K, collecting
several hundred transitions at each temperature. The transition times and relative rate constants have been obtained for both reaction directions. The activation energies extracted from an Arrhenius plot compare well with standard static calculations.



References: *J. Phys. Chem. Lett.,* 8, 2017, 580-583
DOI:10.1021/acs.jpclett.6b02852

Title: Prion protein $\beta 2$–$\alpha 2$ loop conformational landscape

Researchers: E. Caldarulo[1]
A. Barducci[2]
K. Wüthrich[3]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zurich, 8093 Zurich, Switzerland and Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera italiana, 6900 Lugano, Switzerland
[2]Centre de Biochimie Structurale, INSERM, CNRS, Universit ´e de Montpellier, FR-34090 Montpellier, France
[3]Institute of Molecular Biology and Biophysics, Eidgenössische Technische Hochschule Zurich, CH-8093 Zurich, Switzerland; and Department of Integrative Structural and Computational Biology, The Scripps Research Institute, La Jolla, CA 92037

Description:

In transmissible spongiform encephalopathies (TSEs), which are lethal neurodegenerative diseases that affect humans and a wide range of other mammalian species, the normal "cellular" prion protein (PrPC) is transformed into amyloid aggregates representing the "scrapie form" of the protein (PrPSc). Continued research on this system is of keen interest, since new information on the physiological function of PrPC in healthy organisms is emerging, as well as new data on the mechanism of the transformation of PrPC to PrPSc. In this paper we used two different approaches: a combination of the well-tempered ensemble (WTE) and parallel tempering (PT) schemes and metadynamics (MetaD) to characterize the conformational free-energy surface of PrPC. The focus of the data analysis was on an 11-residue polypeptide segment in mouse PrPC(121–231) that includes the $\beta 2$–$\alpha 2$ loop of residues 167–170, for which a correlation between structure and susceptibility to prion disease has previously been described. This study includes wild-type mouse PrPC and a variant with the single residue replacement Y169A. The resulting detailed conformational landscapes complement in an integrative manner the available experimental data on PrPC, providing quantitative insights into the nature of the structural transition-related function of the $\beta 2$–$\alpha 2$ loop.

References: *PNAS,* 1712155114, 114 (36), 2017, 9617-9622
DOI: 10.1073/pnas.1712155114

Title: Identifying Slow Molecular Motions in Complex Chemical Reactions

Researchers: G. M. Piccini[1]
D. Polino[1]
M. Parrinello[1]

Institute/Group: [1] Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule Zurich, 8093 Zurich, Switzerland and
Facoltà di Informatica, Istituto di Scienze Computazionali, Università della Svizzera italiana, 6900 Lugano, Switzerland

Description:

We have studied the cyclization reaction of deprotonated 4-chloro-1-butanethiol to tetrahydrothiophene by means of well-tempered metadynamics. To properly select the collective variables, we used the recently proposed variational approach to conformational dynamics within the framework of metadyanmics. This allowed us to select the appropriate linear combinations from a set of collective variables representing the slow degrees of freedom that best describe the slow modes of the reaction. We performed our calculations at three different temperatures, namely, 300, 350, and 400 K. We show that the choice of such collective variables allows one to easily interpret the complex free-energy surface of such a reaction by univocal identification of the conformers belonging to reactants and product states playing a fundamental role in the reaction mechanism.

References: *J. Phys. Chem. Lett.,* 8, 2017, 4197-4200
DOI: 10.1021/acs.jpclett.7b01889

Institute/Group: Laboratory of Physical Chemistry, ETH Zürich
Group of Martin Quack

Researchers: Prof. Martin Quack
Dr. Sieghard Albert
Dr. Ziqiu Chen
Dr. Csaba Fábri
Dr. Carine Manca Tanner
Dr. Georg Seyfang
Irina Bolotova, Doctoral student (degree ETH obtained 2017)

Description:
Area of Research: Molecular Kinetics and 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.

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.
Key references (reviews), see also www.ir.ETHZ.ch:
M. Quack, Die Spiegelsymmetrie des Raumes und die Chiralität in Chemie, Physik, und in der biologischen Evolution. Nova Acta Leopoldina NF, 412, 119-166 (2016).
M. Quack, Fundamental Symmetries and Symmetry Violations from High Resolution Spectroscopy. In: M. Quack, F. Merkt, (Eds.): Handbook of High Resolution Spectroscopy, Vol. 1, Chapt. 18, Wiley, Chichester, New York, 2011, p. 659-722, ISBN 978-0-470-06653-9.

Institute/Group: Lab. für Physikalische Chemie, Group of Prof. Markus Reiher

Researchers: Prof. Dr. Markus Reiher, Christoph Brunken, Dr. Leon Freitag, Tamara Husch, Dr. Stefan Knecht, Dr. Arseny Kovyrshin, Andrea Muolo, Adrian Mühlbach, Jonny Proppe, Gregor Simm, Jan-Grimo Sobez, Christopher J. Stein, Alain Vaucher, Dr. Thomas Weymuth.

Description: Research in the Reiher group is devoted to general theoretical chemistry. The main focus is on the development of theory and algorithms for the calculation of electronic structures based on the first principles of quantum mechanics. The aim of our efforts is to derive quantitative means as well as concepts for understanding chemical processes. All current projects may be grouped according to four main research directions: Relativistic quantum chemistry, bioinorganic and coordination chemistry, theoretical spectroscopy, and the description of electron–electron interactions and correlations within wavefunction-based and density-functional methods. Our research within relativistic quantum chemistry has been focusing on 4-component and 2-component methods including the development of a relativistic implementation of the quantum chemical density matrix renormalization group (DMRG) algorithm. Recent advances are the development of a relativistic kinetic-balance condition for explicitly correlated basis functions employed in semi-classical relativistic calculations as well as new insight in the definition of electron-correlation energy within 4-component atomic and molecular calculations. Tackling the electron-correlation problem is therefore at the heart of quantum chemistry. Although some methods – such as the notorious B3LYP hybrid density functional theory (DFT) – became standard models in computational chemistry, they may yield unreliable results for special classes of molecules, for example those with dense-lying frontier orbitals such as transition metal complexes. We therefore devised a Bayesian framework for DFT that allows for an error estimation of calculated properties to uncover pathological cases. This allows to find a controlled way to systematically improve these methods. We also developed a new computational software package which implements the DMRG algorithm in an efficient matrix-product operator formalism. One of the key challenges of quantum-chemical multiconfiguration methods is the necessity to manually select orbitals for the active orbital space. In recent works we showed how the iterative nature of DMRG combined with its capability to include up to about 100 orbitals in the active space can be exploited for a systematic assessment and selection of active orbitals. These benefits allowed us to derive a setup that paves the way for routine black-box multiconfiguration calculations. For the exploration of chemical reactivity of complex molecular systems, we developed a new approach which we call Haptic Quantum Chemistry as it exploits our tactile sense to physically experience quantum mechanical forces that are exerted between reactants on molecular fragments. This novel concept opens up a new dimension to the chemist's intuition toward chemical reactivity and reaction mechanisms. In parallel we are developing reliable models of reaction networks based on discrete-time kinetic simulations in discrete state space taking free energy uncertainties into account. An important application of our approach is the detection of regions in a reaction network which require further investigation, given the uncertainties introduced by both approximate electronic structure methods and kinetic models. Such cases can then be studied in greater detail with more sophisticated first-principles calculations.

Institute/Group: Lab. of Physical Chemistry / Theoretical Molecular Quantum Dynamics / group of Prof. Jeremy Richardson

Researchers: Danilo Calderini, Anand Ojha, Jeremy O. Richardson, Johan Runeson, Maximilian Saller, Manish Thapa, Pierre Winter

Description:

The group is devoted to developing new approaches for simulating quantum dynamics in complex molecular systems. We do not use Schrödinger's wave-mechanics approach as this would scale unfavourably with the size of the system, and instead we employ imaginary-time path-integral methods. We show that these methods can give an excellent approximation to the description of quantum effects such as tunnelling, delocalization and coupled electron-nuclear dynamics. They can be evaluated numerically using computer algorithms developed originally for classical statistical mechanics such as local optimization, molecular dynamics and Metropolis Monte Carlo. Our dynamics methods can be combined with Quantum Chemistry programs for on-the-fly evaluation of the electronic structure at each nuclear configuration.

Our current projects are centred around the development of theories for describing tunnelling, the rate of electron-transfer reactions, photoexcited dynamics, and vibronic spectroscopy. We have a particular interest in computing microcanonical rates for use in modelling of atmospheric chemistry and in studying coupled electron-nuclear dynamics in liquids.

As these theories are newly developed, the algorithms we use are not yet optimized and there will be room for improvement in the computational efficiency. Projects for CSE Master's students could involve developing faster algorithms either for minimization or for sampling. With these improvements in efficiency, the student would then be able to study larger and more complex molecules, which are out of reach by current techniques.

A particular interest of our group is understanding tunnelling in water clusters. Tunnelling occurs as the water molecules rearrange to give a permuationally-invariant version. The medium-sized water clusters involving six to 22 water molecules have billions of permutational arrangements. In order to locate and then categorize the different tunnelling pathways, we employ both group theory and graph theory. An automatic procedure for performing this analysis does not yet exist and would be extremely useful to the community of spectroscopists. The development of such a computer program would be an excellent project for an interested CSE student.

Institute/Group: Laboratory of Physical Chemistry, Computational Chemistry Group

Researchers: Dominik Sidler, Sereina Riniker

Description: Recently, we have generalized the replica-exchange EDS (RE-EDS) method to calculate multiple free-energy differences from a single molecular dynamics (MD) simulation [*J. Chem. Phys*., **145**, 154114 (2016)]. In EDS, a reference state is simulated which "envelopes" the end-states. The challenge of this methodology is the determination of optimal reference-state parameters: smoothness parameter(s) and energy offsets. A robust scheme to estimate the energy offsets was developed. The next step is to optimize the distribution of the replicas in the smoothness-parameter space to ensure sufficient transitions and sampling of all end-states. This is especially important for slowly adapting environments such as protein binding pockets.

Researchers: Jagna Witek, Sereina Riniker

Description: Kinetic models of cyclosporine A (CsA) in chloroform and water based on MD data revealed the existence of two "congruent" conformational states which occur in both environments [*J. Chem. Inf. Model*., **56**, 1547 (2016)]. These conformational states may facilitate membrane permeability. A derivative of CsA, cyclosporine E (CsE), contains one backbone *N*-methylation less and is less permeable by an order of magnitude. This pair of peptides represents thus a "permeability cliff". Kinetic models of CsE hint at slower interconversion timescales as a rationale for the lower permeability of CsE. Our approach is further used to investigate the effect of side chains on the conformational behavior. To this end, we study a series of cyclic decapeptides that have the same backbone N-methylation pattern but different side chains at the turns.

Researchers: Annick Renevey, Sereina Riniker

Description: We have recently reparametrized the interactions between atomistic (AT) particles and coarse-grained (CG) water to reproduce the hydration free energy of AT side-chain analogues and water [*J. Chem. Phys*., **146**, 124131 (2017)]. The resulting AT-CG force field can be employed in hybrid AT/CG simulations, where the protein (and potentially a solvent layer around the protein) is treated at the AT level and the surrounding solvent by CG beads, in order to lower the computational cost but retain accuracy in the region of interest. We are currently working on a large-scale benchmarking study of proteins and membranes in CG water, with and without AT water layer.

Researchers: Patrick Bleiziffer, Sereina Riniker

Description: Parametrization of small organic molecules for MD simulations is not trivial due to the vastness of chemical space, which limits the use of building blocks. Partial charges are therefore typically obtained by a quantum-mechanical (QM) calculation of the new molecule, often with low accuracy methods to reduce the computational cost. Instead of performing a QM calculation for each individual molecule, we are training machine-learning (ML) models on high-quality reference electron densities on a large set of molecules, which can predict the partial charges of new molecules outside the training set with high accuracy.

Title: Climate Change and the Water Cycle: Processes and Scenarios

Researchers: Nikolina Ban, Roman Brogli, Erich Fischer, Doris Folini, Laureline Hentgen, Adel Imamovic, Michael Keller, Nico Kröner, David Leutwyler, Daniel Lüthi, Bettina Meyer, Guido Müller, Davide Panosetti, Anna Possner, Jan Rajczak, Christoph Schär, Linda Schlemmer, Matthias Schwarz, Silje Sørland, Martin Wild.

Institute/Group: Institute for Atmospheric and Climate Science
Group of Christoph Schär

Description:

We are using global and regional atmospheric models on a wide range of temporal and spatial scales. The high-resolution regional modeling uses the COSMO-CLM limited-area atmospheric model, and is coordinated by Drs. D. Lüthi, N. Ban, S. Sørland and L. Schlemmer. Comprehensive European-scale climate-change scenario simulations are conducted in the framework of the COordinated Regional climate Downscaling Experiment (Euro-CORDEX) at horizontal resolutions of 12 and 50 km covering the period 1950-2100. Recent work in this context is addressing a standard validation of all models participating in Euro-CORDEX, the calibration of the COSMO-CLM, the analysis of changes in heat-wave, heavy precipitation events and snow cover, the height-dependence of the climate change signals, the representation of aerosol effects, and the quantification of different drivers behind the European summer climate. In addition, we are downscaling a thousand-year-long simulation using COSMO-CLM at horizontal resolution of 50 km, with aim of assessing the role of internal variability for extreme events.

In parallel, we are further developing a high-resolution climate simulation capability with horizontal resolutions at the km-scale. The main motivation behind this work is the desire to explicitly simulate convective clouds (as opposed to using convective cloud parameterization schemes in lower-resolution models). Within the SNF-Sinergia project crCLIM, we are now using a GPU version of the COSMO model. This has enabled us to produce one of the first 10-year long simulations over the European continent at such a high resolution. In addition, we have produced another 10-year long simulation as a Pseudo-Global Warming experiment. The aim of this work is to estimate the effect of thermodynamic changes on climate. The long simulations are complemented by idealized simulations and by detailed analyses of precipitation processes over mountainous terrain, using a combination of satellite data and idealized large-eddy simulations.

The global scale simulations are carried out with the climate model ECHAM6-HAM, developed at the Max Planck Institute in Hamburg, Germany. This work is led by Prof. Martin Wild and Dr. Doris Folini, and it also exploits collaborations with the group of Prof. Ulrike Lohmann. The model contains sophisticated aerosol and cloud microphysics schemes. These are essential for realistic simulations of radiation and precipitation processes in the atmosphere. This model is used to study the link between anthropogenic and natural perturbations of the radiation balance and the intensity of the hydrological cycle. The time period under consideration covers 1870-2100. The global model simulations provide also boundary conditions to drive the regional model. Currently, ECHAM6-HAM is expanded into a coupled atmosphere-ocean climate modeling system, which allows to exploit the full response of the climate system in general and the water cycle in particular to the imposed radiative forcings in transient mode.

References:
A series of papers has been published (see references for further details).

Research Group of Professor Ch. Schwab.

Seminar for Applied Mathematics, D-MATH, ETH Zürich.

Project: Sparse Space-Time solution of Symmetric Linear Hyperbolic Systems

Researchers: Christoph Schwab
Pratyuksh Bansal

Acoustic and elastic wave phenomenon are governed by symmetric linear hyperbolic systems. Numerical methods for solving such systems are well established [1]. However, if the mesh has local refinement, for example - close to the corners in a polygonal domain, numerical solution can be tedious. If an explicit numerical scheme is used, the time step size is severely restricted by the CFL condition corresponding to the smallest cells of the mesh. On the other hand, using an implicit scheme leads to large linear system of equations, which can be computationally expensive to solve.

Griebel et al. [2] developed the sparse grid technology in a spatial setting, which substantially reduces the computational cost for approximating smooth solutions with slight loss of accuracy. We extend this technique to a space-time setting and prove error and work estimates for a discontinuous Galerkin [3] scheme with a suitable time integration. Numerical experiments for acoustic waves with 1d physical space and uniform structured grids confirm the theoretical results. Additional experiments also confirm that the sparse space-time technique requires less degrees of freedom to approximate smooth solutions with the same accuracy as the full grid scheme.

This research is in part supported by the ModCompShock doctoral network under project number 642768.

References:

[1] G. Cohen and S. Pernet, *Finite element and discontinuous Galerkin methods for transient wave equations*, Scientific Computation, Springer (2017)..

[2] H. Bungartz and M. Griebel, *Sparse Grids*, Acta Numerica, vol. 13 (2004), pp. 147–269.

[3] B. Cockburn, G. Karniadakis and C.-W. Shu, *The development of discontinuous Galerkin methods*, Discontinuous Galerkin Methods: Theory, Computation and Applications, Lecture Notes in Computational Science and Engineering, vol. 11, Springer (2000), Part I: Overview, pp. 3–50.

Project: Shape Holomorphy for the Boundary Integral Operators in Acoustic Scattering

Researchers: Christoph Schwab
Fernando Henriquez

Partial differential equations (PDEs) have been extensively used to model complex processes and phenomena in a wide range of applications, for instance: optimal shape design, inverse problems, biomedical imaging and non–destructive testing. These models are subject to

the presence of sources of uncertainty, whose effects we would like to characterize and quantify. Computational Uncertainty Quantification (UQ) is the field of research aiming at understanding how this fluctuations propagate throughout a model.

The numerical approximation of such effects becomes a challenge whenever the number of parameters describing the sources of uncertainty is large or even infinity. This phenomenon corresponds to the so–called *curse of dimensionality*: the computational effort required to perform this analysis grows exponentially with the number of parameters involved in the description of the sources of uncertainty.

Recently in [1], a principle to construct sparse representations of solution manifolds of parametric PDEs has been established. This approach relies on the study of the smooth or, more precisely, the *holomorphic* dependence of the solution of a PDE or other *Quantity of Interest* (QoI) on the set of parameters describing the uncertainties in the mathematical model

Recall that the integral equation method allows us to transform certain classes of PDEs into boundary integral equations (BIEs) by means of boundary integral operators (BIOs). In this project, we study the holomorphic dependence of the BIOs as well as the solution of BIEs in the shape of the boundary on which the BIOs and the BIEs are posed. This property, also known as *shape holomorphy*, has been studied in the context of volume formulations for Helmholtz and Maxwell equations [2, 3]. However, to our knowledge, no work in this subject has been done in the context of BIOs and BIEs for acoustic scattering.

This abstract result allow us to use high–order Quasi–Monte–Carlo quadrature methods [4] and sparse interpolation techniques [5] in the computation of statistical moments or other QoI for the solution of a BIE, a crucial task in Computational UQ. Furthermore, we also exploit shape holomorphy of the BIOs to justify the Bayesian approach to shape inverse problems in acoustic wave scattering, a technique also known as *Bayesian shape inversion* [6].

This work is supported by ETH Grant *"Efficient Computational Bayesian Inversion for Risk and Uncertainty in Engineering and the Sciences"*, number 0-20351-17.

References:

[1] A. Chkifa, A. Cohen and Ch. Schwab, *Breaking the curse of dimensionality in sparse polynomial approximation of parametric PDEs*, 103(2):400–428, 2015.

[2] C. Jerez-Hanckes, Ch. Schwab and J. Zech, *Electromagnetic wave scattering by random surfaces: Shape holomorphy*, 17(12):2229–2259, 2016.

[3] A. Cohen, Ch. Schwab and J. Zech, *Shape Holomorphy of the stationary Navier-Stokes Equations*, echnical Report 2016-45, Seminar for Applied Mathematics, ETH Zu?rich, Switzerland, 2016.

[4] R. N. Gantner and Ch. Schwab, *Computational higher order quasi-Monte Carlo integration*, Monte Carlo and Quasi-Monte Carlo Methods, Springer, 2016.

[5] A. Chkifa, A. Cohenand Ch. Schwab, *High-dimensional adaptive sparse polynomial interpolation and applications to parametric PDEs*, Foundations of Computational Mathematics, 14(4):601–633, 2014.

[6] C. Schillings and Ch. Schwab, *Sparse, adaptive Smolyak quadratures for Bayesian inverse problems*, Inverse Problems, 29(6), 2013.

Project: Numerical analysis of stochastic partial differential equations

Researchers: Christoph Schwab
Lukas Herrmann

Physical systems with random input are used to model uncertainty in science and in engineering applications. In particular statistics of the output quantities are of interest. Approximations of statistics of solutions to physical systems such as PDEs with para- metric or stochastic input entail the problem of the approximation of high-dimensional integrals. Quasi-Monte Carlo (QMC) methods are capable to achieve higher convergence rates than well established Monte Carlo methods for these problems. The known theory was extended with an QMC analysis, which exploits locality of supports of func- tion systems that represent the parametric or stochastic input. As a result QMC rules are applicable with product weights instead of computationally more expensive product and order dependent weights. This has been shown in the case of affine- and lognormal-parametric input. In practice the integrands of these high-dimensional integrals are solutions to PDEs and have to be approximated. Multilevel versions of these algorithms are studied, where the number of sample points and spatial degrees of freedom are coupled. This way in certain cases an overall complexity of the computation of the statistics can be achieved which is asymptotically equal to the complexity of one PDE solve.

The applicability of standard PDE solvers to random operator equations, especially multilevel solvers, which have optimal complexity in the non-parametric, deterministic case, is investigated.

This research is supported by the Swiss National Science Foundation (SNSF) under grant SNF 200021 159940/1.

References:

[1] L. Herrmann, *Strong convergence analysis of iterative solvers for random operator equations*, Technical Report 2017-35, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

[2] L. Herrmann and Ch. Schwab, *Multilevel quasi-Monte Carlo integration with product weights for elliptic PDEs with lognormal coefficients*, Technical Report 2017-19, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

[3] L. Herrmann and Ch. Schwab, *QMC algorithms with product weights for lognormal-parametric, elliptic PDEs*, Technical Report 2017-04, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017. To appear in Proc. MCQMC 2016.

[4] R.N. Gantner, L. Herrmann, and Ch. Schwab, *Multilevel QMC with product weights for affine-parametric, elliptic PDEs*, Technical Report 2016-54, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2016. To appear in: Contemporary Computational Mathematics - a celebration of the 80th birthday of Ian Sloan (J. Dick, F. Y. Kuo, H. Woźniakowski, eds.), Springer-Verlag, 2018.

[5] L. Herrmann and Ch. Schwab, *QMC integration for lognormal-parametric, elliptic PDEs: local supports and product weights*, Technical Report 2016-39, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2016

[6] R.N. Gantner, L. Herrmann, and Ch. Schwab, *Quasi-Monte Carlo integration for affine-parametric, elliptic PDEs: local supports and product weights*, Technical Report 2016-32, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2016. To appear in SIAM J. Numer. Anal.

[7] L. Herrmann, A. Lang, and Ch. Schwab, *Numerical analysis of lognormal diffusions on the sphere*, Stoch PDE: Anal Comp, published online 05 July 2017.

Project: High dimensional multilevel Smolyak approximation

Researchers: Christoph Schwab
Jakob Zech

Parametric partial differential equations (PDEs) allow the modelling of systems subject to varying input data. The parameter may either represent a known but flexible quantity, or reflect uncertainty in the data, in which case it can be treated as a random variable. More precisely, we consider parametric maps $u : U \to X$ taking values in a Banach space X and defined on the parameter domain $U = [-1, 1]^{\mathbb{N}}$. Here $u(\mathbf{y}) \in X$ denotes the PDE solution for each $\mathbf{y} \in U$. The approximation of u as function of $\mathbf{y}$ relies upon the sufficient decrease of the coefficients in infinite expansions such as polynomial chaos expansions. Results of this type yield best N-term rates and have been verified for a large class of PDE models.

Smolyak algorithms based on sparse grid interpolation are known to achieve these rates in the space $L^\infty(U, X)$, i.e. uniformly for all $\mathbf{y} \in U$. In [2] we significantly improve previously known convergence rates of Smolyak *quadrature* for a certain class of functions, by exploiting the fact that all linear terms in the polynomial chaos expansion are integrated exactly by the quadrature operator. This yields a convergence rate which is more than twice the rate obtained for uniform approximation by Smolyak interpolation.

In practice, for a fixed $\mathbf{y} \in U$ the element $u(\mathbf{y}) \in X$ is unknown and must be approximated itself. Assuming algebraic convergence at rate $\alpha > 0$, this yields mappings $u_l : U \to X$ at certain levels $l \in \mathbb{N}$ such that $\sup_{\mathbf{y}\in U} \|u(\mathbf{y}) - u_l(\mathbf{y})\|_X \leq Cl^{-\alpha}$ for some l-independent constant $C < \infty$. As a consequence, an additional source of error connected to the discretization in the Banach space is introduced. Efficient numerical algorithms require to carefully choose the discretization level l for each interpolation point. This amounts to a multilevel method, where differences of sparse grid interpolants of u_l are suitably combined for different levels l to obtain an approximation to u. In [1] we analyze convergence rates for this multilevel Smolyak interpolation. Additionally, employing new results from [2] we obtain improved convergence rates for the corresponding multilevel Smolyak quadrature. A concrete algorithm is proposed which identifies sets of active multiindices and approximation levels for numerical solvers. As an application, we concentrate on the approximation of solutions to parametric linear and nonlinear PDEs, by using Galerkin methods to approximate the PDE solution at a given point in the parameter domain.

References:

[1] D. Dũng, Ch. Schwab and J. Zech, *High dimensional Smolyak approximation*, 2017 (in preparation).

[2] J. Zech and Ch. Schwab *Convergence rates of high-dimensional Smolyak quadrature*, Technical Report 2017-27, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

Institute/Group: Institute of Geophysics / Geophysical Fluid Dynamics Group

Researchers: Profs. Paul Tackley, Taras Gerya; Drs. Antoine Rozel, Maxim Ballmer, Dan Bower, Jie Liao, Kosuke Ueda, Frank Wagner, Patrick Sanan; PhD students D. Balrao, S. Brändli, A. Cordoba, L. Dal Zilio, D. Gebhardt, I. Fomin, R. Herrendörfer, C. Jain, T. Lichtenberg, J. Munch, C. Petrini, C. Pranger, S. Preuss, J. Schierjott, J. Yun

Description: Our research is based on simulations of solid Earth processes using computational fluid dynamics techniques, in particular mixed Eulerian-Lagrangian codes solving the variable-viscosity Stokes equations on fixed grids (finite volume or finite element) while using moving particles to track different materials and properties.

Prof. Paul Tackley and his students, postdocs and international collaborators perform global simulations of Earth and other planets such as Mars, Venus, and extrasolar super-Earth planets. They collaborate on two ERC projects: iGEO, the goal of which is to use neural networks to compare simulations of Earth to actual data, and AUGURY, the goal of which is to use data assimilation to constrain Earth evolution in the last few 100 million years. We are involved with the Swiss-wide PlanetS NCCR, with projects to model coupled interior-atmosphere evolution and to constrain the composition of exoplanets. Key technical developments were made in the GeoPC PASC Co-design project, which brings recent advances in communication-hiding and hybrid computing to geodynamics simulation, working with the StagYY and pTatin3D application codes on the Piz Daint supercomputer. This effort now continues in the PASC-funded Stag_BL project, with Dr. Patrick Sanan being the key computational scientist in the group.

Prof. Taras Gerya and his students, postdocs and international collaborators work on high-resolution thermomechanical modelling (2D and 3D) of plate tectonics processes: subduction, continental collision, oceanic spreading, continental breakup, numerical modeling of Alpine evolution and seismicity, seismo-thermomechanical modeling of seismic cycles at tectonic plate boundaries, tectono-magmatic modeling of Archean geodynamics, modeling of plume-lithosphere interactions and related surface evolution, thermomechanical modeling of planetesimals evolution, modeling of effects of grainsize evolution on subduction, slab breakoff and transform development. They use the 3D thermo-mechanical coupled numerical code I3ELVIS (Gerya, 2013) based on finite differences and marker-in-cell techniques to solve mass, momentum and energy conservation equations in a fully staggered grid, running on the Euler cluster at ETH. Postdoc Dr. Kosuke Ueda engages in geodynamic modelling of lithosphere-crust-surface interaction. To this end, he also maintains code development to improve coupled surface process-tectonic methods that can produce data comparable to natural observables.

Oberassistant Dr. Antoine Rozel is involved in several research projects involving heavy computational resources. His current work requires hundreds of simulations of mantle convection involving complex rheologies including grain size, as well as Archean (early Earth) geodynamics, which involves partial melting and crust production.

Oberassistant Dr. Maxim Ballmer is involved in several projects with a numerical modeling component. He and his students are interested in the evolution of the mantle of terrestrial planets from the magma-ocean stage to the present-day using global-scale 2D models, as well as in the spatio-temporal and chemical patterns of intraplate volcanism using regional-scale high-resolution 2D/3D models.

Group of W.F. van Gunsteren

Title: Interpretation of seemingly contradictory data: low NMR S^2 order parameters observed in helices and high NMR S^2 order parameters in disordered loops of the protein hGH at low pH

Researchers: L. J. Smith*
R. Athill*
W. F. van Gunsteren
N. Hansen[§]

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Switzerland
*Inorganic Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, U.K.
[§] Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart, Stuttgart, Germany

Description:

At low pH, human growth hormone (hGH) adopts a partially folded state, in which the native helices are maintained, but the long loop regions and side-chain packing become disordered. Some of the S^2 order parameters for backbone N-H vectors derived from NMR relaxation measurements on hGH at low pH initially seem contradictory. Three isolated residues (15, 20, and 171) in helices A and D exhibit low order parameter values (<0.5) indicating flexibility, whereas residue 143 in the centre of a long flexible loop region has a high order parameter (0.82). Using S^2 order parameter restraining MD simulations, this paradox has been resolved. Low S^2 values in helices are due to the presence of a mixture of 3_{10}-helical and α-helical hydrogen bonds. High S^2 values in relatively disordered parts of a protein may be due to fluctuating networks of hydrogen bonds between the backbone and the side chains, which restrict the motion of N-H bond vectors.

References: Chem. Eur. J. **23** (2017) 9585-9591, DOI: 10.1002/chem.201700896, incl. suppl. mat.

Title: Using Complementary NMR Data Sets to Detect Inconsistencies and Model Flaws in the Structure Determination of Human Interleukin-4

Researchers: L.J. Smith*
W.F. van Gunsteren
N. Hansen#

Institute/ Group: Laboratory of Physical Chemistry, ETH Zürich, Zurich, Switzerland
*Inorganic Chemistry Laboratory, Department of Chemistry, University of Oxford, Oxford, U.K.
#Institute of Thermodynamics and Thermal Process Engineering, University of Stuttgart, Stuttgart, Germany

Description:

The derivation of protein structure from values of observable quantities measured in NMR experiments is a rather nontrivial task due to (i) the limited number of data compared to degrees of freedom of a protein, (ii) the uncertainty inherent to the function connecting an observable quantity to molecular structure, (iii) the finite quality of bio-molecular models and force fields used in structure refinement, and (iv) the conformational freedom of a protein in aqueous solution, which requires extensive conformational sampling and appropriate conformational averaging when calculating or restraining to sets of NMR data. The protein interleukin-4 (IL-4) has been taken as a test case using NOE distances, S^2 order parameters, and ^{3}J-couplings as test data and the former two types of data as restraints. It is shown that, by combining sets of different, complementary NMR data as restraints in MD simulations, inconsistencies in the data or flaws in the model and procedures used to derive protein structure from NMR data can be detected. This leads to an improved structural interpretation of such data particularly in more mobile loop regions.

References: J. Phys. Chem. **B 121** (2017) 7055-7063, DOI: 10.1021/acs.jpcb.7b03647, incl. suppl. mat.

Title: Validation of Molecular Simulation: An Overview of Issues

Researchers: W. F. van Gunsteren[1]
X. Daura[2]
N. Hansen[3]
A. E. Mark[4]
C. Oostenbrink[5]
S. Riniker[1]
L. J. Smith[6]

Institute/ Group: [1]Laboratory of Physical Chemistry, ETH Zürich, Zurich, Switzerland
[2]Institute of Biotechnology and Biomedicine,
Universitat Autonoma de Barcelona (UAB), Barcelona, Spain
[3]Institute of Thermodynamics and Thermal Process Engineering,
University of Stuttgart, Stuttgart, Germany
[4]School of Chemistry and Molecular Biosciences,
University of Queensland, St. Lucia, Australia
[5]Institute of Molecular Modeling and Simulation,
University of Natural Resources and Life Sciences, Vienna, Austria
[7]Inorganic Chemistry Laboratory, Department of Chemistry,
University of Oxford, Oxford, United Kingdom

Description:

Computer simulation of molecular systems enables structure-energy-function relationships of molecular processes to be described at the sub-atomic, atomic, supra-atomic or supra-molecular level and plays an increasingly important role in chemistry, biology and physics. To interpret results of such simulations appropriately, the quality of the calculated properties must be evaluated. This depends on (1) the degrees of freedom simulated, (2) the accuracy of the molecular model, interaction function or force field, (3) the equations of motion, integration scheme or other method used to sample degrees of freedom as well as the degree of sampling, (4) the boundary conditions, (5) the simulation software, and (6) how the software is used. When validating simulations against values of experimental observable quantities Q^{exp}, one must also consider (1) the accuracy of Q^{exp}, (2) the accuracy of the function $Q(\boldsymbol{r}^N)$ used to calculate Q based on a molecular configuration $\boldsymbol{r}^N$ of N particles, (3) the sensitivity of the function $Q(\boldsymbol{r}^N)$ to the configuration $\boldsymbol{r}^N$, (4) the relative time scales of the simulation and experiment, (5) the degree to which the calculated and experimental properties are equivalent, and (6) the degree to which the system simulated matches the experimental conditions. Validation by comparison between experiment and simulation is seldom straightforward. Experimental data is limited in scope and generally corresponds to averages over both time and space. A critical analysis of the various factors that influence the apparent degree of (dis)agreement between simulations and experiment is presented and illustrated using examples from the literature. What can be done to enhance the validation of molecular simulation is also discussed.

References: Angew. Chem. Int. Ed. (**2017**) on-line

6

High-performance Hardware

5.2 Information Technology Services

The IT Services of ETH are currently operating two large Linux clusters called **Euler** and **Leonhard**. The old **Brutus** cluster was decommissioned in January 2017 after 9 years (!) of operation.

Euler and Leonhard are financed and operated according to the same "shareholder" model as their predecessors. Professors, institutes and even ETH departments can become shareholders by financing a number of compute nodes in the cluster. In return, they get a share of CPU time proportional to their investment. The Euler share financed by the IT Services is made available to the scientific community of ETH at no cost. Leonhard does not have a public share and is therefore reserved to its shareholders.

To make it easy for users to switch back and forth between Euler and Leonhard, both clusters use the same operating system (CentOS), batch system (IBM Spectrum LSF), development tools (GNU and Intel compilers) and applications.

Euler

The first phase (Euler I) was installed at the beginning of 2014. It consists of 448 compute nodes (HP BL460c Gen8), each equipped with 24 cores (two 12-core Intel Xeon E5-2697v2 CPUs) and between 64 and 256 GB of memory. All compute nodes are connected to two high-speed networks:

- 56 Gb/s InfiniBand FDR for inter-node communication (typically MPI);
- 10 Gb/s Ethernet for file access and for global communication (system management, monitoring, batch system, etc.).

A second phase (Euler II) was installed in 2015. It consists of 768 compute nodes of a newer generation (HP BL460c Gen9), each equipped with 24 cores (two 12-core Intel Xeon E5-2680v3 CPUs) and between 64 and 512 GB of memory. Euler II also contains four very-large-memory nodes with 64 cores (four 16-core Intel Xeon E7-8867v3 CPUs) and 3072 GB of memory. Euler II uses similar high-speed networks as Euler I.

A third phase (Euler III), was installed in January 2017. It consists of 1,215 compute nodes of a new generation (HPE m710x), each equipped with 4 cores (Intel Xeon E3-1585Lv5), 32 GB of memory and 256 GB of fast local NVMe storage. These nodes are connected to a special, low-latency 10G/40G Ethernet network. Thanks to its fast CPUs (3.0–3.7 GHz), Euler III is ideal for applications that cannot easily be parallelized.

The cumulated peak performance of Euler I+II+III is about 1.2 PF (double precision).

A fourth phase (Euler IV) will be installed at the end of 2017. It will consist of 288 compute nodes of the latest generation (HPE XL230k Gen10), each equipped with 36 cores (two Intel Xeon Gold 6150 CPUs) and 192 GB of memory. These nodes will increase the cluster's peak performance to 2.1 PF (double precision).

Euler contains two storage systems: a 400-TB Panasas parallel file system for scratch and medium-term storage, and a 1.2-PB NetApp (NFS) cluster for home directories, applications and long-term project storage.

Leonhard

Leonhard (named after Leonhard Euler to reflect the complementarity of these two clusters) is installed in a brand-new computer room at ETH Zurich. Whereas Euler is a traditional HPC cluster, Leonhard is intended for Big Data applications, in particular in the areas of machine-learning and bio-medical research.

Leonhard is divided into two fully independent parts: Leonhard *Open* for applications dealing with open research data, and Leonhard *Med* for applications dealing with confidential medical data.

The first phase of Leonhard was installed at the beginning of 2017. If consists of 36 traditional compute nodes (HP XL170r Gen9), each equipped with 36 cores (two 18-core Intel Xeon E5-2697v4 CPUs) and either 128 or 512 GB of memory. Considering that many Big Data applications require GPUs, this cluster also contains 12 GPU nodes, each equipped with 20 cores (two 10-core Intel Xeon E5-2650v4 CPUs), 8 Nvidia GTX-1080 GPUs and 256 GB of memory.

Fast, scalable and affordable storage is essential for Big Data applications. Therefore, Leonhard contains two separate parallel file systems (DDN GS14K) based on IBM Spectrum Scale Advanced Edition (formerly known as GPFS), with 2.0 PB of usable space in Leonhard Open and 1.5 PB in Leonhard Med.

The compute nodes and storage systems are connected together via high-speed (100 Gb/s) InfiniBand EDR networks. For security reasons, each part of Leonhard has its own InfiniBand network.

The IT Services issued a call for tender in May 2017 for the procurement of additional GPU nodes. These will be installed at the end of 2017 and are expected to increase the cluster's GPU performance to over 5 PF (single-precision).

7

Publications*

*only CSE-related articles
in refereed journals

Group of P. Arbenz

P. Arbenz, D. Hupp, and D. Obrist. *Comparison of parallel time-periodic Navier–Stokes solvers*. Accepted for publication in the proceedings of PPAM 2011, Lublin, Poland, September 10-13, 2017.

D. Hupp, P. Arbenz, and D. Obrist. *A parallel Navier–Stokes solver using spectral discretization in time*. Int. J. Comput. Fluid Dyn., 30 (7-10): 489-494 (2016) doi:10.1080/10618562.2016.1242725.

N. Ohs, F. Keller, O. Blank, W.-Y. W. Lee, C.-Y. J. Cheng, P. Arbenz, R. Müller, and P. Christen. *Towards in silico prognosis using big data*. Current Directions in Biomedical Engineering. 2 (1): 57–60 (2016), doi:10.1515/cdbme-2016-0016,

P. Benedusi, D. Hupp, P. Arbenz, R. Krause: *A parallel multigrid solver for time-periodic incompressible Navier–Stokes equations in 3D*. In: Numerical Mathematics and Advanced Applications - ENUMATH 2015. B. Karasözen, M. Manguoglu, M. Tezer–Sezgin, S. Göktepe, Ö. Ugur (eds.). Lecture Notes in Computational Science and Engineering 112. Springer, 2016. pp. 265-273. doi:10.1007/978-3-319-39929-4_26.

D. Hupp, D. Obrist, P. Arbenz: *Multigrid preconditioning for time-periodic Navier-Stokes problems*. Proc. Appl. Math. Mech. (PAMM) 15, 595–596 (2015), doi:10.1002/pamm.201510287.

S. Pauli, P. Arbenz: *Determining optimal multilevel Monte Carlo parameters with application to fault tolerance*. Comput. Math. Appl. 70 (11): 2638–2651 (2015), doi:10.1016/j.camwa.2015.07.011.

S. Pauli, P. Arbenz, Ch. Schwab: *Intrinsic fault tolerance of multilevel Monte Carlo methods*. J. Parallel Distrib. Comput. 84: 24–36 (2015), doi:10.1016/j.jpdc.2015.07.005.

S. Pauli, R. Gantner, P. Arbenz, A. Adelmann: *Multilevel Monte Carlo for the Feynman–Kac formula for the Laplace equation*. BIT Numer. Math. 55 (4): 1125–1143 (2015), doi:10.1007/s10543-014-0543-8.

Group of K. Boulouchos selected publications

1. K. Giannakopoulos, C.E. Frouzakis, K. Boulouchos, P.F. Fischer, A.G. Tomboulides, Direct numerical simulation of the flow in the intake pipe of an internal combustion engine, *Int. J. Heat Fluid Flow*, 68, 257-268, 2017.

2. G.K. Giannakopoulos, C.E Frouzakis, M. Matalon, A.G. Tomboulides A.G., The Turbulent Flame Speed of Premixed Spherically Expanding Flames. In: Grigoriadis D., Geurts B., Kuerten H., Frhlich J., Armenio V. (eds) Direct and Large-Eddy Simulation X. ERCOFTAC Series, vol 24. Springer, 2018

3. B. O. Arani, C. E. Frouzakis, J. Mantzaras, K. Boulouchos, Three-dimensional direct numerical simulations of turbulent fuel-lean H_2/air hetero-/homogeneous combustion over Pt with detailed chemistry, *Proc. Combust. Inst.*, 36(3), 4355-4363, 2017.

4. B.O. Arani, C.E. Frouzakis, J. Mantzaras, F. Lucci, K. Boulouchos, Direct numerical simulation of turbulent channel-flow catalytic combustion: Effects of Reynolds number and catalytic reactivity, *Combust. Flame*, 187, 52-66, 2018.

5. M. Jafargholi, G. K. Giannakopoulos, C. E. Frouzakis, K. Boulouchos, Laminar syngasair premixed flames in a closed rectangular domain: DNS of flame propagation and flame/wall interactions, *Combust. Flame*, 188, 453-468, 2018.

6. E. Mastorakos, P. Allison, A. Giusti, P. De Oliveira, S. Benekos, Y. Wright, C. Frouzakis, K. Boulouchos, Fundamental Aspects of Jet Ignition for Natural Gas Engines, *SAE Int. J. Eng.*, 10(5), 2429-2438, 2017.

7. T. Kammermann, J. Koch, Y.M. Wright, P. Soltic, K. Boulouchos, Generation of Turbulence in a RCEM towards Engine Relevant Conditions for Premixed Combustion Based on CFD and PIV Investigations, *SAE Int. J. Engines*, 10(4), 2176-2190, 2017.

8. D. Farrace, K. Chung, S. S. Pandurangi, Y. M. Wright, K. Boulouchos, N. Swaminathan, Unstructured LES-CMC modelling of turbulent premixed bluff body flames close to blow-off, *Proc. Combust. Inst.*, 36(2), 1977-1985, 2017.

9. K. Keskinen, M. Nuutinen, O. Kaario, V. Vuorinen, J. Koch, Y.M. Wright, M. Larmi, K. Boulouchos, Hybrid LES/RANS with wall treatment in tangential and impinging flow configurations, *Int. J. Heat Fluid Flow*, 65, 141-158, 2017

10. C. Mandanis, M. Schmitt, J. Koch, Y.M. Wright, K. Boulouchos, Wall Heat Flux and Thermal Stratification Investigations during the Compression Stroke of an engine-like Geometry: A comparison between LES and DNS, *Flow, Turb. Combust.* (to appear)

11. D. Farrace, K. Chung, M. Bolla, Y.M. Wright, K. Boulouchos, E, Mastorakos, A LES-CMC formulation for premixed flames including differential diffusion, *Combust. Theory Model.*, (to appear)

12. G. Xu, Y.M. Wright, P. Kyrtatos, K. Bardis, M.Schiliro, K. Boulouchos, Experimental and Numerical Investigations of the Engine Operational Conditions Influences on a Small Un-scavenged Pre-Chambers Behavior, *SAE Int. J. Engines* 10 (5), 2017

Group Name: Comas-Vives and Copéret

List of publications:

1. Metathesis Activity encoded in Metallacyclobutane Carbon-13 NMR Chemical Shift Tensors, Gordon, C. P. *et. al. ACS Cent. Sci.* **2017**, 3, 759-768.

2. Understanding the Lewis Acidity of Co(II) Sites on a Silica Surface, Estes, D. P. *et. al. Inorg. Chem.* **2017**, *56*, 7731-7736.

3. Orbital Analysis of Carbon-13 Chemical Shift Tensors Reveals Patterns to Distinguish Fischer and Schrock Carbenes, Yamamoto, K. et. al. *Angew. Chem. Int. Ed.* **2017**, *56*, 10127-10131.

4. Local Structures and Heterogeneity of Silica-Supported M(III) Sites Evidenced by EPR, IR, NMR, and Luminescence Spectroscopies, Delley, M. D. et. al. *J. Am. Chem. Soc.*, **2017**, *139*, 8855-8867.

5. Highly Active and Stable Iridium Pyrochlores for Oxygen Evolution Reaction, Lebedev, D. *et. al. Chem. Mater.* **2017**, *29*, 5182-5191.

6. Unraveling Thermodynamics, Stability, and Oxygen Evolution Activity of Strontium Ruthenium Perovskite Oxide, Kim, B. J. *et. al. ACS Catal.* **2017**, *7*, 3245-3256.

7. Understanding surface site structures and properties by first principles calculations: an experimental point of view!, Comas-Vives, A. *et. al. Chem. Commun.* **2017**, *53*, 4296-4303.

8. CO2-to-Methanol Hydrogenation on Zirconia-Supported Copper Nanoparticles: Reaction Intermediates and the Role of the Metal-Support Interface, Larmier, K. *et. al. Angew. Chem. Int. Ed.* **2017**, *56*, 2318-2323.

9. Cooperativity and Dynamics Increase the Performance of NiFe Dry Reforming Catalysts, Kim, S. M. *et. al. J. Am. Chem. Soc.* **2017**, *139*, 1937-1949.

10. Strain effect and dual initiation pathway in CrIII/SiO2 polymerization catalysts from amorphous periodic models. Floryan, L. et. al. *J. Catal.*, **2017**, 346, 50-56.

11. X-H Bond Activation on Cr(III),O Sites (X = R, H): Key Steps in Dehydrogenation and Hydrogenation Processes, Delley, M. F. *Organometallics*, **2017**, *36*, 234-244.

12. Increased Back-bonding explains Step-Edge Reactivity and Particle Size Effect for CO Actvation on Ru Nanoparticles, Foppa, L. et. al. *J. Am. Chem. Soc.* **2016**, *138*, 16655-16668.

13. Surface Sites in Cu Nanoparticles: Chemical Reactivity of Microscopy, Larmier, K. *J. Phys. Chem. Lett.* **2016**, *7*, 3259-3263.

14. Structural Characterization of the EtOH-$TiCl_4$-$MgCl_2$ Ziegler-Natta Precatalyst, D'Anna, V. *J. Phys. Chem. C*, **2016**, 120, 18075-18087.

15. Correlating Synthetic Methods, Morphology, Atomic-Level Structure, and Catalytic Activity of Sn-β Catalysts, Wolf, P. *et. al. ACS Catal.* **2016**, *6*, 4047-4063.

16. CO_2 Activation on Ni/γ–Al_2O_3 Catalysts by First-Principles Calculations: From Ideal Surfaces to Supported Nanoparticles, Silaghi, M. *et. al. ACS Catal.* **2016**, *6*, 4501-4505.

Publications

R. Casagrande (2016), Discontinuous Finite Element Methods for Eddy Current Simulation, Eth dissertation, SAM, ETH Zurich, Switzerland. Submitted.

R. Casagrande, R. Hiptmair and J. Ostrowski (2016), 'An a priori error estimate for interior penalty discretizations of the curl-curl operator on non-conforming meshes', *Journal of Mathematics in Industry* **6**(1), 1–25.

R. Casagrande, C. Winkelmann, R. Hiptmair and J. Ostrowski (2014), DG treatment of non-conforming interfaces in 3D curl-curl problems, Technical Report 2014-32, Seminar for Applied Mathematics, ETH Zürich, Switzerland.

X. Claeys, R. Hiptmair and C. Jerez-Hanckes (2013), Multi-trace boundary integral equations, in *Direct and Inverse Problems in Wave Propagation and Applications* (I. Graham, U. Langer, J. Melenk and M. Sini, eds), Vol. 14 of *Radon Series on Computational and Applied Mathematics*, De Gruyter, Berlin/Boston, pp. 51–100.

X. Claeys, R. Hiptmair and E. Spindler (2015), 'A second-kind Galerkin boundary element method for scattering at composite objects', *BIT Numerical Mathematics* **55**(1), 33–57.

X. Claeys, R. Hiptmair and E. Spindler (2017*a*), 'Second kind boundary integral equation for multi-subdomain diffusion problems', *Adv. Comp. Math.* **43**(5), 1075–1101.

X. Claeys, R. Hiptmair and E. Spindler (2017*b*), 'Second-kind boundary integral equations for electromagnetic scattering at composite objects', *Computers & Mathematics with Applications*. https://doi.org/10.1016/j.camwa.2017.08.014.

X. Claeys, R. Hiptmair and E. Spindler (2018), 'Second-kind boundary integral equations for scattering at composite partly impenetrable objects', *Comm. Computational Physics* **23**(1), 264–295.

X. Claeys, R. Hiptmair, C. Jerez-Hanckes and S. Pintarelli (2014), Novel multi-trace boundary integral equations for transmission boundary value problems, in *Unified Transform for Boundary Value Problems: Applications and Advances* (A. Fokas and B. Pelloni, eds), SIAM, Philadelphia, pp. 227–258.

R. Hiptmair and C. Jerez-Hanckes (2012), 'Multiple traces boundary integral formulation for Helmholtz transmission problems', *Adv. Comput. Math.* **37**(1), 39–91.

R. Hiptmair and L. Kielhorn (2012), BETL – a generic boundary element template library, Report 2012-36, SAM, ETH Zürich, Switzerland.

R. Hiptmair and A. Paganini (2015), 'Shape optimization by pursuing diffeomorphisms', *Comput. Methods Appl. Math.* **15**(3), 291–305.

R. Hiptmair and C. Pagliantini (2017), Splitting-based structure preserving discretizations for magnetohydrodynamics, Technical Report 2017-18, Seminar for Applied Mathematics, ETH Zürich, Switzerland. Submitted to SMAI J. Comp. Math.

R. Hiptmair, C. Jerez-Hanckes, J.-F. Lee and Z. Peng (2014*a*), Domain decomposition for boundary integral equations via local multi-trace formulations, in *Domain Decomposition Methods in Science and Engineering XXI.* (J. Erhel, M. Gander, L. Halpern, G. Pichot, T. Sassi and O. Widlund, eds), Vol. 98 of *Lecture Notes in Computational Science and Engineering*, Springer, Berlin, Proceedings of the XXI. International Conference on Domain Decomposition Methods, Rennes, France, June 25-29, 2012 I, pp. 43–58.

R. Hiptmair, A. Paganini and S. Sargheini (2014*b*), 'Comparison of approximate shape gradients', *BIT Numerical Mathematics* **55**, 459–485.

A. Paganini (2016), Numerical shape optimization with finite elements, Eth dissertation 23212, ETH Zurich.

A. Paganini, S. Sargheini, R. Hiptmair and C. Hafner (2015), 'Shape optimization of microlenses', *Opt. Express* **23**(10), 13099–13107.

S. Sargheini (2016), Shape Sensitivity Analysis of Electromagnetic Scattering Problems, Eth dissertation 23067, ETH Zurich.

E. Spindler (2016), Second Kind Single-Trace Boundary Integral Formulations for Scattering at Composite Objects, Eth dissertation no. 23620, ETH Zurich, Switzerland.

Group name: Prof P.H. Hünenberger - Computer Simulation of Molecular Systems (CSMS)
List of publications:

W. Plazinski, A. Lonardi & P.H. Hünenberger.
Revision of the GROMOS 56A6$_{CARBO}$ force field for hexopyranose-based carbohydrates: Improving the description of ring-conformational equilibria in oligo- and polysaccharide chains.
J. Comput. Chem. **37** (2016) 354-365

Horta, B.A.C., Merz, P.T., Fuchs, P.F.J., Dolenc, J., Riniker, S. & Hünenberger, P.H.
A GROMOS-compatible force field for small organic molecules in the condensed phase: The 2016H66 parameter set.
J. Chem. Theory Comput. **12** (2016) 3825-3850.

Reif, M.M. & Hünenberger, P.H.
Origin of asymmetric solvation effects for ions in water and organic solvents investigated using molecular dynamics simulations: The Swain acity-basity scale revisited.
J. Phys. Chem. B **120** (2016) 8485-8517

Lonardi, A., Oborský, P. & Hünenberger, P.H.
Solvent-modulated influence of intramolecular hydrogen-bonding on the conformational properties of the hydroxymethyl group in glucose and galactose: A molecular dynamics simulation study.
Helvetica Chimica Acta **100** (2017) e1600158/1-e1600158/33

Senac, C., Urbach, P.W., Kurtisovski, E., Hünenberger, P.H., Horta, B.A.C., Taulier, N. & Fuchs, P.F.J.
Simulating bilayers of nonionic surfactants with the GROMOS-compatible 2016H66 force field.
Langmuir, **33** (2017) 10225-10238

Hofer, T.S. & Hünenberger, P.H.
Absolute proton hydration free energy, surface potential of water, and redox potential of the hydrogen electrode from first principles: QM/MM free-energy simulations of sodium and potassium hydration.
J. Chem. Phys., Submitted, - (2017)

Institute of Fluid Dynamics / Prof. Patrick Jenny, Computational Fluid Dynamics and Multi-Scale Modeling

List of submitted manuscripts and publications in-press or having appeared in peer-reviewed journals between July 2016 and July 2017

1. Krzysztoforski, J., P. Jenny, and M. Henczka, Mass transfer intensification in the process of membrane cleaning using supercritical fluids. Theoretical Foundations of Chemical Engineering, 2016. **50**(6): p. 907-913.
2. Müller, F., P. Jenny, and D.W. Meyer, Parallel Multilevel Monte Carlo for Two-Phase Flow and Transport in Random Heterogeneous Porous Media With Sampling-Error and Discretization-Error Balancing. SPE Journal, 2016. **21**(6): p. 2027-2037.
3. Cortinovis, D. and P. Jenny, Zonal Multiscale Finite-Volume framework. Journal of Computational Physics, 2017. **337**: p. 84-97.
4. Küchlin, S. and P. Jenny, Parallel Fokker–Planck-DSMC algorithm for rarefied gas flow simulation in complex domains at all Knudsen numbers. Journal of Computational Physics, 2017. **328**: p. 258-277.
5. Lücker, A., T.W. Secomb, B. Weber, and P. Jenny, The relative influence of hematocrit and red blood cell velocity on oxygen transport from capillaries to tissue. Microcirculation, 2017. **24**(3): p. e12337.
6. Moncorgé, A., H.A. Tchelepi, and P. Jenny, Modified sequential fully implicit scheme for compositional flow simulation. Journal of Computational Physics, 2017. **337**: p. 98-115.
7. Schmid, F., P.S. Tsai, D. Kleinfeld, P. Jenny, and B. Weber, Depth-dependent flow and pressure characteristics in cortical microvascular networks. PLOS Computational Biology, 2017. **13**(2): p. e1005392.
8. Sui, R., E.-t. Es-sebbar, J. Mantzaras, and R. Bombach, Homogeneous ignition during fuel-rich H2/O2/N2 combustion in platinum-coated channels at elevated pressures. Combustion and Flame, 2017. **180**: p. 184-195.
9. Sui, R., J. Mantzaras, and R. Bombach, A comparative experimental and numerical investigation of the heterogeneous and homogeneous combustion characteristics of fuel-rich methane mixtures over rhodium and platinum. Proceedings of the Combustion Institute, 2017. **36**(3): p. 4313-4320.
10. Sui, R., J. Mantzaras, R. Bombach, and A. Denisov, Hetero-/homogeneous combustion of fuel-lean methane/oxygen/nitrogen mixtures over rhodium at pressures up to 12bar. Proceedings of the Combustion Institute, 2017. **36**(3): p. 4321-4328.
11. Xiao, H., J.-X. Wang, and P. Jenny, An Implicitly Consistent Formulation of a Dual-Mesh Hybrid LES/RANS Method. Communications in Computational Physics, 2017. **21**(2): p. 570-599.
12. Deb, R. and P. Jenny, Modeling of shear failure in fractured reservoirs with a porous matrix. Computational Geosciences, 2017. **in press**.
13. Deb, R. and P. Jenny, Finite volume–based modeling of flow-induced shear failure along fracture manifolds. International Journal for Numerical and Analytical Methods in Geomechanics, 2017. **in press**: p. 1-21.

14. Ibrahima, F., H.A. Tchelepi, and D.W. Meyer, An efficient distribution method for nonlinear two-phase flow in highly heterogeneous multidimensional stochastic porous media. Computational Geosciences, 2017. **in press**.
15. Jenny, P. and D.W. Meyer, Non-local generalization of Darcy's law based on empirically extracted conductivity kernels. Computational Geosciences, 2017. **in press**.
16. Khayrat, K. and P. Jenny, A multi-scale network method for two-phase flow in porous media. Journal of Computational Physics, 2017. **342**: p. 194-210.
17. Meyer, D.W., Density estimation with distribution element trees. Statistics and Computing, 2017. **in press**.
18. Schmid, F., M.J.P. Barrett, P. Jenny, and B. Weber, *Vascular density and distribution in neocortex.* NeuroImage, 2017. **in press**.
19. Sui, R., E.-t. Es-sebbar, J. Mantzaras, and N.I. Prasianakis, Experimental and Numerical Investigation of Fuel-Lean H2/CO/Air and H2/CH4/Air Catalytic Microreactors. Combustion Science and Technology, 2017. **in press**: p. 1-27.
20. Deb, R. and P. Jenny, An extended finite volume method and fixed-stress approach for modeling fluid injection induced tensile opening in fractured reservoirs. Computational Geosciences, 2017. **submitted**.
21. Khayrat, K., R. Epp, and P. Jenny, Approximate Multiscale Flow Solver for Unstructured Pore Networks. Journal of Computational Physics, 2017. **submitted**.
22. Küchlin, S. and P. Jenny, Automatic mesh refinement and parallel load balancing for Fokker-Planck-DSMC algorithm. Journal of Computational Physics, 2017. **submitted**.
23. Lücker, A., T.W. Secomb, M.J.P. Barrett, B. Weber, and P. Jenny, The Relation between Capillary Transit Times and Hemoglobin Saturation Heterogeneity. Part 2: Microvascular Networks. Journal of Cerebral Blood Flow & Metabolism, 2017. **submitted**.
24. Lücker, A., T.W. Secomb, B. Weber, and P. Jenny, The Relation between Capillary Transit Times and Hemoglobin Saturation Heterogeneity. Part 1: Theoretical Models. Journal of Cerebral Blood Flow & Metabolism, 2017. **submitted**.
25. Meyer, D.W., A Simple Velocity Random-Walk Model for Macrodispersion in Mildly to Highly Heterogeneous Subsurface Formations. Advances in Water Resources, 2017. **submitted**.
26. Meyer, D.W., (Un)Conditional Sample Generation Based on Distribution Element Trees. Journal of Computational and Graphical Statistics, 2017. **submitted**.

Publications of the research group of Prof. Arnulf Jentzen (July 2016 to July 2017)

[1] Cox, S., Hutzenthaler, M., Jentzen, A., van Neerven, J., & Welti, T., Convergence in Hölder norms with applications to Monte Carlo methods in infinite dimensions. *arXiv:1605.00856* (2017), 48 pages, `https://arxiv.org/abs/1605.00856`. To appear in *IMA J. Numer. Anal.*

[2] Hutzenthaler, M., Jentzen, A., & Wang, X., Exponential integrability properties of numerical approximation processes for nonlinear stochastic differential equations. *arXiv:1309.7657* (2016), 39 pages, `https://arxiv.org/abs/1309.7657`. To appear in *Math. Comp.*

[3] Gerencsér, M., Jentzen, A., & Salimova, D., On stochastic differential equations with arbitrarily slow convergence rates for strong approximation in two space dimensions. *Proc. Roy. Soc. London A* **473** (2017), `https://dx.doi.org/10.1098/rspa.2017.0104`. *arXiv:1702.03229* (2017), 25 pages, `https://arxiv.org/abs/1702.03229`.

[4] Cox, S., Jentzen, A., Kurniawan, R., & Pusnik, P., On the mild Itô formula in Banach spaces. *arXiv:1612.03210* (2016), 27 pages, `https://arxiv.org/abs/1612.03210`. To appear in *Discrete Contin. Dyn. Syst. Ser. B.*

[5] Jacobe de Naurois, L., Jentzen, A., & Welti, T., Lower bounds for weak approximation errors for spatial spectral Galerkin approximations of stochastic wave equations. *arXiv:1701.04351* (2017), 9 pages, `https://arxiv.org/abs/1701.04351`. To appear in the peer-reviewed conference proceedings *Stochastic Partial Differential Equations and Related Fields.*

[6] E, W., Han, J., & Jentzen, A., Deep learning-based numerical methods for high-dimensional parabolic partial differential equations and backward stochastic differential equations. *Commun. Math. Stat.* **5** (2017), no. 4, 349–380, `https://doi.org/10.1007/s40304-017-0117-6`. *arXiv:1706.04702* (2017), 39 pages, `https://arxiv.org/abs/1706.04702`.

[7] Andersson, A., Jentzen, A., Kurniawan, R., & Welti, T., On the differentiability of solutions of stochastic evolution equations with respect to their initial values. *Nonlinear Anal.* **162** (2017), 128–161, `https://doi.org/10.1016/j.na.2017.03.003`. *arXiv:1611.00856* (2016), 41 pages, `https://arxiv.org/abs/1611.00856`.

[8] Jentzen, A., Müller-Gronbach, T., & Yaroslavtseva, L., On stochastic differential equations with arbitrary slow convergence rates for strong approximation. *Commun. Math. Sci.* **14** (2016), no. 6, 1477–1500, `https://doi.org/10.4310/CMS.2016.v14.n6.a1`. *arXiv:1506.02828* (2015), 26 pages, `https://arxiv.org/abs/1506.02828`.

[9] E, W., Jentzen, A., & Shen, H., Renormalized powers of Ornstein-Uhlenbeck processes and well-posedness of stochastic Ginzburg-Landau equations. *Nonlinear Anal.* **142** (2016), 152–193, `https://dx.doi.org/10.1016/j.na.2016.03.001`. *arXiv:1302.5930* (2013), 42 pages, `https://arxiv.org/abs/1302.5930`.

[10] Becker, S., Jentzen, A., & Kloeden, P. E., An exponential Wagner-Platen type scheme for SPDEs. *SIAM J. Numer. Anal.* **54** (2016), no. 4, 2389–2426, https://doi.org/10.1137/15M1008762. *arXiv:1309.4648* (2013), 24 pages, https://arxiv.org/abs/1309.4648.

Computational Polymer Physics, D-MATL, ETH Zurich

Martin Kröger

www.complexfluids.ethz.ch

List of peer-reviewed publications

Z. Shen, M. Röding, M. Kröger, Y. Li,
Carbon nanotube length governs viscoelasticity and permeability of buckypaper,
Polymers **9** (2017) 115.

Z. Shen, H. Ye, M. Kröger, Y. Li,
Self-assembled core-polyethylene glycol-lipid shell nanoparticles demonstrate high stability in shear flow,
Phys. Chem. Chem. Phys. **19** (2017) 13294-13306.

X. Shang, M. Kröger, B. Leimkuhler,
Assessing numerical methods for molecular and particle simulation,
Soft Matter **13** (2017) 8565-8578.

P.S. Stephanou, T. Schweizer, M. Kröger,
Communication: Appearance of undershoots in start-up shear: Experimental findings captured by tumbling-snake dynamics,
J. Chem. Phys. **146** (2017) 161101.

C. Luo, M. Kröger, J.-U. Sommer,
Molecular dynamics simulations of polymer crystallization under confinement: Entanglement effect,
Polymer **109** (2017) 71-84.

Z. Shen, D.T. Loe, J.K. Awino, M. Kröger, J.L. Rouge, Y. Li,
Self-assembly of core-polyethylene glycol-lipid shell (CPLS) nanoparticles and their potential as drug delivery vehicles,
Nanoscale **8** (2016) 14821-14835.

Y.R. Sliozberg, M. Kröger, T.L. Chantawansri,
Fast equilibration protocol for million atom systems of highly entangled linear polyethylene chains,
J. Chem. Phys. **144** (2016) 154901.

Y. Li, S. Tang, M. Kröger, W.K. Liu,
Molecular simulation guided constitutive modeling on finite strain viscoelasticity of elastomers,
J. Mech. Phys. Solids **88** (2016) 204-226.

M. Schuppler, F.C. Keber, M. Kröger, A.R. Bausch,
Boundaries steer the contraction of active gels,
Nat. Commun. **7** (2016) 13120.

S.H. Jeong, J.M. Kim, J. Yoon, C. Tzoumanekas, M. Kröger, C. Baig,
Influence of molecular architecture on the entanglement network: topological analysis of entangled linear, long- and short-chain branched polyethylene melts via Monte Carlo simulation,
Soft Matter **12** (2016) 3770-3786.

S. Costanzo, L.F. Scherz, T. Schweizer, M. Kröger, G. Floudas, A.D. Schlüter, D. Vlassopoulos,
Rheology and packing of dendronized polymers,
Macromolecules **49** (2016) 7054-7068.

P.S. Stephanou, M. Kröger,
Solution of the complete Curtiss-Bird model for polymeric liquids subjected to simple shear flow,
J. Chem. Phys. **144** (2016) 124905.

M.K. Singh, P. Ilg, R.M. Espinosa-Marzal, N.D. Spencer, M. Kröger,
Influence of chain stiffness, grafting density and normal load on the tribological and structural behavior of polymer brushes: a nonequilibrium-molecular-dynamics study,
Polymers **8** (2016) 254.

M.K. Singh, P. Ilg, R.M. Espinosa-Marzal, M. Kröger, N.D. Spencer,
Effect of crosslinking on the microtribological behavior of model polymer brushes,
Tribol. Lett. **63** (2016) 17.

C. Luo, M. Kröger, J.-U. Sommer,
Entanglements and crystallization of concentrated polymer solutions: molecular dynamics simulations,
Macromolecules **49** (2016) 9017-9025.

A. Karatrantos, N. Clarke, M. Kröger,
Modeling of polymer structure and conformations in polymer nanocomposites from atomistic to mesoscale: A Review,
Polym. Rev. **56** (2016) 385-428.

Group of M. Luisier

1. S. Brück, M. Calderara, M. H. Bani-Hashemian, J. VandeVondele, and M. Luisier, “Efficient algorithms for large-scale quantum transport calculations”, J. Chem. Phys. 147, 074116 (2017).

2. D. Bauer, T. Bunjaku, A. Pedersen, and M. Luisier, “Electronic properties of lithiated SnO-based anode materials”, J. Appl. Phys. 122, 055105 (2017).

3. C. Stieger, A. Szabo, T. Bunjaku, and M. Luisier, “Ab-initio quantum transport simulation of self-heating in single-layer 2-D materials”, J. Appl. Phys. 122, 045708 (2017).

4. A. Daus, C. Vogt, N. Münzenrieder, L. Petti, S. Knobelspies, G. Cantarella, M. Luisier, G. A. Salvatore, and G. Tröster, “Charge Trapping Mechanism Leading to Sub-60-mV/decade-Swing FETs”, IEEE Trans. Elec. Dev. 64, 2789 (2017).

5. Y. Lee, M. Bescond, N. Cavassilas, D. Logoteta, L. Raymond, M. Lannoo, and M. Luisier, “Quantum treatment of phonon scattering for modeling of three-dimensional atomistic transport”, Phys. Rev. B 95, 201412 (2017).

6. A. Pedersen, M. Bieri, M. Luisier, and L. Pizzagalli, “Lithiation of Silicon Nanoclusters”, Physical Review Applied 7, 054012 (2017).

7. J. Gooth, M. Borg, H. Schmid, V. Schaller, S. Wirths, K. E. Moselund, M. Luisier, S. Karg, and H. Riel, “Ballistic one-dimensional InAs nanowire cross-junction interconnects”, Nano Letters 17, 2596-2602 (2017).

8. S. Jin, H.-H. Park, M. Luisier, W. Choi, J. Kim, and K.-H. Lee, “Band-to-Band Tunneling in SiGe: Influence of Alloy Scattering”, IEEE Elec. Dev. Lett. 38, 422 (2017).

9. R. Rhyner and M. Luisier, “Influence of thermal losses at the gate contact of Si nanowire transistors: A phenomenological treatment in quantum transport theory”, Appl. Phys. Lett. 110, 103508 (2017).

10. A. K. A. Lu, G. Pourtois, M. Luisier, I. P. Radu, and M. Houssa, “On the electrostatic control achieved in transistors based on multilayered MoS_2: A first-principles study”, J. Appl. Phys. 121, 044505 (2017).

11. S. N. Raja, R. Rhyner, K. Vuttivorakulchai, M. Luisier, and D. Poulikakos, “Length Scale of Diffusive Phonon Transport in Suspended Thin Silicon Nanowires”, Nano Lett. 17, 276 (2017).

12. A. Daus, C. Vogt, N. Münzenrieder, L. Petti, S. Knobelspies, G. Cantarella, M. Luisier, G. A. Salvatore, and G. Tröster, “Positive Charge Trapping Phenomenon in n-Channel Thin-Film Transistors with Amorphous Alumina Gate Insulators”, J. Appl. Phys. 120, 244501 (2016).

13. S. Sant, M. Luisier, and A. Schenk, “DFT-based analysis of the origin of traps at the InAs/Si (111) interface”, Proceedings of the 2017 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 17-20, Kamakura, Japan, September 2017.

14. S. Andermatt, M. H. Bani-Hashemian, S. Brück, J. VandeVondele, and M. Luisier, “Transport simulations with density-matrix-based real-time time-dependant density functional theory”, Proceedings of the 2017 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 177-180, Kamakura, Japan, September 2017.

15. M. Rau, M. Luisier, and H.-H. Park, “Modeling of crystal impurities in III-V ultra-thin body field-effect transistors within the empirical tight-binding”, Proceedings of the 2017 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 353-356, Kamakura, Japan, September 2017.

16. H.-H. Park, S. Jin, W. Choi, M. Luisier, J. Kim, and K.-H. Lee, “Atomistic simulation of band-to-band tunneling in SiGe: Influence of alloy scattering”, Proceedings of the 2017 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 173-176, Kamakura, Japan, September 2017.

17. A. Ziegler and M. Luisier, “Phonon confinement effects in diffusive quantum transport simulations with the effective mass approximation and k·p method”, Proceedings of the 2017 International Conference on Simulation of Semiconductor Processes and Devices (SISPAD), pp. 25-28, Kamakura, Japan, September 2017.

18. C. Stieger, T. Bunjaku, A. Szabo, and M. Luisier, “Ab-initio Modeling of Self-Heating in Single-Layer MoS_2 Transistors”, Proceedings of the 75 Device Research Conference (DRC), doi: 10.1109/DRC.2017.7999505, 2017, Notre Dame, IN, USA, June 2017.

19. M. Luisier, A. Szabo, C. Stieger, C. Klinkert, S. Brück, A. Jain, and L. Novotny, “First-principles Simulations of 2-D Semiconductor Devices: Mobility, *I-V* Characteristics, and Contact Resistance”, Proceedings of the IEDM 2016, pp. 5.4.1-5.4.4, San Francisco, CA, USA, December 2016.

20. H. Carrillo-Nuñez, C. Stieger, M. Luisier and A. Schenk, “Performance Predictions of Single-layer In-V double-gate *n*- and *p*-type Feld-effect Transistors”, Proceedings of the IEDM 2016, pp. 14.5.1-14.5.4, San Francisco, CA, USA, December 2016.

21. M. Rau, E. Caruso, D. Lizzit, P. Palestri, D. Esseni, L. Selmi, A. Schenk and M. Luisier, “Performance Projection of III-V Ultra-Thin-Body, FinFET, and Nanowire MOSFETs for two Next- Generation Technology Nodes”, Proceedings of the IEDM 2016, pp. 30.6.1-30.6.4, San Francisco, CA, USA, December 2016.

Group of S. Mishra

Published papers

1. A. BelJadid, P. G. LeFloch, S. Mishra and C. Pares, Schemes with well-controlled dissipation-Hyperbolic systems in non-conservative form, *Commun, Comput. Phys.,* 21 (4), 2017, 913-946.

2. F. Leonardi, S. Mishra and Ch. Schwab, Numerical approximation of statistical solutions of incompressible flow. *Math. Mod. Meth. Appl. Sci. (M3AS)*, 2016, 26 (13), 2471-2524.

3. U. S. Fjordholm, R. Käppeli, S. Mishra and E. Tadmor, Construction of approximate entropy measure valued solutions for hyperbolic systems of conservation laws. *Found. Comput. Math.,* 17 (3), 2017, 763-827.

4. U. S. Fjordholm, S. Lanthaler and S. Mishra, Statistical solutions of hyperbolic conservation laws I: Foundations, *Arch. Rat. Mech. Anal.,*226, 2017, 809-849.

5. K. G. Pressel, S. Mishra, T. Schneider, C. M. Kaul and Z. Tan, Numerics and Subgrid-Scale Modeling in Large Eddy Simulations of Stratocumulus Clouds, *Journal of Advances in Modeling Earth Systems (JAMES)*, 9 (2), 2017, 1342-1365.

6. R. Abgrall and S. Mishra Uncertainty quantification for hyperbolic systems of conservation laws, *Handbook of numerical methods for hyperbolic problems*, 507544, Handb. Numer. Anal., 18, Elsevier/North-Holland, Amsterdam, 2017

7. S. Mishra, Numerical methods for conservation laws with discontinuous coefficients, *Handbook of numerical methods for hyperbolic problems*, 479506, Handb. Numer. Anal., 18, Elsevier/North-Holland, Amsterdam, 2017.

In Press

8. A. Hiltebrand, S. Mishra and C. Pares, Entropy stable space-time DG schemes for non-conservative hyperbolic systems, *ESIAM Math. Model. Num. Anal.,* 2018, to appear.

9. S. Mishra and Ch. Schwab, Monte-Carlo Finite-Volume methods in uncertainty quantification for hyperbolic conservation laws, 2018, to appear.

Preprints

10. U. S. Fjordholm, K. Lye and S. Mishra, Numerical approximation of statistical solutions of scalar conservation laws, *Preprint*, 2017.

Group name: Laboratory for Bone Biomechanics, Prof. Ralph Müller

List of publications:

N. Ohs, F. Keller, O. Blank, W.-Y. W. Lee, C.-Y. J. Cheng, P. Arbenz, R. Müller and P. Christen. Towards in silico prognosis using big data. *Current Directions in Biomedical Engineering*, 2(1):57-60, 2016.

J. R. Vetsch, R. Müller and S. Hofmann. The influence of curvature on three-dimensional mineralized matrix formation under static and perfused conditions: An in-vitro bioreactor model. *Journal of the Royal Society Interface*, 13:20160425, 2016.

S. D. Badilatti, P. Christen, I. Parkinson and R. Müller. Load-adaptive bone remodeling simulations reveal osteoporotic microstructural and mechanical changes in whole human vertebrae. *Journal of Biomechanics*, 49(16):3770-3779, 2016.

S. D. Badilatti, P. Christen, Stephen J. Ferguson and R. Müller. Computational modeling of long-term effects of prophylactic vertebroplasty on bone adaptation. *Proceedings of the Institution of Mechanical Engineers, Part H: Journal of Engineering in Medicine*, 231(5):423-431, 2017.

J. R. Vetsch, D. C. Betts, R. Müller and S. Hofmann. Flow velocity-driven differentiation of human mesenchymal stromal cells in silk fibroin scaffolds: A combined experimental and computational approach. *PLoS One*, 12(7), 2017.

J. J. A. de Jong, P. Christen, S. Boutroy, P. P. Geusens, J. P. W. van den Bergh, R. Müller and B. van Rietbergen. Feasibility of rigid 3D image registration of high-resolution peripheral quantitative computed tomography images of healing distal radius fractures. *PLoS One*, 12(7), 2017.

P. Christen and R. Müller. In vivo visualisation and quantification of bone resorption and bone formation from time-lapse imaging. *Current Osteoporosis Reports*, 5:311-317, 2017.

Parrinello Group

"Communication: Role of explicit water models in the helix folding/unfolding processes"
F. Palazzesi, M. Salvalaglio, A. Barducci and M. Parrinello
J. Chem. Phys., **145**, 121101 (2016), DOI: 10.1063/1.4963340

"Overcoming time scale and finite size limitations to compute nucleation rates from small scale well tempered metadynamics simulations"
M. Salvalaglio, P. Tiwary, G. M. Maggioni, M. Mazzotti and M. Parrinello
The Journal of Chemical Physics **145**, 211925 (2016); DOI: 10.1063/1.4966265

"A variational conformational dynamics approach to the selection of collective variables in metadynamics"
J. McCarty and M. Parrinello
Cond-mat-stat-mech. arXiv: 1703.08777vl (2017)

"Conformational Entropy as Collective Variable for Proteins"
F. Palazzesi, O. Valsson and M. Parrinello
Physics-chem-ph, arXiv: 1704.03344vl (2017)

"Unbinding Kinetics of a p38 MAP Kinase Type II Inhibitor from Metadynamics Simulations"
R. Casasnovas, V. Limongelli, P. Tiwary, P. Carloni and M. Parrinello
J. Am. Chem. Soc., **139**, 4780-4788 (2017), DOI: 10.1021/jacs.6b12950

"Variational Flooding Study of a S_N2 Reaction"
G. M. Piccini, J. McCarty, O. Valsson and Michele Parrinello
J. Phys. Chem. Lett., **8**, 580-583 (2017), DOI: 10.1021/acs.jpclett.6b02852

"Prion protein β2-α2 loop conformational landscape"
E. Caldarulo, A. Barducci, K. Wüthrich and M. Parrinello
PNAS, 1712155114, **114** (36), 9617-9622 (2017), DOI: 10.1073/pnas.1712155114

"Identifying Slow Molecular Motions in Complex Chemical Reactions"
GM Piccini, D. Polino and M. Parrinello
J. Phys. Chem. Lett., **8**, 4197-4200 (2017), DOI: 10.1021/acs.jpclett.7b01889

Group name: **Molecular Kinetics and Spectroscopy,**
Group of Prof. M. Quack

List of publications:

A Combined Gigahertz and Terahertz (FTIR) Spectroscopic Investigation of Meta-D-phenol: Observation of Tunneling Switching
S. Albert, Z. Chen, C. Fábri, Ph. Lerch, R. Prentner, and M. Quack
Mol. Phys. 114, 2751 – 2768 (2016)

Eingriffe in der Evaluation und Förderung der naturwissenschaftlichen Grundlagenforschung,
M. Quack,
VSH Bulletin Heft 3/4, November 2016 (Vereinigung der schweizerischen Hochschuldozierenden ISSN 1663-9898), Seiten 61 – 69.

Symmetrie und Asymmetrie in Wissenschaft und Kunst
J. Hacker und M. Quack (Hrsg.)
Nova Acta Leopoldina NF Band 127, Nr. 412 (2016)
(Seite 7, Vorwort zum Buch mit total 275 Seiten)

Die Spiegelsymmetrie des Raumes und die Chiralität in Chemie, Physik, und in der biologischen Evolution.
Quack, M.
Nova Acta Leopoldina NF, 412, 119-166 (2017)

Leitsätze für eine gute wissenschaftliche Publikationspraxis
M. Quack,
Bunsen-Magazin, 19, 52 – 54 (2017)

Combined Synchrotron-Based High Resolution FTIR and IR-Diode Laser Supersonic Jet Spectroscopy of the Chiral Molecule CDBrClF
S. Albert, K. Keppler, V. Boudon, Ph. Lerch, and M. Quack
J. Mol. Spectr. 337, 105 – 123 (2017).

High-resolution FTIR spectroscopy of trisulfane HSSSH: A candidate for detecting parity violation in chiral molecules
S. Albert, I. Bolotova, Z. Chen, C. Fábri, M. Quack, G. Seyfang and D. Zindel,
Phys. Chem. Chem. Phys. (PCCP) 19, 11738 – 11743 (2017)

High resolution Fourier transform infrared spectroscopy of the ground state, ν_3, $2\nu_3$ and ν_4 levels of $^{13}CHF_3$
I. B. Bolotova, O. N. Ulenikov, E. S. Bekhtereva, S. Albert, Z. Chen, H. Hollenstein, D.Zindel, and M. Quack
J. Mol. Spectr. 337, 96 – 104 (2017)

Isotope effects on the resonance interactions and vibrational quantum dynamics of fluoroform $^{12,13}CHF_3$
S. Albert, E. Bekhtereva, I. Bolotova, Z. Chen, C. Fábri, H. Hollenstein, M. Quack, and O. Ulenikov
Phys. Chem. Chem. Phys. 19, 26527 –26534 (2017)

On the use of nonrigid-molecular symmetry in nuclear motion computations employing a discrete variable representation: a case study of the bending energy levels of CH_5^+
C. Fábri, M. Quack, and A. G. Császár
J. Chem. Phys. 147, 134101 (2017)

High resolution FTIR Spectroscopy of Fluoroform ^{12}CHF and critical analysis of the Infrared Spectrum from 25 to 1500 cm^{-1}
S. Albert, S. Bauerecker, E. S. Bekhtereva, I. B. Bolotova, H. Hollenstein, M. Quack, and O. N. Ulenikov
Mol. Phys. 000, 00 – 00 (2017), DOI: 10.1080/00268976.2017.1392628

Institute/Group: Lab. für Physikalische Chemie, Group of Prof. Markus Reiher

List of Publications:

1. Erik D. Hedegård and Markus Reiher. Polarizable Embedding Density Matrix Renormalization Group. *J. Chem. Theory Comput.*, **2016**, *12*, 4242 – 4253.

2. Stefan Knecht, Sebastian Keller, Jochen Autschbach, and Markus Reiher. A Nonorthogonal State-Interaction Approach for Matrix Product State Wave Functions. *J. Chem. Theory Comput.*, **2016**, *12*, 5881 – 5894.

3. Arseny Kovyrshin and Markus Reiher. Tensor Network States with Three-Site Correlators. *New J. Phys.*, **2016**, *18*, 113001.

4. Florian Krausbeck, Jochen Autschbach, and Markus Reiher. Calculated Resonance Vibrational Raman Optical Activity Spectra of Naproxen and Ibuprofen. *J. Phys. Chem. A*, **2016**, *120*, 9740 – 9748.

5. Jonny Proppe, Tamara Husch, Gregor N. Simm, and Markus Reiher. Uncertainty Quantification for Quantum Chemical Models of Complex Reaction Networks. *Faraday Discuss.*, **2016**, *195*, 497 – 520.

6. Gonzalo Angulo, Raymond D. Astumian, Vijay Beniwal, Peter G. Bolhuis, Christoph Dellago, John Ellis, Bernd Ensing, David R. Glowacki, Sharon Hammes-Schiffer, Johannes Kästner, Tony Lelièvre, Nancy Makri, David Manolopoulos, Georg Menzl, Thomas F. Miller, Adrian Mulholland, Ewa A. Oprzeska-Zingrebe, Michele Parrinello, Eli Pollak, Jonny Proppe, Markus Reiher, Jeremy Richardson, Priyadarshi R. Chowdhury, Eduardo Sanz, Christof Schütte, Dmitry Shalashilin, Rafał Szabla, Srabani Taraphder, Ambuj Tiwari, Eric Vanden-Eijnden, Adithya Vijaykumar, and Kirill Zinovjev. New Methods: General Discussion. *Faraday Discuss.*, **2016**, *195*, 521 – 556.

7. Christopher J. Stein and Markus Reiher. Measuring Multi-Configurational Character by Orbital Entanglement. *Mol. Phys.*, **2017**, *115*, 2110 – 2119.

8. Leon Freitag, Stefan Knecht, Celestino Angeli, and Markus Reiher. Multireference Perturbation Theory with Cholesky Decomposition for the Density Matrix Renormalization Group. *J. Chem. Theory Comput.*, **2017**, *13*, 451 – 459.

9. Yingjin Ma, Stefan Knecht, and Markus Reiher. Multiconfigurational Effects in Theoretical Resonance Raman Spectra. *ChemPhysChem*, **2017**, *18*, 384 – 393.

10. Alain C. Vaucher and Markus Reiher. Steering Orbital Optimization Out of Local Minima and Saddle Points Toward Lower Energy. *J. Chem. Theory Comput.*, **2017**, *13*, 1219 – 1228.

11. Florian Krausbeck, Jan-Grimo Sobez, and Markus Reiher. Stabilization of Activated Fragments by Shell-Wise Construction of an Embedding Environment. *J. Comput. Chem.*, **2017**, *38*, 1023 – 1038.

12. Gregor N. Simm, Jonny Proppe, and Markus Reiher. Error Assessment of Computational Models in Chemistry. *Chimia*, **2017**, *71*, 202 – 208.

13. Christopher J. Stein and Markus Reiher. Automated Identification of Relevant Frontier Orbitals for Chemical Compounds and Processes. *Chimia*, **2017**, *71*, 170 – 176.

14. Denis G. Artiukhin, Christopher J. Stein, Markus Reiher, and Johannes Neugebauer. Quantum Chemical Spin Densities for Radical Cations of Photosynthetic Pigment Models. *Photochem. Photobiol.*, **2017**, *93*, 815 – 833.

15. Stefan Knecht, Sebastian Keller, Yingjin Ma, and Markus Reiher. Second-Order Self-Consistent-Field Density-Matrix Renormalization Group. *J. Chem. Theory Comput.*, **2017**, *13*, 2533 – 2549.

16. Peter Becker, Thomas Duhamel, Christopher J. Stein, Markus Reiher, and Kilian Muñiz. Cooperative Light-Activated Iodine and Photoredox Catalysis for the Amination of C_{sp^3}–H bonds. *Angew. Chem. Int. Ed.*, **2017**, *56*, 8004 – 8008.

17. Jonny Proppe and Markus Reiher. Reliable Estimation of Prediction Uncertainty for Physicochemical Property Models. *J. Chem. Theory Comput.*, **2017**, *13*, 3297 – 3317.

18. Markus Reiher, Nathan Wiebe, Krysta M. Svore, Dave Wecker, and Matthias Troyer. Elucidating Reaction Mechanisms on Quantum Computers. *Proc. Natl. Acad. Sci.*, **2017**, *114*, 7555 – 7560.

19. Shashi Bhushan Sinha, Dimitar Y. Shopov, Liam S. Sharninghausen, Christopher J. Stein, Brandon Q. Mercado, David Balcells, Thomas B. Pedersen, Markus Reiher, Gary W. Brudvig, and Robert H. Crabtree. Redox Activity of Oxo-Bridged Iridium Dimers in an N,O-Donor Environment: Characterization of Remarkably Stable Ir(IV,V) Complexes. *J. Am. Chem. Soc.*, **2017**, *139*, 9672 – 9683.

20. Tamara Husch, Dieter Seebach, Albert K. Beck, and Markus Reiher. Rigorous Conformational Analysis of Pyrrolidine Enamines with Relevance to Organocatalysis. *Helv. Chim. Acta*, **2017**, in press.

21. Tamara Husch and Markus Reiher. Mechanistic Consequences of Chelate Ligand Stabilization on Nitrogen Fixation by Yandulov–Schrock-type Complexes. *ACS Sustainable Chem. Eng.*, **2017**, in press.

Institute/Group: Lab. of Physical Chemistry / Theoretical Molecular Quantum Dynamics / group of Prof. Jeremy Richardson

List of publications:

- J. O. Richardson. "Microcanonical and thermal instanton rate theory for chemical reactions at all temperatures." *Faraday Discuss.* **195**, 49 (2016).
- J. O. Richardson, P. Meyer, M.-O. Pleinert, and M. Thoss. "An analysis of nonadiabatic ring-polymer molecular dynamics and its application to vibronic spectra." *Chem. Phys.* **482**, 124 (2017); arXiv:1609.00644 [physics.chem-ph].
- A. N. Beyer, J. O. Richardson, P. J. Knowles, J. Rommel, and S. C. Althorpe. "Quantum tunneling rates of gas-phase reactions from on-the-fly instanton calculations." *J. Phys. Chem. Lett.* **7**, 4374 (2016).
- J. O. Richardson. "Full- and reduced-dimensionality instanton calculations of the tunnelling splitting in the formic acid dimer." *Phys. Chem. Chem. Phys.* **19**, 966 (2017); arXiv:1611.04816 [physics.chem-ph].

PUBLICATION LIST

Group name: Computational Chemistry Group (Prof. Sereina Riniker)

List of publications:

A. Renevey, S. Riniker, "The importance of N-methylations for the stability of $\beta^{6.3}$-helical conformation of polytheonamide B", *Eur. Biophys. J.*, **46**, 363 (2016).

D. Sidler, A. Schwaninger, S. Riniker, "Replica exchange enveloping distribution sampling (RE-EDS): A robust method to estimate multiple free-energy differences from a single simulation", *J. Chem. Phys*., **145**, 154114 (2016).

A. Renevey, S. Riniker, "Improved accuracy of hybrid atomistic/coarse-grained simulations using reparametrised interactions", *J. Chem. Phys*., **146**, 124131 (2017).

S. Riniker, "Molecular dynamics fingerprints (MDFP): Machine-learning from MD data to predict free-energy differences", *J. Chem. Inf. Model*., **57**, 726 (2017).

D. Sidler, M. Cristòfol-Clough, S. Riniker, "Efficient round-trip time optimisation for replica-exchange enveloping distribution sampling (RE-EDS)", *J. Chem. Theory Comput*., **13**, 3020 (2017).

W. F. van Gunsteren, X. Daura, N. Hansen, A. E. Mark, C. Oostenbrink, S. Riniker, L. Smith, "Validation of molecular simulation: An overview of issues", *Angew. Chem. Int. Ed*., online, DOI: 10.1002/anie.201702945 (2017).

S. Riniker, G. A. Landrum, F. Montanari, S. D. Villalba, J. Maier. J. M. Jansen, P. W. Walters, A. A. Shelat, "Virtual-screening workflow tutorials and prospective results from the Teach-Discover-Treat competition 2014 against malaria", *F1000Research*, **6**, 1136 (2017).

Group: Group of Christoph Schär

List of publications:

Bartok, B., Wild, M., Folini, D., Lüthi, D., Kotlarski, S., Schär, C., Vautard, R., Jerez, S., and Imecs, Z., 2017: Projected changes in surface solar radiation in CMIP5 global climate models and in EURO-CORDEX regional climate models for Europe. Clim. Dyn., 49, 2665–2683, doi:10.1007/s00382-016-3471-2

Bellprat, O., Kotlarski S., Lüthi D., De Elìa R., Frigon A., Laprise R., Schär C., 2016: Objective Calibration of Regional Climate Models: Application over Europe and North America. *Journal of Climate*, 39, 819-838, doi: 10.1175/JCLI-D-15-0302.1

Belušić, A., M.T. Prtenjak, I. Güttler, N. Ban, D. Leutwyler, and C. Schär, 2017: Near-surface wind variability over the broader Adriatic region: insights from an ensemble of regional climate models. *Clim Dyn,* doi: 10.1007/s00382-017-3885-5

Dallafior, T. N., Folini, D., Knutti, R., and Wild, M., 2016: Mixed-layer ocean responses to anthropogenic aerosol dimming from 1870 to 2000, *J. Geophys. Res. Atmos.*, 121, 49–66, doi:10.1002/2015JD024070.

Folini, D., Dallafior, T. N., Hakuba, M. Z., and Wild, M., 2017: Trends of surface solar radiation in unforced CMIP5 simulations. *J. Geophys. Res.*, 122, 469–484, doi:10.1002/2016JD025869.

Giorgi F., C. Torma, E. Coppola, N. Ban, C. Schär and S. Somot, 2016: Enhanced summer convective rainfall at Alpine high elevations in response to climate warming, *Nature Geoscience*, doi:10.1038/ngeo2761

Hakuba, M.Z., D. Folini, and M. Wild, 2016: On the Zonal Near-Constancy of Fractional Solar Absorption in the Atmosphere. *J. Climate* 29, 3423–3440, doi: 10.1175/JCLI-D-15-0277.1.

Hassanzadeh, H., Schmidli, J., Langhans, W., Schlemmer, L., and Schär, C., 2016: Impact of topography on the diurnal cycle of summertime moist convection in idealized simulations. *Meteorologische Zeitschrift*, Vol. 25 No. 2, p. 181-194, doi: 10.1127/metz/2015/0653

Hourdin, F., Mauritsen,T., Gettelman, A., Golaz, J-C., Balaji, V., Duan, Q., Folini, D., Ji, D., Klocke, D., Qian, Y., Rauser, F., Rio, C., Tomassini, L., Watanabe, M., and Williamson, D. 2017: The Art and Science of Climate Model Tuning, Bull. Amer. Meteor.Soc., 98, 589–602, DOI:10.1175/BAMS-D-15-00135.2

Imamovic, A., Schlemmer, L., and Schär, C., 2017: Collective impacts of orography and soil moisture on the soil moisture-precipitation feedback. *Geophysical Research Letters*, 44, doi: 10.1002/2017GL075657

Ivanov, M. A. and Kotlarski, S., 2017: Assessing distribution-based climate model bias correction methods over an alpine domain: added value and limitations. *Int. J. Climatol.*, 37: 2633–2653. doi:10.1002/joc.4870

Keller, M., Fuhrer, O., Schmidli, J., Stengel, M., Stöckli, R. and Schär, C., 2016: Evaluation of convection-resolving models using satellite data: The diurnal cycle of summer convection over the Alps. *Meteorologische Zeitschrift*, Vol. 25 No. 2, p. 165 – 179, doi: 10.1127/metz/2015/0715

Kendon, E.J., Ban, N., Roberts, N. M., Fowler, H. J., Roberts, M. J., Chan, S. C., Evans, J. P., Fosser, G., and Wilkinson, J. M., 2017: Do convection-permitting regional climate models improve projections of future precipitation change? *Bulletin of the American Meteorology Society*, doi: http://dx.doi.org/10.1175/BAMS-D-15-0004.1

Keuler, K., Radtke, K., Kotlarski, S., and Lüthi, D., 2016: Regional climate change over Europe in COSMO-CLM: Influence of emission scenario and driving global model., *Meteorologische Zeitschrift*, Vol. 25 No. 2, p. 121-136, doi: 10.1127/metz/2016/0662

Kröner, N., Kotlarski, S., Fischer, E., Lüthi, D., Zubler, E., and Schär, C., 2017: Separating climate change signals into thermodynamic, lapse-rate and circulation effects: Theory and application to the European summer climate. *Climate Dynamics*, 48: 3425. doi: 10.1007/s00382-016-3276-3

Lembo, V., Folini, D., Wild, M, Lionello, P., 2017: Energy budgets and transports: global evolution and spatial patterns during the twentieth century as estimated in two AMIP-like experiments, *Climate Dynamics*, 48, 1793–1812, doi:10.1007/s00382-016-3173-9

Leutwyler, D., D. Lüthi, N. Ban, O. Fuhrer, and C. Schär, 2017: Evaluation of the convection-resolving climate modeling approach on continental scales, *J. Geophys. Res. Atmos.*, 122, 5237–5258, doi:10.1002/2016JD026013.

Leutwyler, D., Fuhrer, O., Lapillonne, X., Lüthi, D., and Schär, C., 2016: Towards European-Scale Convection-Resolving Climate Simulations, *Geosci. Model Dev. Discuss.* doi:10.5194/gmd-2016-119.

Marmy, A., Rajczak, J., Delaloye, R., Hilbich, C., Hoelzle, M., Kotlarski, S., Lambiel, C., Noetzli, J., Phillips, M., Salzmann, N., Staub, B., and Hauck, C., 2016: Semi-automated calibration method for modelling of mountain permafrost evolution in Switzerland, *The Cryosphere*, 10, 2693-2719, https://doi.org/10.5194/tc-10-2693-2016

Müller Schmied, H. Müller, R., Sanchez-Lorenzo, A., Ahrens, B., and Wild, M., 2016: Evaluation of Radiation Components in a Global Freshwater Model with Station-Based Observations, Water, 8, 450; doi:10.3390/w8100450.

Panosetti, D., S. Böing, L. Schlemmer, and J. Schmidli, 2016: Idealized Large-Eddy and Convection-Resolving Simulations of Moist Convection over Mountainous Terrain. *Journal of the Atmospheric Sciences.* 73:10, 4021-4041

Possner A., E. M. Zubler, U. Lohmann, and C. Schär, 2016: The resolution dependence of cloud effects and ship-induced aerosol-cloud interactions in marine stratocumulus, *J. Geophys. Res. Atmos.*, 121, 4810–4829, doi:10.1002/2015JD024685.

Rajczak, J. and C. Schär, 2017: Projections of future precipitation extremes over Europe: a multi-model assessment of climate simulations. *J. Geophys. Res. Atmos.*, doi:10.1002/2017JD027176.

Rajczak, J., Kotlarski, S., and Schär, C., 2016: Does Quantile Mapping of Simulated Precipitation Correct for Biases in Transition Probabilities and Spell Lengths? *Journal of Climate*, 29:5, 1605-1615

Raschke, E., Kinne, S., Rossow, W.B.,Stackhouse, P.W., and Wild, M., 2016: Comparison of Radiative Energy Flows in Observational Datasets and Climate Modeling, *J. Applied Meteorol. Climatol.*, 55, 93-117, doi: 10.1175/JAMC-D-14-0281.1

Schär, C. and N. Kröner, 2017: Sequential Factor Separation for the Analysis of Numerical Model Simulations. *Journal of the Atmospheric Sciences*, 74:5, 1471-1484

Schär, C., N. Ban, E.M. Fischer, J. Rajczak, J. Schmidli, C. Frei, F. Giorgi, T.R. Karl, E.J. Kendon, A.M.G. Klein Tank, P.A. O'Gorman, J. Sillmann, X. Zhang, F.W. Zwiers, 2016: Percentile indices for assessing changes in heavy precipitation events. *Climatic Change* 137: 201, doi:10.1007/s10584-016-1669-2

Schlemmer, L., P. Bechtold, I. Sandu, and M. Ahlgrimm, 2017: Uncertainties related to the representation of momentum transport in shallow convection, *J. Adv. Model. Earth Syst.*, 9, 1269–1291, doi:10.1002/2017MS000915.

Schlemmer, L. and Hohenegger, C., 2016: Modifications of the atmospheric moisture field as a result of cold-pool dynamics. *Q.J.R. Meteorol. Soc*., 142: 30–42. doi: 10.1002/qj.2625

Sørland, S. L., A. Sorteberg, C. Liu, and R. Rasmussen, 2016: Precipitation response of monsoon low-pressure systems to an idealized uniform temperature increase, *J. Geophys. Res. Atmos.*, 121, 6258–6272, doi:10.1002/2015JD024658.

Storelvmo, T., T. Leirvik, U. Lohmann, P.C.B. Phillips and M. Wild, 2016: Disentangling greenhouse warming and aerosol cooling to reveal Earth's climate sensitivity. *Nature Geoscience* 9, 286–289, doi:10.1038/ngeo2670

Wild, M., 2017: Towards Global Estimates of the Surface Energy Budget, Curr. Clim. Change Rep, 3, 87–97. DOI 10.1007/s40641-017-0058-x

Wild, M., 2017: Changes in shortwave and longwave radiative fluxes as observed at BSRN Sites and simulated with CMIP5 models, AIP Conf. Proc., 1810, 090014 (2017); doi: 10.1063/1.4975554.

Wild, M., Folini, D., and Henschel, F., 2017: Impact of climate change on future Concentrated Solar Power (CSP) production, AIP Conf. Proc., 1810, 100007 (2017); doi: 10.1063/1.4975562.

Winter, K.J.-.M., Kotlarski, S., Scherrer, S.C., and Schär, C, 2017: The Alpine snow-albedo feedback in regional climate models. *Clim. Dyn.*, 48: 1109. doi:10.1007/s00382-016-3130-7

Group of Professor Ch. Schwab

List of publications:

R. N. Gantner, L. Herrmann and Ch. Schwab
Multilevel QMC with Product Weights for Affine-Parametric, Elliptic PDEs, Contemporary Computational Mathematics - a celebration of the 80th birthday of Ian Sloan, accepted (2017), SAM Report 2016-54.

A. Cohen, Ch. Schwab and J. Zech
Shape Holomorphy of the stationary Navier-Stokes Equations, SIAM J. Math. Analysis, accepted (2017), SAM Report 2016-45.

D. Devaud and Ch. Schwab
Space-time hp-approximation of parabolic equations, Technical Report 2017-38, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

S. Mishra and Ch. Schwab
Monte-Carlo Finite-Volume Methods inUncertainty Quantification for Hyperbolic Conservation Laws, Technical Report 2017-50, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

L. Banjai, J. Melenk, R. Nochetto, E. Otarola, A. Salgado and Ch. Schwab
Tensor FEM for spectral fractional diffusion, Technical Report 2017-36, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

J. Zech and Ch. Schwab
Convergence rates of high dimensional Smolyak quadrature, Technical Report 2017-27, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

L. Herrmann and Ch. Schwab
Multilevel quasi-Monte Carlo integration with product weights for elliptic PDEs with lognormal coefficients, Technical Report 2017-19, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

M. Bachmayr, A. Cohen, D. Düng and Ch. Schwab
Fully discrete approximation of parametric and stochastic elliptic PDEs, SIAM J. Numer. Analysis, accepted (2017), SAM Report 2017-08.

L. Herrmann and Ch. Schwab
QMC Algorithms with Product Weights for Lognormal-Parametric, Elliptic PDEs, Technical Report 2017-04, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

J.-L. Bouchot, H. Rauhut and Ch. Schwab
Multi-level Compressed Sensing Petrov-Galerkin discretization of high-dimensional parametric PDEs, Technical Report 2017-01, Seminar for Applied Mathematics, ETH Zürich, Switzerland, 2017.

R. N. Gantner, L. Herrmann and Ch. Schwab

Quasi-Monte Carlo integration for affine-parametric, elliptic PDEs: local supports and product weights, SIAM J. Numer. Analysis, accepted (2017), SAM Report 2016-32.

V. Kazeev and Ch. Schwab
Quantized tensor-structured finite elements for second-order elliptic PDEs in two dimensions, Numer. Math., accepted (2017), SAM Report 2015-24.

U. Koley, N.H. Risebro, Ch. Schwab and F.Weber
A Multilevel Monte Carlo Finite Difference Method for Random Scalar Degenerate Convection Diffusion Equations, Journal of Hyperbolic Differential Equations, accepted (2017), SAM Report 2013-32.

F. Müller, D. Schötzau and Ch. Schwab
Symmetric Interior Penalty Discontinuous Galerkin Methods for Elliptic Problems in Polygons, SIAM J. Numer. Anal., 55/5 (2017), pp. 2490-2521, SAM Report 2017-15.

C. Jerez-Hanckes, Ch. Schwab and J. Zech
Electromagnetic Wave Scattering by Random Surfaces: Shape Holomorphy, Math. Mod. Meth. Appl. Sci., 27/2229 (2017), SAM Report 2016-34.

J. Dick, R. N. Gantner, Q. T. Le Gia and Ch. Schwab
Multilevel higher-order quasi-Monte Carlo Bayesian estimation, Math. Mod. Meth. Appl. Sci., 27/5 (2017), pp. 953-995, SAM Report 2016-34.

D. Schötzau and Ch. Schwab
Exponential Convergence of hp-FEM for Elliptic Problems in Polyhedra: Mixed Boundary Conditions and Anisotropic Polynomial Degrees, Journ. Found. Comput. Math. (2017), pp. 1-66, SAM Report 2016-05.

L. Herrmann, A. Lang and Ch. Schwab
Numerical Analysis of Lognormal Diffusions on the Sphere, Stochastics and Partial Differential Equations: Analysis and Computations (2017), pp. 1–44, SAM Report 2016-02.

Ch. Schwab and R. Stevenson
Fractional space-time variational formulations of (Navier-) Stokes equations, SIAM Journ. Math. Analysis, 49/4 (2017), pp. 2442–2467, SAM Report 2015-43.

C. Jerez-Hanckes and Ch. Schwab
Electromagnetic wave scattering by random surfaces: uncertainty quantification via sparse tensor boundary elements, IMA Journal of Numerical Analysis, 37/3 (2017), pp. 1175-1210, SAM Report 2015-23.

F. Y. Kuo, R. Scheichl, Ch. Schwab, I. H. Sloan and E. Ullmann
Multilevel Quasi-Monte Carlo Methods for Lognormal Diffusion Problems, Math. Comp., 86/308 (2017), pp. 2827–2860, SAM Report 2015-22.

H. Rauhut and Ch. Schwab
Compressive sensing Petrov-Galerkin approximation of high-dimensional parametric operator equations, Mathematics of Computation, 86/304 (2017), pp. 661-700, SAM Report 2014-29.

J. Dölz, H. Harbrecht and Ch. Schwab
Covariance regularity and H-matrix approximation for rough random fields, Numerische Mathematik, 135/4 (2017), pp. 1045-1071, SAM Report 2014-19.

Group name: Geophysical Fluid Dynamics, Institute of Geophysics, D-ERDW

List of publications:

Atkins, S., P. J. Tackley, J. Trampert and A. P. Valentine (2016) Using pattern recognition to infer parameters governing mantle convection, Phys. Earth Planet. Inter. 257, 171-186, doi:10.1016/j.pepi.2016.05.016.

Baes, M.; Gerya, T.; Sobolev, S. V. (2016) 3-D thermo-mechanical modeling of plume-induced subduction initiation. Earth and Planetary Science Letters, 453, 193-203.

Ballmer, M. D., D. Lourenço, K. Hirose, R. Caracas, and R. Nomura (2017): Reconciling Magma-Ocean Crystallization Models with the present-day Structure of the Earth's mantle, *Geochemistry Geophysics Geosystems*, 18, doi:10.1002/2017GC006917

Ballmer, M. D., C. Houser, J. W. Hernlund, R. Wentzcovitch, K. Hirose (2017): Persistence of Strong Silica-Enriched Domains in the Earth's Lower Mantle. *Nature Geoscience*, 10, 236-240, doi:10.1038/ngeo2898

Ballmer, M. D., L. Schumacher, V. Lekic, C. Thomas, and G. Ito (2016): Compositional layering within the Large Low Shear-wave Velocity Provinces in the lower mantle, *Geochem. Geophys. Geosys.*, 17, 5056-5077, doi:10.1002/2016GC006005

Buiter, S.J.H., Schreurs, G., Albertz, M., Gerya, T.V., Kaus, B., Landry, W., le Pourhiet, L., Mishin, Y., Egholm, D.L., Cooke, M., Maillot, B., Thieulot, C., Crook, T., May, D., Souloumiac, P., Beaumont, C. (2016) Benchmarking numerical models of brittle thrust wedges. Journal of Structural Geology, 92, 140-177.

Chen, L., Capitanio, F., Liu, L., Gerya, T. (2017) Crustal rheology controls on the Tibetan plateau formation during India-Asia convergence. Nature Communications, 8 Article Number: 15992.

Crameri, F. and P. J. Tackley (2016) Subduction initiation from a stagnant lid and global overturn: New insights from numerical models with a free surface, Progress in Earth and Planetary Science 2016 3:30 doi:10.1186/s40645-016-0103-8.

Crameri, F., C. Lithgow-Bertelloni and P. J. Tackley (2017) The dynamical control of subduction parameters on surface topography, Geochem. Geophys. Geosyst. 18, doi:10.1002/2017GC006821.

Duretz, Thibault , Dave A. May, and Phillipe Yamato, "A free surface capturing discretiza-tion for the staggered grid finite difference scheme", 2016, Geophysical Journal International, 204(3), 1518-1530.

Fischer, R., Gerya, T. (2016) Regimes of subduction and lithospheric dynamics in the Precambrian: 3D thermomechanical modeling. Gondwana Research, 37, 53-70.

Fischer, R., Gerya, T. (2016) Early Earth plume-lid tectonics: A high-resolution 3D numerical modelling approach. Journal of Geodynamics, 100, 198-214.

Gonzalez, C.M., Gorczyk, W., Gerya, T.V. (2016) Decarbonation of subducting slabs: Insight from petrological–thermomechanical modeling. Gondwana Research, 36, 314-332.

Guerri, M., F. Cammarano and P. J. Tackley (2016) Modelling Earth's surface topography: decomposition of the static and dynamic components, Phys. Earth Planet. Inter., 261, 172-186, doi:10.1016/j.pepi.2016.10.009.

Huangfu, P., Wang, Y., Cawood, P.A., Li, Z.H., Fan, W.M., Gerya, T.V. (2017) Thermo-mechanical controls of flat subduction: Insights from numerical modeling. Gondwana Research, 40, 170-183.

Li, Z.H., Liu, M., Gerya, T. (2016) Lithosphere delamination in continental collisional orogens: A systematic numerical study. Journal of Geophysical Research, 121, 5186-5211.

Liao, J., Gerya, T. (2017) Partitioning of crustal shortening during continental collision: 2-D thermomechanical modeling. Journal of Geophysical Research, 122, 592-606.

Lichtenberg, T., Golabek, G.J., Gerya, T.V., Meyer, M.R. (2016) The effects of short-lived radionuclides and porosity on the early thermo-mechanical evolution of planetesimals. Icarus, 274, 350-365.

Malatesta, C., Gerya, T., Crispini, L., Federico, L., Capponi, G. (2016) Interplate deformation at early-stage oblique subduction: 3-D thermomechanical numerical modeling. Tectonics, 35, 1610-1625.

Mallard, C., N. Coltice, M. Seton, R. D. Mueller and P. J. Tackley (2016) Subduction drives the organisation of Earth's tectonic plates, Nature doi:10.1038/nature17992.

Mannu, U., Ueda, K., Willett, S.D., Gerya, T.V., Strasser, M. (2017) Stratigraphic signatures of forearc basin formation mechanisms. Geochemistry Geophysics Geosystems, 18, 2388-2410.

Patocka, V., O. Cadek, P. J. Tackley and H. Cizkova (2017) Stress memory effect in viscoelastic stagnant lid convection, Geophys. J. Int. 209(3), 1462-1475, doi:10.1093/gji/ggx102.

Rozel, A. B., G. J. Golabek, C. Jain, P. J. Tackley and T. V. Gerya (2017) Continental crust formation on early Earth controlled by intrusive magmatism, Nature 545, 332-335.

Ruh, J.B., Gerya, T., Burg, J.-P. (2017) Toward 4D modeling of orogenic belts: Example from the transpressive Zagros Fold Belt. Tectonophysics, 702, 82-89.

Ruh, J.B., Sallares, V., Ranero, C.R., Gerya, T. (2016) Crustal deformation dynamics and stress evolution during seamount subduction: High-resolution 3-D numerical modeling. Journal of Geophysical Research, 121, 6880-6902.

Sanan, Patrick , Sascha M. Schnepp, Dave A. May, “Pipelined, Flexible Krylov Sub-space Methods,” SIAM Journal on Scientific Computing, 2016, 38:5, C441-C470

Sternai, P., Avouac, J.P., Jolivet, L., Faccenna, C., Gerya, T., Becker, T.W., Menant, A. (2016) On the influence of the asthenospheric flow on the tectonics and topography at a collision-subduction transition zones: Comparison with the eastern Tibetan margin. Journal of Geodynamics, 100, 184-197.

Zheng, L., May, D., Gerya, T., Bostock, M. (2016) Fluid-assisted deformation of the subduction interface: Coupled and decoupled regimes from 2-D hydromechanical modeling. Journal of Geophysical Research,121, 6132-6149.

Group of W.F. van Gunsteren

Z. Lin, W.F. van Gunsteren
A comparison of pathway independent and pathway dependent methods in the calculation of conformational free enthalpy differences
Protein Science **25** (2016) 184-191, DOI: 10.1002/pro.2695

J. Dolenc, B.H. Meier, V.H. Rusu, W.F. van Gunsteren
Investigation of the structural preference and flexibility of the loop residues in amyloid fibrils of the HET-s prion
Phys.Chem.Chem.Phys. **18** (2016) 5860-5866, DOI: 10.1039/c6cp00057f, incl. suppl. mat.

V.H. Rusu, S.J. Bachmann, W.F. van Gunsteren
GROMOS polarisable model for acetone
Mol. Phys. **114** (2016) 845-854, DOI: 10.1080/00268976.2015.1126366

W.F. van Gunsteren
Going for a PhD: Joys and Pitfalls
Helv. Chim. Acta **99** (2016) 1-5

L. J. Smith, G. Rought Whitta, J. Dolenc, D. Wang, W. F. van Gunsteren
A molecular dynamics simulation investigation of the relative stability of the cyclic peptide octreotide and its deprotonated and its (CF_3)-Trp substituted analogs in different solvents
Bioorg. Med. Chem. **24** (2016) 4936-4948, DOI: 10.1016/j.bmc.2016.08.001, incl. suppl. mat.

L.J. Smith, W.F. van Gunsteren, N. Hansen
On the Use of Time-Averaging Restraints when Deriving Biomolecular Structure from ^3J-coupling Values Obtained from NMR Experiments
J. Biomol. NMR **66** (2016) 69-83, DOI: 10.1007/s10858-016-0058-5, incl. suppl. mat.

W.F. van Gunsteren, J.R. Allison, X. Daura, J. Dolenc, N. Hansen, A.E. Mark,
C. Oostenbrink, V.H. Rusu, L.J. Smith
Deriving structural information from experimentally measured data on biomolecules: a review
Angew. Chem. Int. Ed. **55** (2016) 15990-16010, DOI: 10.1002/anie.201601828
Angew. Chem. **128** (2016) 16222-16244, DOI: 10.1002/ange.201601828

W.F. van Gunsteren
Publication of Research Results: Use and Abuse
Infozine, Special Issue **1** (2016) 27-28, DOI: 10.3929/ethz-a-010745085

L.J. Smith, R. Athill, W.F. van Gunsteren, N. Hansen
Interpretation of seemingly contradictory data: low NMR S^2 order parameters observed in helices and high NMR S^2 order parameters in disordered loops of the protein hGH at low pH
Chem. Eur. J. **23** (2017) 9585-9591, DOI: 10.1002/chem.201700896, incl. suppl. mat.

L.J. Smith, W.F. van Gunsteren, N. Hansen
Using Complementary NMR Data Sets to Detect Inconsistencies and Model Flaws in the Structure Determination of Human Interleukin-4
J. Phys. Chem. B **121** (2017) 7055-7063, DOI: 10.1021/acs.jpcb.7b03647, incl. suppl. mat.

W.F. van Gunsteren, X. Daura, N. Hansen, A.E. Mark, C. Oostenbrink, S. Riniker, L.J. Smith
Validation of Molecular Simulation: An Overview of Issues
Angew. Chem. Int. Ed. (2017) on-line

Computational Science and Engineering (CSE)
Annual Report
2016/2017

ETH Zurich
Rämistrasse 101
8092 Zurich

www.rw.ethz.ch