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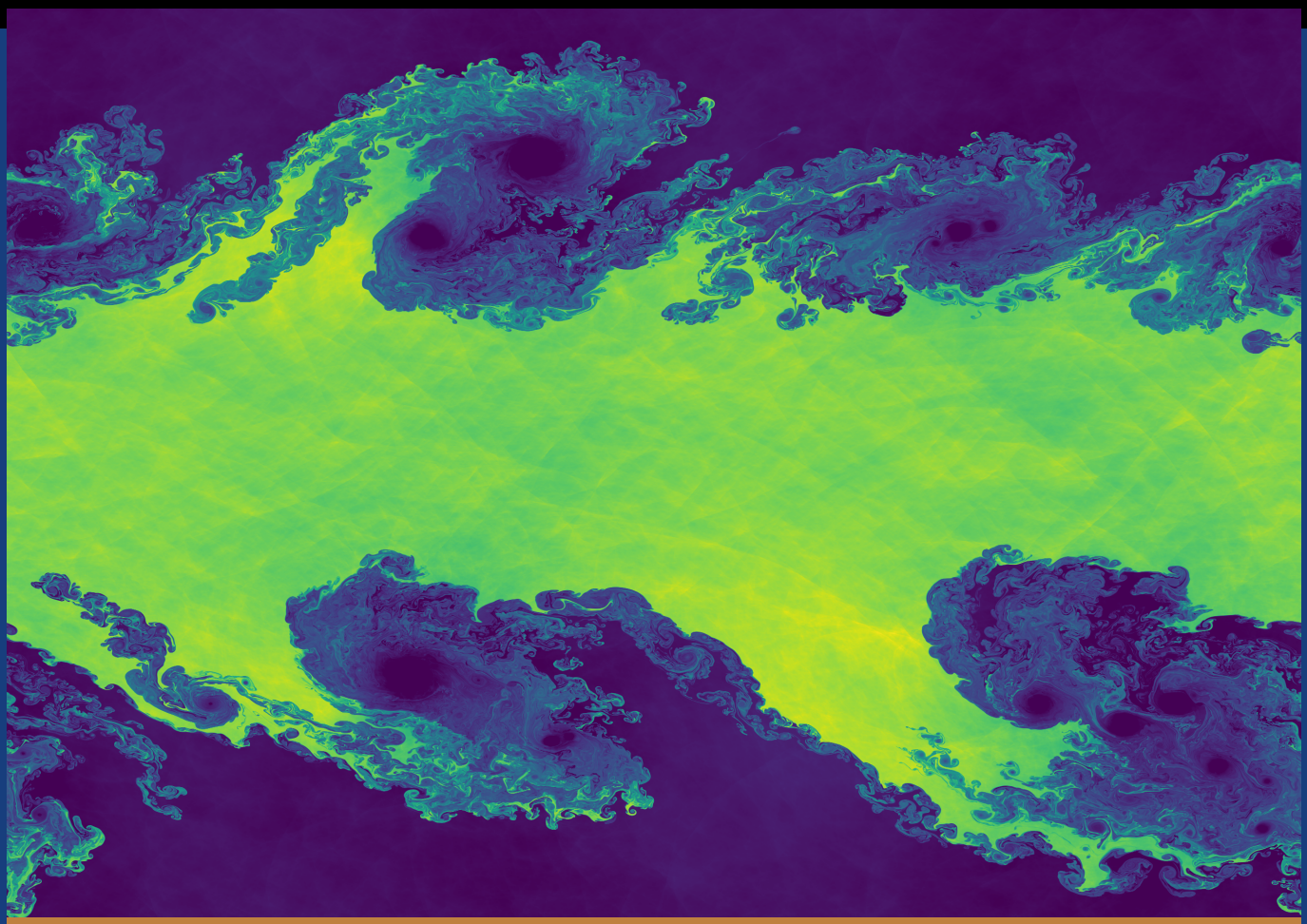

Computational Science and Engineering (CSE)

Annual Report 2018/2019

CSE

Computational Science and Engineering

Annual Report
2018 / 2019

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

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Cover:
Kelvin–Helmholtz instability, see chapter 4.

Groups having contributed to this report

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Introduction

CSE Report 2019: Editorial

R. Hiptmair*

Rico Zenklusen

Before joining D-MATH of ETH Zurich, **Prof. Dr. Rico Zenklusen** was Assistant Professor at the Johns Hopkins University. Prior to that he had worked several years at MIT as a postdoc, and also shortly at EPFL. He holds a master's degree in Mathematics from EPFL, and a PhD from the Department of Mathematics at ETH Zurich.
He has a broad interest in Combinatorial Optimization and its applications. A main focus of his is the design of fast algorithms for complex (mathematical) optimization problems by leveraging a variety of techniques and combinatorial structures, like matroids, submodular functions, and polyhedral methods. He also works on problems in various related fields such as Theoretical Computer Science and Graph Theory.

Prof. Dr. Bernd Gärtner studied mathematics at Freie Univerität Berlin, where he also did his PhD in Computer Science. In 1997 he moved to ETH Zürich as a senior researcher, where he became Adjunct Professor in 2013.
His research interests are in computational geometry, optimization, as well as computer science education. In optimization, he is mostly interested in trying to understand and extract the "combinatorial essence" of problems and algorithms that is responsible for things to work (efficiently). In education, he is is researching effective ways of teaching computer science to children.

Bernd Gärtner

David Steurer

Prof. Dr. David Steurer studied computer science at Saarland University and Princeton University, where he acquired his PhD in 2010. After a stint a Microsoft Research he became Assistant Professor at Cornell University, then at IAS, Princeton, until, in 2017, he joined ETH Zurich as an assistant professor in D-INFK.
His research interests are approximation algorithms, mathematical programming, and the computational complexity of high-dimensional estimation problems that arise in machine learning, e.g., tensor decomposition.

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

I would like to thank the three colleagues for taking the time to meet me. We spoke German and the conversation on the topic of "Optimization" took place on December 4, 2019. I am now giving a translated and edited summary in the format of an interview.

1. "Optimization" is a fuzzy term. How would you define it in light of your research activities?

   B.G.: In most general terms optimization is about finding in a set those elements that are "optimal" or, at least, satisfy certain quality criteria, and provably so. A special, but very common, case is that those quality criteria are derived from a real-valued objective function that we want to minimize.

   D.S.: "Optimization" also provides a versatile language for mathematical modeling: problems from completely different domains can be described in a way that highlights their common mathematical structure

   R.Z.: Optimization is about techniques to intelligently explore extremely large sets of options with the goal to quickly find a solution of high quality. Being amenable to and tractable for optimization is also an important guideline for mathematical modeling in applications.

2. What are the main directions in the field of optimization as researched by mathematicians and computer scientists and how have they evolved over time?

   B.G.: A major trend in the field of optimization is surging interest in very large, high-dimensional, and non-convex optimization problems.

   R.Z.: Nowadays, huge amounts of data are constantly being collected and processed. This not only entails the need for fast procedures being able to deal with very large data sets but also leads to "online" optimization problems, where information about the optimization problem trickles in over time.

   D.S.: Modern machine learning (ML), e.g., learning deep neural networks, heavily uses ideas from optimization. Interestingly, there are many open questions about what really happens in these use cases from an optimization perspective. For example, the underlying optimization problems often have a large number of spurious optimal solutions that are not useful for the learning task. The mystery is that empirically gradient-descent optimization algorithms seem to avoid those spurious optimal solutions and find optimal solutions that are useful for the learning task.

3. What is the role of algorithm development and implementation versus theory in (computational) optimization?

   R.Z.: Lack of theory, including in some areas of ML, can be worrisome, because theoretical insights are often essential for reliability and interpretability of the results returned by optimization algorithms.

   B.G.: It is an important role of theory to tell us what is possible and what is not. It can give rigorous bounds for the quality of solutions and the efficiency of algorithms.

4. Stochastic optimization: What is it and what is its importance?

   R.Z.: Classical stochastic optimization tackles problems for which the data includes random variables. This is distinct from the use of so-called randomized algorithms.

   B.G.: Nevertheless, randomized algorithms are gaining importance due to superior robustness and efficiency.

   R.Z.: Stochastic considerations also play a central role when making statistical predictions about the behavior of algorithms.

5. What are the mathematical foundations that students have to master when they want to specialize in optimization?

   R.Z.: Optimization theory and algorithms are built upon the usual mathematical foundations of linear algebra, analysis, and basic numerical methods.

   D.S.: Students who want to work in optimization must master rigorous mathematical reasoning and must not be afraid of proofs. The students should also have a basic understanding of computational complexity (e.g., polynomial vs exponential running time, NP-hardness).

6. "Just push the optimize button": Can optimization in science and engineering be farmed out to software tools?

   R.Z.: Indeed, powerful optimization software has become available. Nevertheless, mathematical modeling, which is about casting real-world problems as well-defined mathematical optimization problems that can be solved quickly, crucially needs a strong expertise in optimization.

   B.G.: Moreover, the selection of algorithms and the choice of good parameters will require expertise.

Zürich, December 4, 2019

Ralf Hiptmair,

Director of Studies CSE, member of the CSE Committee

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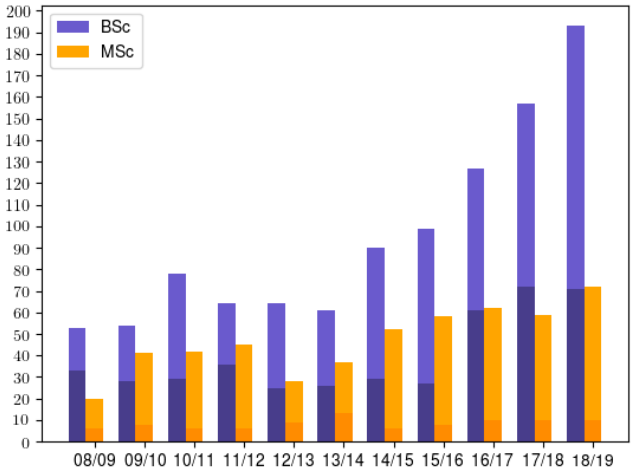
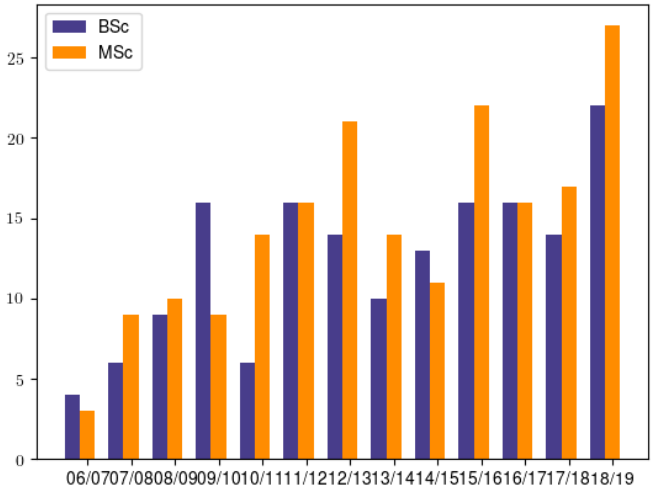
Education

In September 2018, 71 new students started their CSE Bachelor studies, 63 in the first semester, 8 in the third semester. From outside CSE 10 students (9 from overseas) entered the CSE Master curriculum.
The total number of CSE students enrolled at 24 Oktober 2018 was 257 (headcount): 193 in the BSc program and 72 in the MSc program, 8 in both.

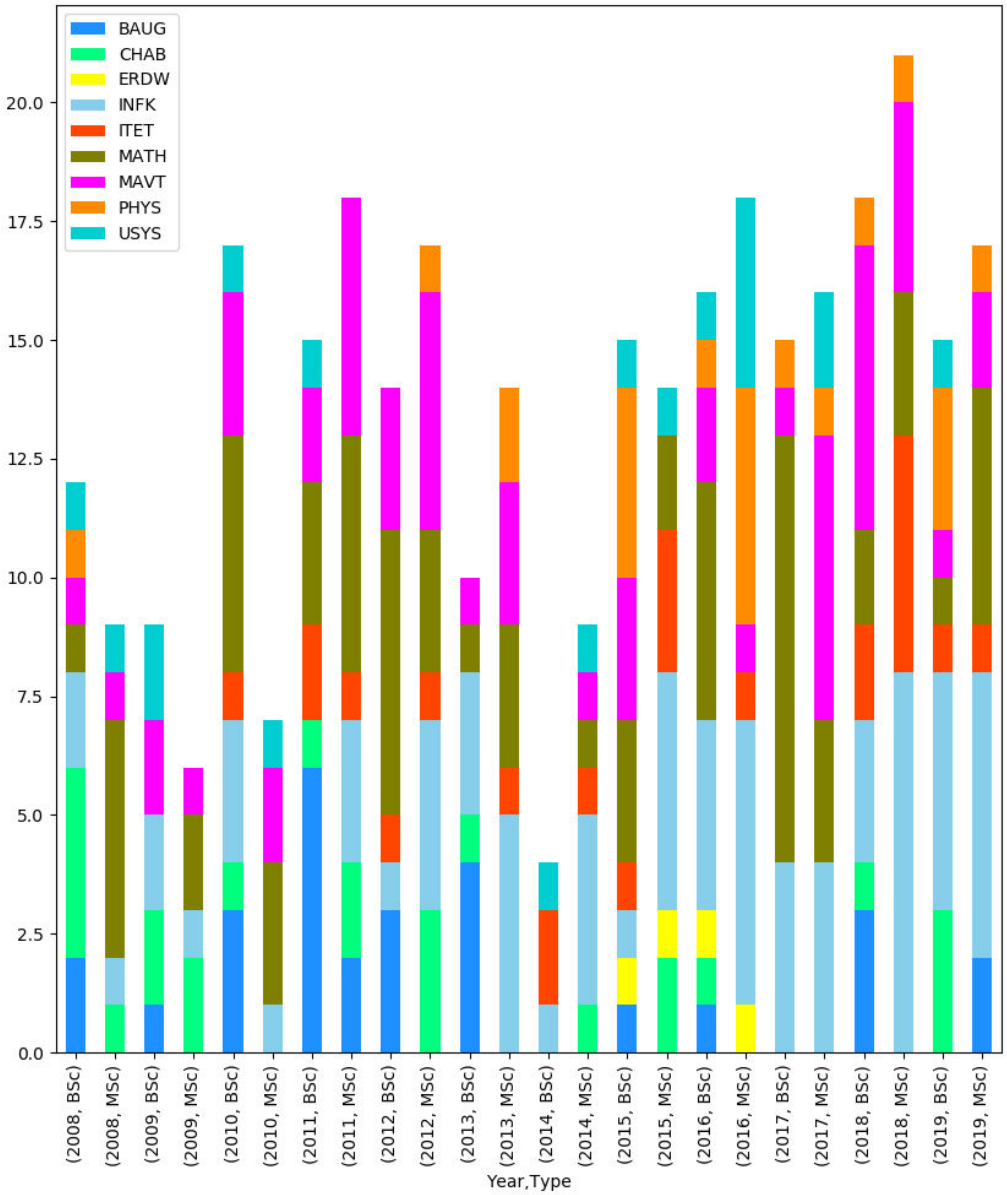
In the past academic year 49 students have successfully finished a CSE curriculum, 22 Bachelor students and 27 Master students, and have received a CSE degree, some with very good scores. In the following list we give the name of the student, the title of the Bachelor/Master/Term thesis and the name and the department of the advisor.
The Willi Studer Preis 2019 for the best CSE Master Diploma in the past academic year was awarded to Bian Wu.



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



Number of CSE graduates



Departments with groups where CSE students wrote BSc- or MSc-Theses

Bachelor Theses

Andrej Blaser
Untersuchung der Abhängigkeit von Mischphasenwolken im Klimamodell ECHAM-HAM von der vertikalen Auflösung
(Ulrike Lohmann, D-USYS)

Cyrill Cedric Hedinger
Improving Phase-Based Frame Interpolation for Video
(Markus Gross, D-INFK)

Valentin Jacot-Descombes
Simulation of branching morphogenesis on growing domains
(Dagmar Iber, D-BSSE)

Philipp Fischer
The Variational Monte Carlo optimization of the correlator product states ansatz
(Markus Reiher, D-CHAB)

Clemens Giuliani
A dual-level approach to the GPR-aided instanton method
(Jeremy Richardson, D-CHAB)

Sebastian Heinekamp
Calculation of ion trap DC voltages with fine-grained control over competing objectives in a trap-agnostic framework
(Jonathan Home, D-PHYS)

Luca Andrea Lavarini
Tendon Sparsification for Plush Robots
(Stelian Coros, D-INFK)

Lasse Lingens
Enhanced Design Through Augmented Reality
(Stelian Coros, D-INFK)

Emanuel Isaac Malvetti
Decomposition of Arbitrary Isometries into Elementary Gates Implemented in C++
(Renato Renner, D-PHYS)

Silvia Nauer
Simulation and Characterization of Granular Networks
(Manfred Sigrist, D-PHYS)

Anian Patrick Ruoss
Evaluation of Adversarial Attack Methods on Neural Networks
(Rima Alaifari, D-MATH)

Leonardo Schwarz
Tetrahedral Mesh Registration for Labeled Medical Images
(Orcun Goksel, D-ITET)

Joel Uster
Interactive Segmentation of Medical Images
(Joachim Buhmann, D-INFK)

Krispin Wandel
Advanced Finite Element Simulation for Viscoelastic Foam
(Stelian Coros, D-INFK)

Ang Ye
Numerical simulation of the behaviour of water droplets suspended in the air
(Petros Koumoutsakos, D-MAVT)

Master Theses

Dinesh Acharya
Towards High Resolution Video Generation with Progressive Growing of Sliced Wasserstein GANs
(Luc Van Gool, D-ITET)

Pierre Beckmann
Story Understanding and Generation with Deep Learning
(Markus Gross, D-INFK)

Daphne Chopard
Sentiment Analysis of Suicide Notes: a Deep Learning Approach
(Peter Bühlmann, D-MATH)

Laurent Eriksen
Efficient AC Field-Circuit Coupling
(Ralf Hiptmair, D-MATH)

Jernej Fink
Uncertainty Quantification Using Neural Networks
(Petros Koumoutsakos, D-MAVT)

Florian Frei
Adaptive Hierarchical Deep Reinforcememt Learning
(Roger Wattenhofer, D-INFK)

Lorenzo Giacomel
Boundary Element Method on Complex Screens
(Ralf Hiptmair, D-MATH)

Linus Groner
Trust Region Methods for Training Neural Networks
(Thomas Hofmann, D-INFK)

David Haldimann
This is not what I imagined: Error Detection for Semantic Segmentation through Visual Dissimilarity
(Roland Siegwart, D-MAVT)

Fabian Hillebrand
Algorithm for the Simulation of HR-STM within the Two Probe Particle Model
(Vasile Gradinaru, D-MATH)

Andreas Hug
Unsupervised Learning of Representations for Lexical Entailment Detection
(Thomas Hofmann, D-INFK)

Mara Iosif
Randomized Algorithms for Online Matching with Delay for Two Sources
(Roger Wattenhofer, D-INFK)

Franziska Krummenacher
The Structural DNA of Cities
(Rudolf Heinimann, D-ENV)

Mathis Lamarre
Probabilistic Word Embeddings for Intent Classification
(Ce Zhang, D-INFK)

Yi Liu
Super-resolution and Wasserstein bound
(Sara Van de Geer, D-MATH)

Fabio Luchsinger
Optimized real-time orbit determination of cube satellites with low-cost GNSS receivers
(Markus Rothacher, D-BAUG)

Lukas Strebel
Automatic domain decomposition for HPC stencil codes in heterogeneous systems
(Christoph Schulthess, D-PHYS)

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

Term Papers

Niklaus David Bamert
Two-stage (semi-)dense real-time 3D depth estimation
(Marc Pollefeys, D-INFK)

Christian Baumann
A Review on Fusion Techniques Applied to Semantic Segmentation
(Roland Siegwart, D-MAVT)

Abhimanyu Bhadauria
Discrete Adjoint Method for 2D Problems in OpenFOAM : Optimisation and Regularisation
(Patrick Jenny, D-MAVT)

Luzius Brogli
Conditional variance regularization for data Augmentation
(Nicolai Meinshausen, D-MATH SfS)

Jingqiu Ding
Semidefinite Programming and Low Degree Moment Estimation in Stochastic Block Model
(David Steuerer, D-INFK)

Till Ehrengruber
GPU Parallel Computing in Reactive Transport Simulations for Geothermal Energy Systems
(Martin Saar, D-ERDW)

Anna Eigenmann
Answer Reranking for Open-Domain Question Answering
(Stefan Feuerriegel, D-MTEC)

Laurent Eriksen
Metropolis-Hastings
(Vasile Gradinaru, D-MATH)

Julien Sebastian Gacon
On Properties of Cosmic Filaments
(Sebastiano Cantalupo, D-PHYS)

Pedro Partida Guitron
Bitcoin Bubbles: Epidemic-Diffusion Analyses and Models
(Didier Sornette, D-GESS)

Bjarni Hannesson
Vector Field Topology in the Circular Restricted Three Body Problem
(Markus Gross, D-ITET)

Ramona Emilie Hohl
Lorentz-force based imaging
(Habib Ammari, D-MATH)

Filip Michael Janicki
Explaining the decision made by a black box model
(Rainer Andreas Krause, D-INFK)

Fabian Keller
Application of the Lattice Boltzmann Method to the Shallow Water Equations
(Ilya Karlin, D-MAVT)

Evgenii Kolesnikov
A Machine Learning Framework for Acceleration of Computations of the Burgers' Equation
(Siddhartha Mishra, D-MATH)

Lasse Lingens
Perceiving Autonomous Agents for Emergent Narratives in Video Games
(Robert Sumner, D-INFK)

Kay Sebastian Müller
Training for rotational invariance and applications to SDF recognition
(Roland Siegwart, D-MAVT)

Philipp Thomas Müller
M-Hompack and its Application to Counterfactual Analysis in Dynamic Games
(Karl Schmedders, UZH)

Piyush Panchal
Shape Calculus Enabled Force Computation
(Ralf Hiptmair, D-MAHT)

Max Rossmannek
Martin: Chatting about Computational Chemistry
(Markus Reiher, D-CHAB)

Fabian Schwarz
Coarse-grained MD simulation of polymer melts & end-crosslinked polymer networks
(Andrej Gusev, D-MATL)

Dominic Christoph Stemmler
Coupling of a 2-D visco-elasto-plastic geodynamical code with a biological diversification model of lineages through time
(Taras Gerya, D-ERDW)

Shruti Thota
Place Recognition using 3D lines
(Roland Siegwart, D-MAVT)

Erik Träff
Numerical Implementation of a continuum model for 3D truss metamaterials
(Dennis Kochmann, D-MAVT)

Yiqing Zhu
Ice Formation on Liquid Simulations
(Markus Gross, D-INFK)

Zürich, November 1, 2019
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

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CSE Case Studies Seminar

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

Case Studies Seminar HS18

20.09.18	Ralf Hiptmair, Seminar für Angewandte Mathematik (SAM) Presenting in the Case Studies
27.09.18	Stefan Wörner, Quantum Technologies Group, IBM Research - Zurich Quantum Computing & Applications
18.10.18	Santiago Badia, Universitat Politècnica de Catalunya and CIMNE, Barcelona The FEMPAR Project: Scaling up Computational Science and Engineering
15.11.18	Simon Scheidegger, Department of Finance, University of Lausanne Peta-scalable Dynamic Stochastic Economic Modeling
22.11.18	Michael Steinlechner, Ziemer Ophthalmic Systems AG, Port CSE for MedTech: Image-Guided Eye Surgeries
29.11.18	Carlos Jerez Hanckes, Mathematical and Computational Engineering, Pontificia Universidad Católica de Chile, and Seminar für Angewandte Mathematik (SAM) Application of Boundary Element Methods in Biomedical Engineering

Case Studies Seminar FS19

21.02.19	Andreas Elsener, FirmTec Solutions AG, Pfäffikon Performance Challenges in Business IT
28.02.19	Tobias Grosser, Computing Platforms, D-NFK Presburger Arithmetic at the Core of Compilers and Deep Learning
21.03.19	Fernando Perez Cruz & Luis Salamanca, ETH Swiss Data Science Center An Introduction to Machine Learning & Latent Variable Models for TE4Med
28.03.19	Roman Vetter, Computational Biology, D-BSSE Simulation of Proton Exchange Membrane Fuel Cells
04.04.19	Christoph Winkelmann, ABB Corporate Research, Baden-Dättwil Force Computation for Magnetic Actuation of Switching Devices

4

Computational Highlight

ALSVINN: A FAST MULTI-GPGPU FINITE VOLUME SOLVER WITH A STRONG EMPHASIS ON REPRODUCIBILITY

KJETIL OLSEN LYE

Abstract. We present the Alsvinn simulator, a fast multi general purpose graphical processing unit (GPGPU) finite volume solver for hyperbolic conservation laws in multiple space dimensions. Alsvinn has native support for uncertainty quantifications, and exhibits excellent scaling on top tier compute clusters.

1. Introduction

We are interested in approximating solutions to systems of non-linear hyperbolic conservation laws of the form

$$\begin{cases} \mathbf{u}_t + \nabla_x \cdot \mathbf{F}(\mathbf{u}) = 0 & \text{on } D \times [0,T] \\ \mathbf{u}(x,0) = \mathbf{u}_0(x) & \text{on } D. \end{cases} \tag{1.1}$$

Examples include the compressible Euler equations of gas dynamics, the shallow water equations of oceanography, and the Magnetohydrodynamics equations of plasma physics. For a complete review, consult [1].

It is well-known that solutions of (1.1) develop discontinuities in finite time, making the design of efficient numerical schemes challenging. The finite volume method has shown great success in dealing with these discontinuities, and will the method of choice for this paper.

Additionally, instabilities, turbulence and multi-scale phenomena develop, and recent numerical and theoretical evidence [4] show that deterministic solutions to (1.1) are ill-posed, and one is forced to consider a probabilistic formulation. There are several popular frameworks available for uncertainty quantifications (UQ) for hyperbolic conservation laws, but due to the ill-posed nature of the equations, the measure valued solutions [4] and statistical solutions [2, 3, 5] are well suited for hyperbolic equations.

The probabilistic formulations typically involve a sampling method, requiring multiple evaluations of the (very expensive) numerical scheme, which in turn creates the need for fast numerical solvers of hyperbolic conservation laws. While there are several multi-node CPU-based numerical finite volume codes, the largest computing clusters in the world often use general-purpose graphical processing units (GPGPUs) as their main accelerator, and thus one has a need for fast multi-GPGPU numerical codes for hyperbolic equations. Indeed, even highly optimized CPU codes are often limited by the lower memory bandwidth the CPU offers. Furthermore, since the intrinsic nature of the equations is probabilistic, the numerical solvers should have built-in support for uncertainty quantifications. On Switzerland's, and Europe's, largest supercomputer, the CSCS Piz Daint, the typical runtime difference of a highly optimized CPU finite volume code and an optimized GPGPU finite volume code can be an order of magnitude in favour of the GPGPU version. For three dimensional datasets, a single GPGPU does not have enough on-board memory to hold the whole dataset, and one is forced to develop multi-GPGPU finite volume solvers. While there are GPGPU finite volume solvers available, they are either often only available on single GPGPUs, or they do not have built-in support for UQ. Indeed, for high performance UQ on GPGPUs, one needs to take care that the statistics evaluation is done on GPGPU, minimzing overhead and storage requirements.

Alsvinn, presented in this paper, is a fast, multi-GPGPU-based finite volume solver with UQ support built-in, written in C++ with CUDA and MPI, made to address the concerns in the above paragraph. Alsvinn supports a wide range of numerical finite volume solvers, and various sampling methods including Monte Carlo (MC), Quasi Monte Carlo (QMC) and Multilevel Monte Carlo (MLMC). Alsvinn is open source software freely available from `https://alsvinn.github.io`.

Seminar for Applied Mathematics, ETH Zürich, Rämistrasse 101, 8092 Zürich, Switzerland
E-mail address: `kjetil.lye@sam.math.ethz.ch`.
Date: November 2018.

2. Implementation of Alsvinn

In this section we briefly describe the implementation and numerical methods used in Alsvinn. Alsvinn contains two core components: The finite volume solver, and the uncertainty quantification module.

2.1. Finite Volume Methods.

The finite volume method (FVM) is by far the most widely used method for approximating solutions of hyperbolic conservation laws. This section briefly reviews the finite volume method, for a full review, consult [8].

We discretize the computational spatial domain as a collection of cells marked as $\mathbf{i}$, and we let $u_{\mathbf{i}}^{\Delta}(t)$ denote the averaged value in the cell at time $t \geqslant 0$. The semi-discrete case satisfies the following equation

$$\frac{\mathrm{d}}{\mathrm{d}t} u_{\mathbf{i}}^{\Delta}(t) + \sum_{k=1}^{3} \frac{1}{\Delta} \left(F^{k,\Delta}_{\mathbf{i}+1/2\mathbf{e}_k}(t) - F^{k,\Delta}_{\mathbf{i}-1/2\mathbf{e}_k}(t) \right) = 0. \tag{2.1}$$

Here $F^{k,\Delta}$ is a *numerical flux function* in the direction k for $k = 1, 2, 3$. Alsvinn supports a large array of numerical fluxes, including the well-known HLLC flux[10], the Godunov flux, the Rusanov flux, the Roe flux, and high order entropy conservative fluxes described in [7]. We then use a strong stability preserving Runge-Kutta time stepping scheme [6] to discretize (2.1), moreover, we also add a high order reconstruction, such as a the ENO or WENO reconstructions [9], to estimate the cell interface values.

In Alsvinn, we use a smart mixture of compile-time and run-time polymorphism to support a multitude of equations, numerical fluxes, time steppers and reconstructions on both the CPU and the GPGPU. Moreover, the compile time polymorphism works akin to a compile time *domain specific language*, allowing domain specialists to write their equations without interacting with any GPGPU specific code. Indeed, any of the mentioned components can be written once, but will automatically be translated into a version on the CPU and on the GPGPU.

To minimize the overhead of internode communication when running in a multi-GPGPU setup, Alsvinn overlaps communication with computation, and both the communication and compactification of the halo domain is done in parallel with the computation of the inner domain.

2.2. Uncertainty quantifications in Alsvinn.

Uncertainty quantifications are built into the Alsvinn simulator. We support a wide variety of sampling methods, both built in, but also user specified through external libraries. At the core, the UQ module of Alsvinn can approximate stochastic integrals through either single-level or multilevel sampling of the form

$$\int_{\Omega} G(u(\omega, \cdot))\, d\mathbb{P}(\Omega) \approx \frac{1}{M} \sum_{k=1}^{M} G(u_k) \qquad \text{and} \qquad \int_{\Omega} G(u(\omega, \cdot))\, d\mathbb{P}(\Omega) \approx \sum_{l=1}^{L} \frac{1}{M_l} \sum_{k=1}^{M_l} (G(u_k^l) - G(u_k^{l-1})),$$

respectively. The random samples $1, \ldots, M$ are distributed over MPI by a load balancing algorithm.

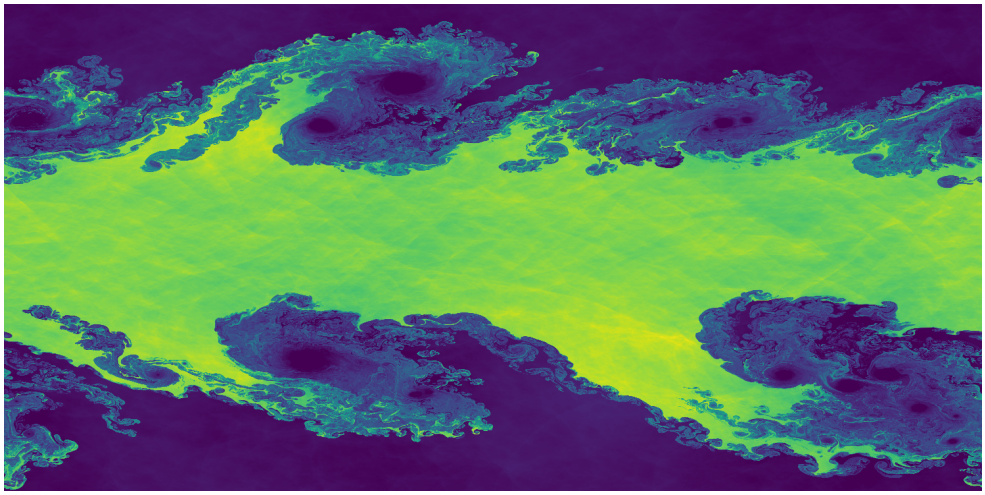
We also support a wide range of statistical functionals, such as mean, variance, point PDFs, two-point structure functions, joint PDFs and multi-point correlators [3]. And finally, a large variety of sampling methods are available, including Monte Carlo and Quasi Monte Carlo sampling.

Alsvinn furthermore computes all statistics on the GPGPU when available, minimizing overhead, computational time and disk storage. Since each stochastic sample is independent, Alsvinn is able to perfectly parallelize over the stochastic dimensions for Monte Carlo and Quasi Monte Carlo, while for MLMC, it can utilize effective load balancing algorithms.

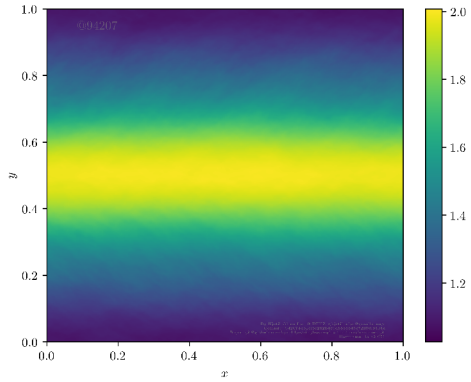
2.3. Reproducibility.

Alsvinn is written with reproducibility in mind. It uses a range of modern software techniques to be as robust as possible. There are to date over 200 unit tests covering most of Alsvinn's functionality. To make the experiments easy to reproduce in other simulators, the input data is specified in an XML file specifying simulator parameters (for example numerical flux and grid size), while the initial data is specified in a Python, both of which could potentially be read from any other finite volume simulator.

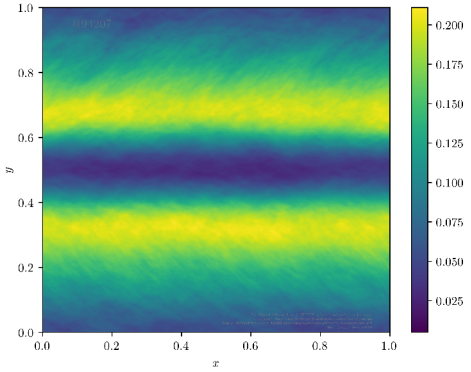
Furthermore, every output file of Alsvinn is marked with the revision number of Alsvinn, the library versions used and the input parameters and initial data.



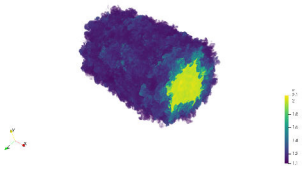
(A) Single sample 2D



(B) Mean 2D

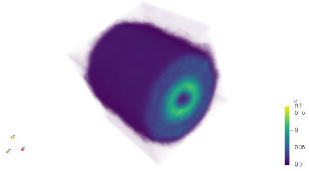


(C) Variance 2D



(D) Single sample 3D.

(E) Mean 3D



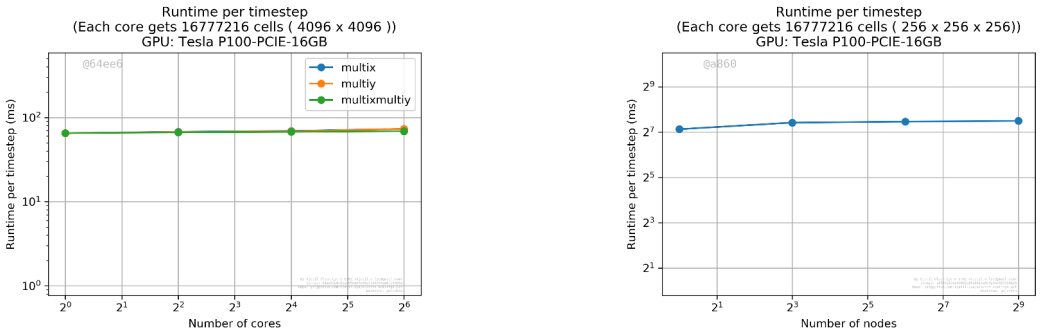
(F) Variance 3D

FIGURE 1. Numerical results for the Kelvin–Helmholtz instability in 2D and 3D. We plot the approximate density (ρ) (A and E) in 2D and 3D, with a mesh resolution of 32768^2 and 1024^3 respectively, together with the mean and variance of the density (B, C, F and G). We also plot hte The numerical flux used is the HLLC flux, a third order WENO reconstruction is used, along with a third order SSP Runge-Kutta time stepper

3. Examples and performance analysis

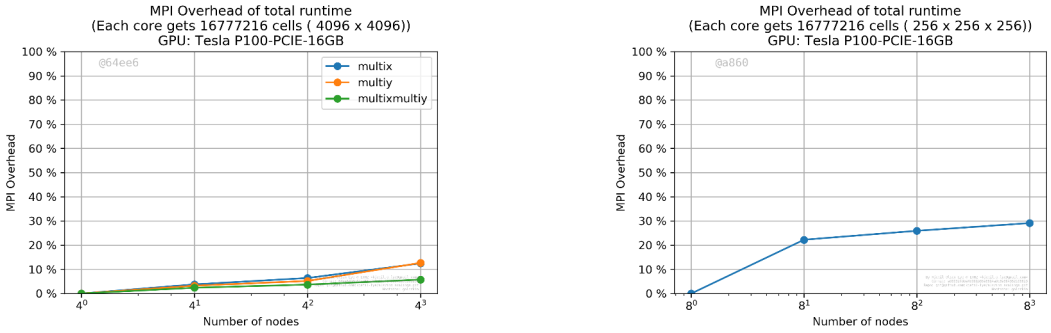
The Kelvin–Helmholtz initial data is given as a shear flow with two states, see [4] for details. Here we use Alsvinn to simulate the Kelvin–Helmholtz initial data in two and three spatial dimensions, see Figure 1 for an illustration.

3.1. **Spatial scalability.** We measure the performance of the communication implementation for 2 and 3 spatial dimensions for the Kelvin–Helmholtz experiment described in the above section. All runs are performed on the super computer CSCS Piz Daint.



(A) 2D (B) 3D

FIGURE 2. Weaking scaling of the Kelvin-Helmholtz experiment in 2D and 3D. In 2D, we can decompose either in the x-direction (multix), y-direction (multiy) or both (multixmultiy). In all experiments, an HLLC flux with a third order WENO reconstruction was used. Performed on CSCS Piz Daint.



(A) 2D (B) 3D

FIGURE 3. MPI overhead for the Kelvin-Helmholtz experiment in 2D and 3D. In 2D, we can decompose either in the x-direction (multix), y-direction (multiy) or both (multixmultiy). In all experiments, an HLLC flux with a third order WENO reconstruction was used. Performed on CSCS Piz Daint.

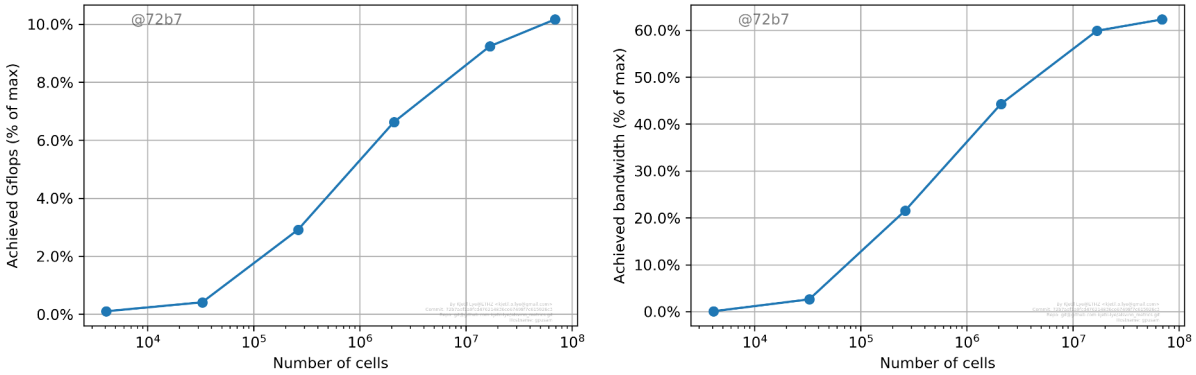
As parallel in time simulations of finite volume methods are still in its infancy, we focus our scalability study on the spatial decomposition. We perform two experiments to measure the weak scalability of Alsvinn. We run the Kelvin–Helmholtz experiment 2D and 3D with varying number of spatial cells, where we keep the number of cells per GPGPU constant (each GPGPU gets 2^24 cells), and we measure the runtime per timestep in Figure 2. From both plots it is evident that Alsvinn obtains excellent scaling, and scales across 512 GPGPUs for a single sample. Here we note that even at a resolution of 2048^3, we only use 0.105 seconds per timestep.

We furthermore measure the performance impact of the MPI communication compared to the overall runtime of the base configuration in Figure 3, that is, the MPI overhead of K nodes is defined as

$$\text{MPI Overhead}(K) = \frac{\text{Runtime per timestep}(K) - \text{Runtime per timestep (1)}}{\text{Runtime per timestep}(1)}.$$

As we can see, in 2D, we get less than 10 % overhead, while in 3D, we get roughly 30% overhead while utilizing 512 GPGPUs, which is to be expected for 3D GPGPU codes, where the dataset to communicate grows as $\mathcal{O}(N^2)$ where N is the number of cells in each spatial direction.

3.2. **Utilization of hardware.** While the figures in the previous section showed that Alsvinn is able to scale over multiple compute nodes, it still remains to show that the code utilizes a single node effectively.



(A) FLOPS, P100

(B) Bandwidth, P100

FIGURE 4. Hardware utilization in Alsvinn. We measure the ratio between the achieved memory bandwidth and the maximum peak memory bandwidth (left), and the ratio between the achieved number of floating point operations per second (FLOPS) and the maximum number of floating point operations per second achievable by the GPGPU (right). In all experiments, an HLLC flux with a third order WENO reconstruction was used. Performed on CSCS Piz Daint with an NVIDIA Tesla P100.

We benchmark our implementation on an NVIDIA Tesla P100. All experiments utilize double precision (64 bits) floating point numbers.

We plot the a ratio between the achieved number of floating point operations per second (FLOPS) and the maximum FLOPS achievable on the GPGPU in Figure 4 (A). We see that we achieve 10 % of peak floating point performance, which is to be expected from a finite volume algorithm, which usually is memory bandwidth bounded.

In Figure 4 (B) we measure the ratio between the achieved memory bandwidth, and the theoretical maximum memory bandwidth of the GPGPU. From the figure, we see that we achieve above 60 % memory bandwidth utilization, which confirms that the code is memory bandwidth bounded, and that we achieve close to peak performance in terms of the memory bandwidth.

4. Conclusion

We have presented Alsvinn, a robust, fast, efficient and highly scalable multi-GPGPU code for simulating and performing UQ for systems of conservation laws, such as the Euler equations of gas dynamics, in two and three space dimensions. It has been well-established [4] that purely deterministic simulations of multi-dimensional conservation laws may not converge on mesh refinement. Hence, UQ simulations have to be performed even of deterministic initial data. Given the prohibitive cost of simulating complex three-dimensional problems with state of the art multi-CPU codes on leadership class hardware platfroms, it is imperative to design scale multi-GPGPU codes. Alsvinn satisfies these requirements as it is shown to scale very well on state of the art GPGPU clusters and incorporates various efficient numerical schemes and sampling based UQ techniques in one platform. In particular, we are able to perform UQ, within the framework of statistical solutions, for very complex three dimensional compressible flows at high spatio-temporal and statistical resolutions, with Alsvinn, providing the first such results globally.

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5

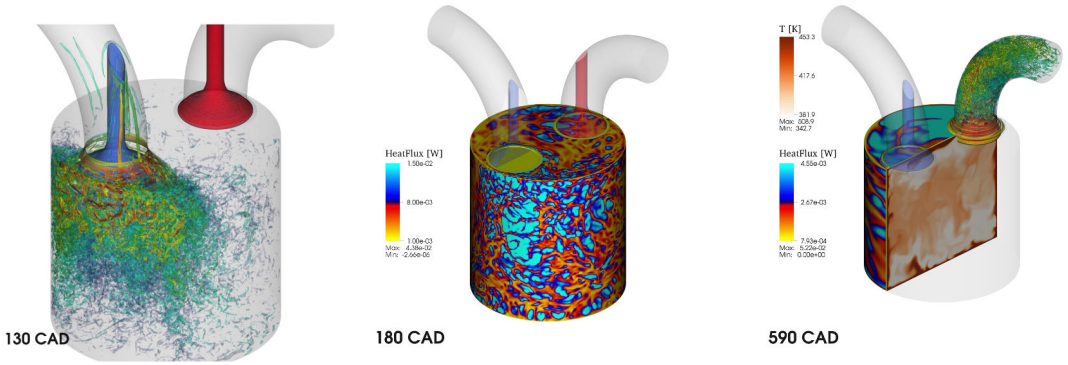
CSE Research Projects

Group of Prof. K. Boulouchos
(Aerothermochemistry and Combustion Sytems Laboratory)

Title: LES of the Gas-Exchange Process Inside an Internal Combustion Engine Using a High-Order Method

Institute/ Group: G.K. Giannakopoulos[1], C.E. Frouzakis[1], P.F. Fischer[2], A.G. Tomboulides[3], K. Boulouchos[1]
[1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ
[2]Dept. Computer Science, U. Illinois, Urbana-Champaign, USA
[3]Dept. Mechanical Engineering, Aristotle U., Thessaloniki, Greece

High-order, wall-resolved large eddy simulations (LES) using the spectral element method (SEM) were performed to investigate the gas-exchange process inside a laboratory-scale internal combustion engine (ICE) and study the in-cylinder flow evolution. Using a stabilizing filter, over 30 engine cycles were simulated to generate data for statistical analysis, which demonstrated good agreement in the mean and root mean-squared (rms) phase-averaged velocity fields across three different filter parameter/resolution combinations. The large scale flow motion was characterized during each stage of the engine cycle. Tumble ratio profiles indicate peak values during the intake stroke which decay during compression and are almost non-existent thereafter. The tumble breakdown process is quantified by investigating the evolution of the mean and turbulent kinetic energy over the full cycle, and its effect on the evolution of the momentum and thermal boundary layers is discussed. Algorithmic advances to the computational fluid dynamics (CFD) solver Nek5000, employed in the current study, resulted in significant reduction in the wall-time needed for the simulation of each cycle for mesh resolutions of at least an order of magnitude higher than the current state-of-the-art.



(a) (b) (c)

(a) Vortical flow structures during the intake stroke, and distribution of (b) heat flux on the walls at 180 crank angle degrees (CAD), and (c) of temperature inside the cylinder, heat flux on the walls and vortical structures in the exhaust manifold at 590 CAD.

References:

G.K. Giannakopoulos, C.E. Frouzakis, P.F. Fischer, A. G. Tomboulides, K. Boulouchos, LES of the Gas-Exchange Process Inside an Internal Combustion Engine Using a High-Order Method *Flow, Turbulence and Combustion*, 198, 1–20, 2019

Title:	Consumption and displacement speeds of stretched premixed flames – Theory and simulations
Institute/ Group:	G.K. Giannakopoulos[1], C.E.Frouzakis[1], S. Mohan[2], A.G.Tomboulides[3], M. Matalon[2] [1]Aerothermochemistry and Combustion Systems Laboratory, ETHZ [2]Dept. Mechanical Science and Engineering, U. Illinois, Urbana-Champaign, USA [3]Dept. Mechanical Engineering, Aristotle U. Thessaloniki, Greece

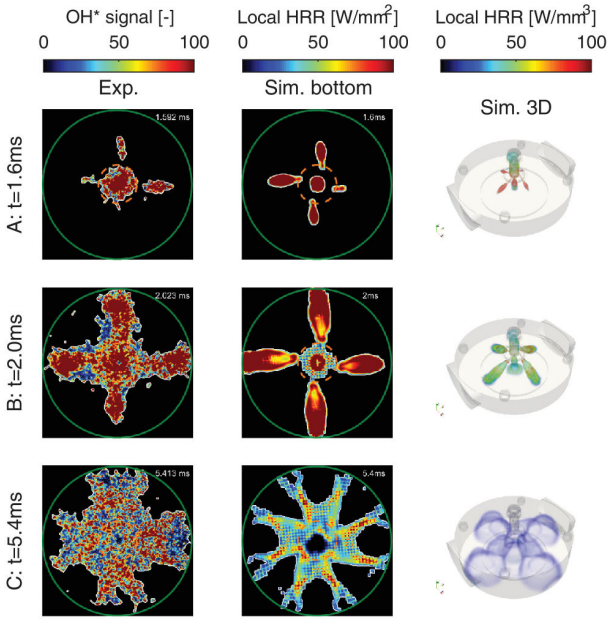
The flame displacement speed (FDS) and flame consumption speed (FCS) are commonly used in numerical studies to characterize flame dynamics. Although for a planar configuration they are both well defined and accurately represent the propagation speed of the flame into the combustible mixture, their definition in more general circumstances is ambiguous. The FDS and FCS are local quantities: the FDS is associated with the displacement of an arbitrarily selected iso-surface, and the FCS is an integrated quantity throughout a region that needs to be approximated, in a direction that is not always uniquely defined. The only unambiguously defined quantity is the global (volumetric) consumption rate obtained by integrating the rate of reactant consumption over the entire combustion volume. However, using it to determine the FCS requires a proper identification of the flame surface area which introduces uncertainty in the results. Indeed, numerical simulations show that combustion properties depend significantly on the choices made in the determination of the FDS and FCS. In order to utilize these quantities in a meaningful way, their limitations are explored by providing a detailed comparison between predictions of numerical simulations and theoretical expressions obtained for weakly-stretched flames. The theory is based on the assumption that the flame is thin relative to the representative hydrodynamic length scale and in this asymptotic limit both, the FDS (commonly referred to as the flame speed) and the FCS, are uniquely and unambiguously defined. Two configurations are examined in this paper: (i) spherical flames, unsteady expanding as well as stationary, where the flow is unidirectional and (ii) steadily propagating cusp-like flames (resulting from the Darrieus-Landau instability) whose structures are spatially varying and where the flow through the flame is nonuniform. The presented comparison validates the accuracy of the asymptotic expressions for the dependence of the FDS and FCS on stretch for one-step chemistry, and demonstrates that the theoretical predictions remain qualitatively, and to a large extent quantitatively valid for detailed chemistry for both, lean and rich flames.

References:

G.K. Giannakopoulos, C.E.Frouzakis, S. Mohan, A.G.Tomboulides, M. Matalon, Consumption and displacement speeds of stretched premixed flames – Theory and simulations *Combustion and Flame*, 208, 164–181, 2019

Title:	Experimental and numerical investigations of the unscavenged prechamber combustion in a rapid compression and expansion machine under engine-like conditions
Institute/ Group:	G. Xu, M. Kotzagianni, P. Kyrtatos, Y.M. Wright, K. Boulouchos Aerothermochemistry and Combustion Systems Laboratory, ETHZ

The unscavenged prechamber combustion of lean methane/air mixtures in a Rapid Compression Expansion Machine is investigated using optical diagnostics (high-speed OH*-chemiluminescence and Schlieren imaging) and 3D Computational Fluid Dynamic (CFD) simulations. The comparison of the Schlieren and the OH* images confirm the hypothesis that inherent reacting flame jets exit the prechamber, which justifies the applicability of a level set combustion modeling framework for the investigated operating conditions. The employed G-equation combustion model has been extended to account for the specifics of spark ignition and flame wall interaction present in the prechamber. Validation of the developed model by means of the experimental data shows good agreements in terms of (i) jet exit timing, (ii) main chamber heat release rate and (iii) projected reactive flame area, evidencing encouraging predictive capability of the proposed modeling approach. The subsequent analysis on a single flame jet, using OH*-chemiluminescence and CFD images, indicates that the jet head tends to be more reactive due to a higher turbulence levels and larger eddy size.



Comparison of the reactive region at three time instants: experiments (left column), simulation (middle column), simulation with 3D view (right column).

References:

G. Xu, M. Kotzagianni, P. Kyrtatos, Y.M. Wright, K. Boulouchos Experimental and numerical investigations of the unscavenged prechamber combustion in a rapid compression and expansion machine under engine-like conditions, *Combustion and Flame*, 204, 68–84, 2019

Title:	Experimental and numerical investigations of the unscavenged prechamber combustion in a rapid compression and expansion machine under engine-like conditions
Institute/ Group:	M. Banholzer[1], W. Vera-Tudela[2], C. Traxinger[1], M. Pfitzner[1], Y. Wright[2], and K. Boulouchos[2] [1]DInstitute for Thermodynamics, Department of Aerospace Engineering, Bundeswehr University Munich, Neubiberg, Germany [2]Aerothermochemistry and Combustion Systems Laboratory, ETHZ

Numerical simulations are carried out to investigate underexpanded methane jets with phase separation effects. In order to predict the fuel injection and the mixture formation in the constant volume chamber, a hybrid, pressure-based solver is combined with a vapor-liquid equilibrium model and a moving mesh methodology. The thermodynamic models are based on the cubic equation of state of Soave, Redlich, and Kwong. A compressibility correction for the widely known k-ω SST turbulence model is implemented additionally. Application-relevant simulations with a total fuel pressure of 300 bars and five different chamber pressures ranging from 12 to 60 bars were defined. Furthermore, the influence of two fuel and chamber temperatures, 294 and 363 K, is analyzed. Depending on the chamber pressure, two different flow structures of the potential core can be distinguished: (1) A series of typical shock barrels for small pressure ratios and moderately underexpanded jets and (2) a shear layer consisting of a two-phase mixture which enfolds the potential core for high pressure ratios and highly underexpanded jets. Increasing the fuel temperature leads to less significant phase separations, while an increase in the chamber pressure does not affect the structure of the potential core. A comparison with experimental measurements shows a very good agreement of the simulated structure of the potential core, providing evidence that the underlying phenomena are predicted correctly and suggesting that a moving mesh strategy and consistent two-phase thermodynamics implementation are necessary for a physical representation of high-pressure injections.

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Institute/Group: Computer-assisted Applications in Medicine (CAiM), D-ITET, ETH Zurich
Group of Prof. Orcun Goksel

Researchers: Dr. Baran Gözcü, Dr. Sabine Kling (SNSF Ambizione), Dr. Tiziano Portenier, Dr. Richard Rau, Dr. Valery Vishnevskiy, Bhaskara Chintada, Matija Ciganovic, Alvaro Gomariz**,** Firat Ozdemir, Pushpak Pati, Fabien Péan, Dieter Schweizer, Kevin Thandiackal, Lin Zhang

Description: Basic and applied research in CAiM involve data analysis and information extraction, on topics lying at the intersection of multiple disciplines: *engineering*, *computer science*, and *medicine*. With the involvement of group members with diverse and cross-disciplinary skill-set, the group aims to devise novel imaging and image analysis techniques, and develop them for clinical translation. The group's efforts push the boundaries of diagnostic and surgical procedures as well as minimally-invasive interventions.

A first line of work focuses on *quantitative imaging* and *image reconstruction* in diagnostic and interventional clinical applications, with research extending to areas such as *tissue characterization*, *inverse problems in imaging*, and *signal processing*. Novel imaging contrast techniques, especially based on ultrasound physics, is a major interest in the group.
A second line of work is devoted to *computer-assisted interventions* and *image-guided therapy*, with research in *image analysis*, *machine learning*, *patient-specific finite-element simulations*, *personalized anatomical meshing*, and *virtual-reality in clinical training*.
These closely integrated lines of work cross-fertilize each other, for instance on the development of neural network approaches for inverse problems of imaging or with the expertise in imaging physics for highly realistic simulations in VR.

Research in CAiM is conducted in close collaboration with clinical as well as industrial partners, where the research results have a strong translational component, both clinically and commercially. To that end, CAiM aims to develop innovative diagnostic and interventional applications, focusing on data analysis from imaging to abstracting patient-specific models and representations, and from there to optimal intervention planning and intra-operative execution.

A novel ultrasound imaging contrast modality, speed-of-sound, developed in CAiM received the 2016 ETH Spark Award (for the most promising innovation of the year) and the 2017 Swiss Venture Award (for the best idea). This contrast marker has so far been tested in clinical studies on the breast and on muscles, e.g. for the quantification of breast density and muscular degeneration, as well as for differential diagnosis of breast cancer.

Semester and master projects can be defined in discussion from a wide range of exciting topics, based also on the interests and background of the student.
Some sample topics can be found at: www.caim.ee.ethz.ch
Nevertheless, due to the dynamic nature of research in the field, potential students are encouraged to contact Prof. Goksel for up-to-date project topics.

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 Coupling of Finite Elements and Multiple-Based Trefftz Approximation

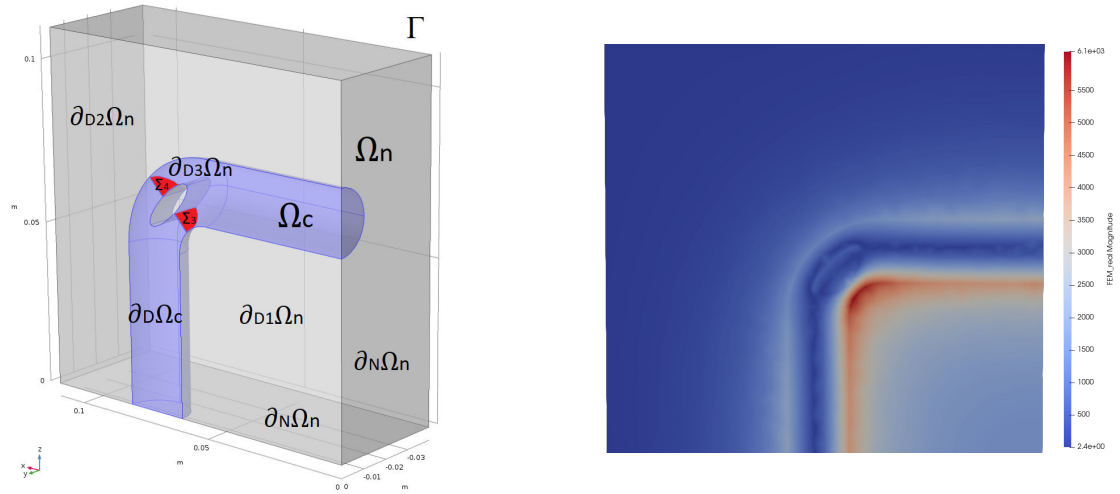

Figure 1: lefgt: geometric setup for a time-harmonic eddy current problem (reduced to an octant by symmetry), right: magnitude of the real part of the magnetic field, computations used DtN-based coupling.

This project considers linear electromagnetic field problems in frequency domain. In the case of piecewise homogeneous materials Trefftz approximation has been employed successfully for the discretization of the corresponding field problems. These techniques rely on approximation spaces comprising functions that are solution of the homogeneous Maxwell equations. They offer an alternative to the use of boundary element methods.

However, Trefftz methods cannot deal with inhomogeneous and non-linear materials. If those are confined to bounded regions of space, volume based finite element discretizations have to be used locally. This project investigates how to couple Trefftz spaces generated by spatially distributed multipoles with standard low-order conforming finite element methods for electromagnetic field problems.

This is a joint project with Prof. em. Ch. Hafner and Prof. J. Smajic (D-ITET), conducted by D. Casati as his PhD project.

This research was supported by SNF under grant 2000021_165674/1 "Coupling of Finite Elements and Multiple Multipoles for Computational Electromagnetism"

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.

Initially 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 other is a suitable representation of shape deformations. We use a volume based encoding

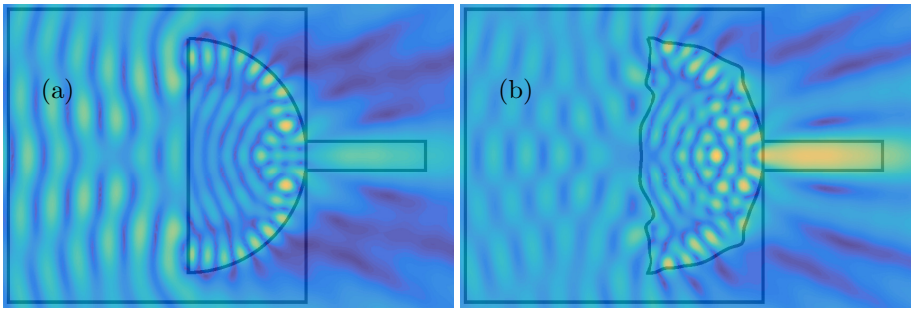

Figure 2: Shape optimization of microlenses An incoming plane wave hits (from the left) a cylindrical lens with semi-circular cross section (a). The shape of the lens is optimized to maximize the focused light in the thin rectangle on the back of the lens (b).

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.

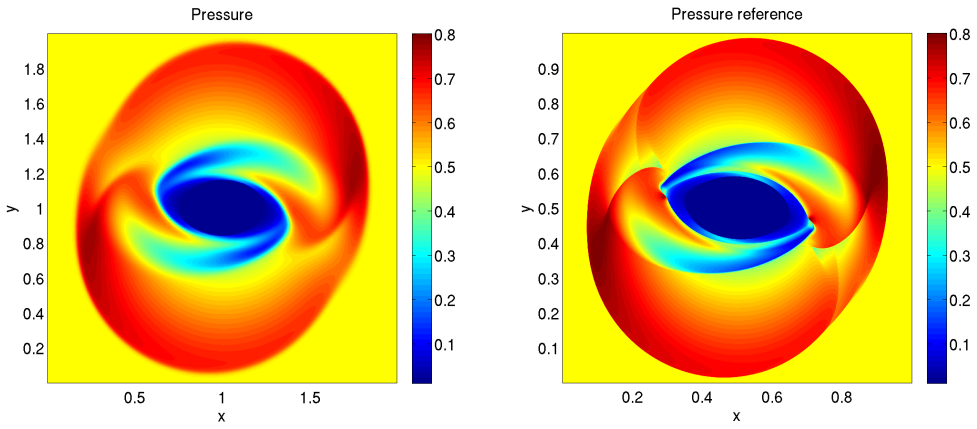

Figure 3: XXX

Figure 4: Ad ❻: Rotor problem. 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.

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Institute/Group: Institute of Virtual Manufacturing

Researchers: Dr. Bekim Berisha, Michele Crosio, Sebastian Hirsiger, Maximilian Neuhauser, Prof. Dr. Pavel Hora

Description:

1.) Using advanced deep-learning algorithms for surface quality control in industrial extrusion processes

Surface defect control is still challenging in the metal working industry. Production facilities such as extrusion companies conduct quality control using the human eye. In order to make quality control faster, less cost intensive and more reliable, research is done in the question of how to implement an automated surface defect detection system. In this context, the institute focuses on the detection using deep convolutional neural networks. A hardware system in the form of a light tunnel has been developed that illuminates extruded profiles all around their cross section to optimally capture surface defects in images taken with industrial cameras. Pure classification (various high performance network architectures), object detection (Faster R-CNN) and instance segmentation (Mask R-CNN) algorithms are then the key technologies from computer science used to detect surface defects on flawed profiles.

2.) Virtual analysis of welds through particle-tracking methods in the special-purpose extrusion simulation software PF-Extrude

Given the complex boundary conditions and process characteristics, the numerical analysis of the extrusion process still presents many challenges. As the workpiece is pressed through the die, a complex velocity field is formed due to the complex thermal/pressure-influenced contact conditions. Process-bounded defects have to be carefully inspected in order to ensure the mechanical integrity of the produced part: Charge welds are formed when material from different billets merge together in the profile. These sections of the extrudate must be removed from the product. On the other hand, seam welds are the unavoidable defects of the extrusion of hollow profiles: the material from the billet is divided into different streams, which re-join together within a welding chamber. As this happens, the streams weld together and form the shape of the final product. A particle-tracking algorithm has been implemented in the FE-code PF-Extrude, enabling a detailed analysis of the simulated material stream and the investigation of how the material from the new loaded billet develops in the extruded profile. Moreover, the seam welds analysis routine allows to identify the welding zones, where the material streams weld together and determine the quality of the welding condition. The results offers insights on how to optimize the die, even before being manufactured.

3.) Computational modelling of sheet metal anisotropy based on crystal plasticity models

Crystal plasticity (CP) models in combination with efficient numerical methods, like the FFT-based spectral solver, are used as a complementary modelling strategy to macroscopic models. Focus of the current research is to replace cumbersome experiments by virtual experiments and secondly to perform virtual experiments which are not directly possible in reality such as the biaxial compression test for metal sheets. The CP simulations results are used for a better calibration of the common constitutive models in order to improve the numerical results of finite element simulations. All numerical crystal plasticity simulations are performed in a highly parallelised open-source environment – DAMASK. Computations in the framework of fast Fourier transformations are considerably faster than the classical FEM.

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

Researchers: Prof P.H. Hünenberger / Dr Sadra Gheta / Marina Pereira
Alzbeta Kubincová / Salomé Rieder(-Walthard)

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* :

- Force-field calibration (incl. development of an experimental database, of a fragment-based topology builder, of a molecular-dynamics engine, and of systematic parameter optimization procedures for compound families)
- Treatment of electrostatic interactions under periodic boundary conditions
- Thermodynamic boundary conditions and extended-system methods
- Enhanced conformational sampling and free-energy calculations
- Development of new simulation algorithms and trajectory analysis procedures

and in terms of *applications* :

- Development of a thermodynamically consistent fragment-based force field for organic compounds
- Single-ion solvation (book: www.csms.ethz.ch/publications/book), role of electrostatic interactions (hydrogen bonding, salt bridges) in molecular systems, and properties of ionic systems (electrolyte solutions, crystals)
- Simulation of biomolecular systems (with a main focus on carbohydrates and lipids)

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

Researchers: Prof. Dr. Patrick Jenny, Nemanja Andric, Amir Ashrafi Habibabadi, Oliver Brenner, Kyoungseoun Chung, Dr. Rajdeep Deb*, Dr. Amir Droudian, Robert Epp, Valentin Giddey, Lorenz Hulfeld, Dr. Karim Khayrat, Thomas Kummer, Dr. Stephan Küchlin, Michael Liem, Dr. Adrien Lücker, PD Dr. Daniel W. Meyer, Dr. Arthur Moncorgé*, Ranit Monga, Daniel Oberle, Pasha Piroozmand, Dr. Franca Schmid*, Philipp Weiss *) external

Description:
Our research projects are essentially grouped into the following four major directions:

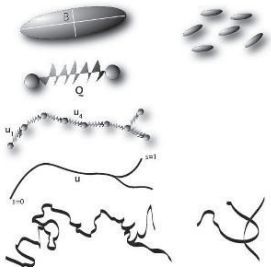
(1) Fluid dynamics in biomedical systems: We are collaborating with researchers from the Universities of Arizona, Berlin, Bern, San Diego, and Zürich. A first research effort is focused on the heterogeneity of capillary transit times of red blood cells and the neurovascular coupling, which links neuronal activity to cerebral blood flow. More specifically, we study the adjustment mechanisms of blood flow and energy supply in, respectively to, different regions of the brain. Our second focus deals with the development of numerical and experimental models of the human hearth that account for electrophysiology as well as structure mechanics. We use these models for the investigation of novel heart assist device concepts.

(2) 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. Related developments include new techniques for adaptive mesh refinement. 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.

(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. More specifically, we investigate the role of droplet clusters and voids on, e.g., overall turbulence conditions or evaporation rates. Our DNS results provide valuable data that guide a model development effort focused on representing clustering effects in CFD models.

(4) Flow and transport in porous and fractured media: This is a collaborative research effort with researchers from Total and Stanford University. Subsurface flows of water or oil are determined by the spatially heterogeneous permeability $K(\mathbf{x})$, which is typically a very heterogeneous quantity. With $K(\mathbf{x})$ being a highly uncertain quantity, we are developing numerical methods that translate given statistics for $K(\mathbf{x})$ 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 are working on models and algorithms for single- and multi-phase transport that enable a simplified representation and computationally efficient prediction of pore-scale effects at larger scales.

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



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

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

Description:

Computational Polymer Physics @ ETH recently focused its attention on the effect of nanoparticle geometry during cellular uptake [1], the tumbling-snake model [2], efficient hybrid algorithms for the creation of semiflexible polymers and glasses [3], the emergence of stationary uphill currents in 2D Ising models [4], 3D conformations of thick synthetic polymer chains [5], the gas-liquid phase equilibrium of a model Langmuir monolayers via a multiscale approach [6], the modeling of entangled polymer diffusion in melts and nanocomposites [7], mechanical properties of 3D graphene foams [8], the ordering and crystallization of entangled melts [9], the dynamics and wetting behavior of soft particles at a fluid-fluid interface [10], crosslinked polymer brushes under shear [11], surface disentanglement and slip in a model polymer melt [12], and topological constraints of lamellae-forming block copolymers [13]. Details available at www.complexfluids.ethz.ch

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Title: Novel 2-D materials as building blocks for advanced logic switches

Researchers: Cedric Klinkert
Christian Stieger
Aron Szabo
Mathieu Luisier

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

Description:

With the continuous down-scaling of the field-effect transistors (FETs), the 7nm technology node has been reached in 2018. FinFET, the current transistor architecture, is getting closer to its fundamental limits, calling for the emergence of novel concepts to be used as logic switches. Out of the various candidates that are currently investigated by the semiconductor industry, those based on 2-D materials such as the single-layer (SL) MoS_2 shown in Fig.1 appear as very promising. 2-D materials are in effect relatively straightforward to process and a large palette of SL 2-D crystals may exist, more than 1,800 according to a recent theoretical study.

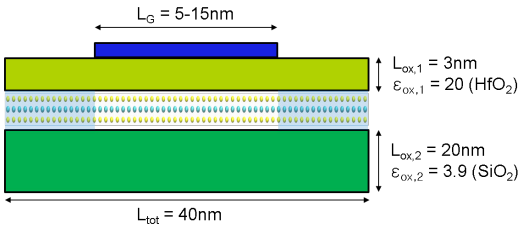


Fig.1: Schematic view of a planar FET implementing a single-layer 2-D materials as channel (here: MoS_2).

The anticipated number of attractive novel 2-D materials makes the evaluation of their potential as FET very time consuming from an experimental point of view. This is why a pre-screening of their device characteristics should be performed via simulation. In this study, density functional theory has been combined with the Wannier90 tool and our own *ab initio* quantum-transport solver to shed light on the properties of FETs with a 2-D channel material. Both n-type and p-type transistors have been simulated for gate lengths ranging from 15 down to 5 nm. Several materials that can outperform conventional transition metal dichalcogenides such as MoS_2 or WSe_2 have been identified. ON-current and scalability results are presented in Figs. 2-3.

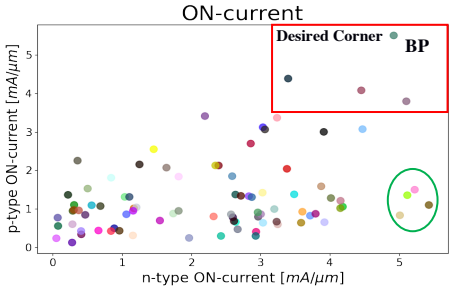


Fig.2. ON-currents of n- and p-type FETs at V_{GS}=0.7V and V_{DS} = 0.7V. Materials providing high ON-current values for both transistor types are desired.

In terms of computational effort, our in-house quantum transport simulator relies on a massive parallelization of the workload through 3 levels of parallelism. Each simulation is typically run on 225 nodes of the Piz Daint Supercomputer at CSCS, taking advantage of all available CPUs and GPUs per hybrid node. More than 1500 node hours per parameter set are needed. So far, 100 2-D materials have been explored, but the search for the optimal compound is still on-going.

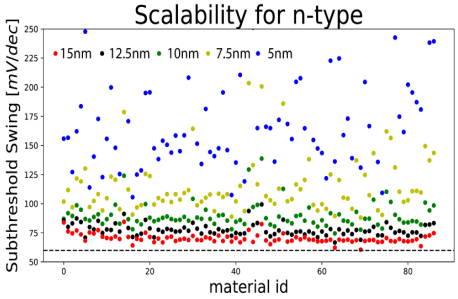
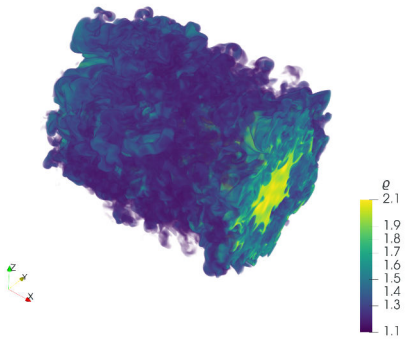


Fig. 3. Sub-threshold slope (SS) of the simulated 2-D FETs for gate lengths ranging from 15 down to 5 nm. A good SS scalability down to 10 nm can be observed.



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

Researchers: S. Mishra, K. Lye, C. Pares Pulido, S. Gurjar, L. Grosheintz Laval, M. Petrella, S. Lanthaler, K. Rutsch, R. Molinaro, A. Ruf.

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 2018-19, the main research projects carried out in the group are

- Efficient computation, mathematical and numerical analysis of the novel framework of statistical solutions for turbulent fluid flows.
- Uncertainty quantification in computational fluid dynamics.
- Machine learning, particularly Deep learning techniques for the approximation of solutions of nonlinear PDEs.
- Modeling and simulation of multiphase compressible flow.
- Bayesian inverse problems and data assimilation.
- Simulation of powder cloud avalanches.
- Computational astrophysics by using well-balanced high-resolution finite volume schemes.

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

Researchers: Prof. Dr. Markus Reiher, Dr. Alberto Baiardi, Franceso Bosia, Christoph Brunken, Dr. Leon Freitag, Stephanie Grimmel, Stefan Gugler, Tamara Husch, PD Dr. Stefan Knecht, Dr. Arseny Kovyrshin, Andrea Muolo, Adrian Mühlbach, Jan-Grimo Sobez, Dr. Jan Unsleber, Vera von Burg, 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 calculation as well new insight in the definition of electron-correlation energy within 4-component atomic and molecular calculations.

Tackling the so-called 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 in turn opens up for finding a controlled way to systematically improve these methods. We also developed a new computational software package which implements the quantum chemical DMRG algorithm in an efficient matrix-product operator formalism. One of the key challenges of quantum-chemical multi-configuration 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 set-up 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 and kinetic simulations.

References to research papers are given in Chapter 7.

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

Researchers: Wei Fang, Eric Heller, Andrea Lidberg, Jonathan Mannouch, Jeremy 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. We have recently employed machine learning techniques to reduce the number of these evaluations necessary without making any compromise to the efficiency.

Our current projects are centred around the development of theories for describing quantum tunnelling, nonadiabatic chemical reactions, photoexcited dynamics, and vibronic spectroscopy. We have a particular interest in scaling up our approaches to study dynamics of the condensed phase including reactions in liquids.

As these theories are newly developed, the algorithms we use are not yet fully optimized and there will be room for improvement in the computational efficiency. Projects for CSE Master's students could involve developing faster numerical algorithms or for improving the machine learning methodology. With these improvements in efficiency, the student would then be able to study larger and more complex molecules, which are out of reach by our current approach. This would give an excellent project for an interested CSE student to bring techniques studied in their course into the field of theoretical chemistry.

Institute/Group: Laboratory of Physical Chemistry, Computational Chemistry Group, Group of Prof. Sereina Riniker

Researchers: Annick Renevey, Dominik Sidler, Patrick Bleiziffer, Shuzhe Wang, Lennard Böselt, Benjamin Schroeder, Thomas Stadelmann, Gregor Weiss, Carmen Desposito, Gerhard König

Description: The research of the group is centered on the development of methods and software for classical molecular dynamics simulations and cheminformatics, and their application to gain insights into challenging biological and chemical questions.

To enhance sampling efficiency in molecular dynamics (MD) simulations, neighboring atoms can be grouped into so-called coarse-grained (CG) beads, which reduces the number of particles in the system and results in a smoother potential-energy surface. Coarse-graining leads, however, to a loss in information. Hybrid approaches, which combine an atomistic (AT) of the protein with a CG description of the solvent, allow us to lower the computational cost but retain accuracy in the region of interest. We have tested our hybrid scheme in a large-scale benchmarking on 23 proteins and found that a small but consistent increase of intra-molecular hydrogen bonds occurs for the proteins. This can be circumvented by introducing a AT solvent layer around charged side chains.

A major application area of the group is the investigation of the conformational behavior of cyclic peptides in order to improve our understanding of their passive membrane permeability. Cyclization and selected backbone N-methylations are found to be often necessary but not sufficient conditions for peptidic drugs to have a good bioavailability. Thus, the design of cyclic peptides with good passive membrane permeability and good solubility remains a challenge. For this, we have developed a workflow to construct kinetic models based on multi-microsecond MD data of the peptides in chloroform and water. By looking at "permeability cliffs", i.e. pairs or series of peptides with small structural variation but large changes in the permeability we were able to establish the importance of the population of the membrane-permeable conformation in water as well as the time scales of the conformational interconversion processes.

The prediction of conformational ensembles of molecules is also important for spectroscopy. Using vibrational circular dichroism (VCD) spectroscopy, the absolute configuration of chiral molecules can be determined in solution, making it an attractive alternative to X-ray crystallography. The interpretation of experimental VCD spectrum and thus the assignment of the absolute configuration rely on quantum-mechanical (QM) calculations. While such calculations are straightforward for rigid molecules with a single conformation, the need to estimate the correct conformational ensemble and energy landscape to obtain the appropriate theoretical spectra poses significant challenges for flexible molecules. In this work, we present the development of a VCD spectra alignment (VSA) algorithm to compare theoretical and experimental VCD spectra. The approach considers a spectrum as a sequence of peaks with associated intensities such that a Needleman-Wunsch type algorithm can be used to align the spectra, followed by a quantitative measure of the resulting alignment. The VSA algorithm determines which enantiomer is more likely to reproduce the experimental spectrum and thus allows the correct assignment of the absolute stereochemistry. The VSA algorithm was applied successfully to determine the absolute chirality of highly flexible molecules, including commercial drug substances.

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

Researchers: Nikolina Ban, Roman Brogli, Christophe Charpilloz Marie-Estelle Demory, Doris Folini, Christoph Heim, Laureline Hentgen, Adel Imamovic, David Leutwyler, Davide Panosetti, Daniel Regenass, Christoph Schär, Linda Schlemmer, Matthias Schwarz, Silje Sørland, Christian Steger, Jesus Vergara, Martin Wild, Christian Zeman.

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 at resolutions between 500 m and 50 km. The work includes regional climate scenario simulations covering decadal to centennial time periods, as well as case and process studies using shorter simulations. Recent work is addressing the generation, validation and analysis of Euro-CORDEX model scenarios (http://www.cordex.org/), investigations of the amplified Mediterranean drying and warming, analysis and projections of heavy precipitation events and snow cover in high-resolution simulations, and research about the Atlantic cloud cover.

The main thrust of recent work is the further development and exploitation of a high-resolution climate modeling capability at horizontal resolutions of 2 km. 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). We are among the first groups that are using a GPU version of the COSMO model for this purpose (see https://crclim.ch). This has enabled us to produce 10-year long simulations over the European continent at such a high resolutions, covering current and future climatic conditions. 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. In addition to Europe, this work is also addressing cloud cover in the tropical Atlantic, which is a key feedback of climate change.

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.

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

Title: Sparse space-time discontinuous Galerkin method for the acoustic wave equation in polygons.

Researchers: Pratyuksh Bansal[1], Andrea Moiola[2], Ilaria Perugia[3], Christoph Schwab[1]

Institutes: [1]Seminar for Applied Mathematics, ETH Zürich;
[2]University of Pavia, Italy; [3]University of Vienna, Austria.

Description:

Acoustic and linear elastic wave propagation phenomena observed in nature can be modelled by the linear, second-order, hyperbolic partial differential equation (PDE):

$$\partial_{tt}\mathbf{u}(\mathbf{x},t) - \mathcal{A}[\mathbf{u}](\mathbf{x},t) = \mathbf{f}(\mathbf{x},t), \quad \forall (\mathbf{x},t) \in Q := \mathcal{D} \times (0,T), \tag{1}$$

called the *Wave equation*, where $\mathcal{D} \subset \mathbb{R}^d$ is a bounded spatial domain and T is the time horizon, for $d \in \{1,2,3\}$. Initial and boundary conditions are also supplied. In equation 1, $\mathbf{u} \in \mathbb{R}^m$ represents the unknown solution, the operator $\mathcal{A}$, defined as

$$\mathcal{A} = \sum_{j,j'=1}^{d} \partial_{j'} A_{j,j'} \partial_j, \quad A_{j,j'} \in \mathbb{R}^{m\times m}, \tag{2}$$

is elliptic and the source $\mathbf{f} \in \mathbb{R}^m$ is specified, for $m \in \mathbb{N}$. In general, as a closed form solution to the wave equation is not available, numerical methods are widely used to compute an approximate solution, for example - continuous and discontinuous Galerkin finite element methods (FEM) [7, 6, 2].

It is well known by now that the presence of non-convex corners in a 2D polygon domain may lead to singularities in the solution of the wave equation. These singularities can be resolved using meshes with appropriate local refinement near the corners, [5]. We propose a novel non-Trefftz space-time discontinuous Galerkin method for the acoustic wave equation, based on the previous work of some of the authors [4], which yields *optimal* asymptotic rates of convergence with these locally refined meshes in polygons. It is *unconditionally stable*, thus, no restriction needs to be imposed on the size of the space-time cells. We prove a priori error estimates for the proposed method.

Use of hierarchies of locally, corner-refined meshes in the spatial, polygonal domain (e.g. by bisection-tree refinement [3]) and corresponding adapted multi-level time-stepping allows to apply the combination formula [1] to approximate the wave propagation in polygons in time-domain at work vs. accuracy scaling as one elliptic solve on the finest spatial grid. Our numerical experiments confirm the theory.

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

Researchers: Fernando Henríquez
Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

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) [2]. 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 [3, 4, 5]. However, to our knowledge, no work in this subject has been done in the context of BIOs and BIEs for acoustic scattering.

Furthermore, this abstract result allow us to use high–order Quasi–Monte–Carlo quadrature methods [6, 7] and sparse interpolation techniques [8] 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* [9, 10, 11].

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Title: Numerical analysis of stochastic partial differential equations

Researchers: Lukas Herrmann [(1)]
Christoph Schwab [(1)]

Institute: [(1)] Seminar for Applied Mathematics
ETH Zürich

Description:

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 parametric 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 a QMC analysis, which exploits locality of supports of function 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 rigorously analyzed also in the case of unbounded parameteric input.

In the case of lognormal inputs, different representation systems are avialable that entail different consequences for the QMC weights. We analyze fast multilevel methods to sample Gaussian random inputs with possible non-stationary covariance. These methods can be incorporated in multilevel QMC algorithms for PDEs with lognormal inputs, where the underlying Gaussian random input is non-stationary.

Measured data of a PDE model may need to be assimilated to a certain quantity of interest. We treat this task in the framework of Bayesian estimation. As we show QMC Bayesian estimation techniques can accomodate so called Besov prior function space measures, which generalized the frequently used Gaussian priors.

This research is supported by the Swiss National Science Foundation (SNSF) under grant SNF 200021_159940/1.

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Title: Multilevel Approximation of Gaussian Random Fields

Researchers: Kristin Kirchner [(1)]
Christoph Schwab [(1)]

Institute: [(1)] Seminar for Applied Mathematics
ETH Zürich.

Description:

Stochastic partial differential equations (SPDEs) are frequently used in statistics for approximating Gaussian random fields (GRFs) of Matérn type. Specifically, a Gaussian Matérn field on $\mathcal{D} = \mathbb{R}^d$ can be described as the solution u to the fractional-order SPDE

$$\left(\kappa^2 - \Delta\right)^{\beta} (\tau u(\mathbf{x})) = \mathcal{W}(\mathbf{x}), \quad \mathbf{x} \in \mathcal{D}, \tag{1}$$

where Δ denotes the Laplacian and $\mathcal{W}$ is Gaussian white noise on $\mathbb{R}^d$. This relation between Gaussian Matérn fields and SPDEs was exploited in [6] to construct Markov random field approximations of Matérn fields on bounded domains $\mathcal{D} \subsetneq \mathbb{R}^d$ if $2\beta \in \mathbb{N}$ by augmenting the differential operator $\kappa^2 - \Delta$ with Neumann boundary conditions on $\partial\mathcal{D}$ and using a finite element method for the numerical solution of the resulting problem.

Later on, the numerical solution of the stochastic fractional-order equation $L^\beta u = \mathcal{W}$ has been considered in the general framework of an elliptic operator L and white noise $\mathcal{W}$ on a separable Hilbert space H [2, 3]. Note that (1) and the (generalized) Whittle–Matérn fields, where $\kappa, \tau \colon \mathcal{D} \to \mathbb{R}$ may be spatially varying, are members of this class of equations (there: $H = L_2(\mathcal{D})$, $\mathcal{D} \subsetneq \mathbb{R}^d$). A practical numerical approximation u_h of the Gaussian solution process u which is computable for the whole parameter range $\beta > 0$ has been proposed, supported by rigorous convergence analysis for the strong mean-square error with respect to various norms [3, 4] and the weak error [2]. In addition, the method has been applied to kriging (spatial prediction) and likelihood-based inference in statistics [1].

The purpose of this project is twofold: Firstly, we have formulated multilevel algorithms to solve for the approximation introduced in [3] at a computational cost in work and memory which is essentially linear in the degrees of freedom and at a certified accuracy [5]. Since these algorithms allow not only for bounded Euclidean domains, but also for more general physical domains such as the sphere, they facilitate simulating a wide class of GRFs in (essentially) linear complexity. Secondly, we are currently investigating, how covariance matrices of GRFs can be compressed while maintaining a prescribed accuracy. More specifically, we are proving that $N \times N$ covariance matrices corresponding to generalized Whittle–Matérn GRFs can be compressed (after setting negligible entries to zero) to sparse matrices with only $\mathcal{O}(N)$ non-zero entries when considered with respect to multi-resolution bases.

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Title: Richardson extrapolation for Multi-Level Quasi-Monte Carlo Finite Element discretization of parametric elliptic PDEs.

Researchers: Joseph Dick [(1)]
Marcello Longo [(2)]
Christoph Schwab [(2)]

Institute: [(1)] School of Mathematics and Statistics
University of New South Wales, Sydney
[(2)] Seminar for Applied Mathematics
ETH Zürich

Description:

We analyze Richardson extrapolation of Quasi-Monte Carlo (QMC) integration rules to approximate expected values of quantities of interest of the solutions of a class of countably parametric elliptic PDEs. We consider the differential model problem of [4] that, to mention one example, arises from the diffusion in uncertain heterogeneous media.

The uncertainty lies in the diffusion coefficient, that takes an expansion such as the Karhunen-Loève (KL) or wavelet expansions. A set of positive weights models the varying importance of the different uncertain parameters. The key idea to treat globally supported expansions, as in the case of KL, is to extend the Richardson extrapolation of polynomial lattice rules introduced in [1] to smoothness and order-dependent (SPOD) weights, introduced in [2]. In this work, we adapt this methodology to construct a set of QMC sampling points with a fast component-by-component construction, cf. [3]. Moreover, thanks to an Euler-McLaurin formula, we obtain higher order QMC rules by Richardson extrapolation.

Next, we study the convergence of the combined higher order QMC FE approximation to the exact solution, exploiting smooth dependence of the solution on the parameters. Both the order of convergence and the underlying constant result to be independent of the parametric dimension of the problem. The analysis is extended to Multi-Level discretization to reduce further the computational cost. Finally, we perform numerical experiments to confirm the theoretical convergence rates.

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Title: Quantized tensor approximations for problems with point singularities in $\mathbb{R}^3$

Researchers: Carlo Marcati
Maxim Rakhuba
Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Functions that exhibit point singularities in $\mathbb{R}^3$ arise in a variety of scientific applications: nonlinear Schrödinger equations, Hartree-Fock and density functional theory equations, continuum models of point defects to name but a few. Due to the presence of singularities, approximating such functions can be computationally challenging.

In this project, we are concerned with the approximation of such functions using tensor-structured representations. In particular, we approximate, using quantized tensor decompositions, three-dimensional arrays of coefficients associated with the finite element projection of functions over basis functions. Here, *quantization* refers to the reshaping of an array of coefficients of size $2^\ell \times 2^\ell \times 2^\ell$ into a multidimensional array of size $2 \times \ldots \times 2$. The application of tensor decompositions (e.g., the Tensor-Train decomposition, which leads to the QTT—quantized tensor train decomposition) to such an array can lead to a reduction in complexity and number of parameters.

The main result we obtain [1] is that quantized, tensor-structured approximations of functions with isolated point singularities converge exponentially, i.e., admit tensor ranks bounded polylogarithmically with respect to the accuracy $\epsilon \in (0, 1)$ of the approximation, measured in the Sobolev space H^1. This leads to the overall exponential convergence of the tensor-structured approximation with respect to the effective number of parameters of the tensor decomposition. Having this a priori knowledge, allows for the application of tensor-structured algorithms that avoid working with full arrays of coefficients, and thus significantly reduces complexity of computations.

We emphasize the fact that we do not need to know a priori the type and exact location of the singularity of the solution to solve PDEs in quantized tensor-structured formats. The nonlinear structure of the decomposition allows for an "automatic" adaptation of the tensor compressed representation to the regularity of the function.

Note, however, that due to the extremely refined underlying virtual meshes, finite element discretization matrices of certain PDEs can become severely ill-conditioned. Therefore, in order to overcome the effect of ill-conditioning and to accurately solve arising equations, particular attention has to be devoted to technical details of the computation [2].

The work was parially supported by ETH Grant ETH-44 17-1.

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Title: Weighted analytic regularity for nonlinear problems in polygons

Researchers: Carlo Marcati
Christoph Schwab

Institute: Seminar for Applied Mathematics
ETH Zürich

Description:

Solutions to partial differential equations (PDEs) set in polygonal domains have low regularity in classical Sobolev spaces, in particular if the domain is not convex. This has led to the development, in the last fifty years, of the analysis of regularity of PDEs in weighted Sobolev spaces.

We are interested in the derivation of analytic-type regularity results, and to their consequences for numerical approximation. While the linear case has been thoroughly analyzed, less results are available for nonlinear problems. We have therefore considered, in [1], the regularity of solutions to the Navier-Stokes equation in polygonal domains. We proved, for the steady-state, incompressible equation with analytic right hand side, that the solution is analytic in weighted Sobolev spaces.

Mathematical regularity results on the solutions of the Navier-Stokes equations have immediate consequences in a wide range of applications, from aerodynamics to hemodynamics. The precise mathematical characterization of solution regularity in function spaces of Sobolev or Besov type is essential in the analysis of numerical schemes for the approximate solution of these equations. Analytic regularity in weighted Sobolev spaces implies, among others, exponential convergence of *hp* finite element and spectral element methods. In addition, the technique we use in proving these analytic-type estimates in polygons can be seen as the basis for the proof of analytic regularity in three dimensional polyhedra.

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[1] Carlo Marcati and Christoph Schwab, Analytic regularity for the Navier-Stokes equations in polygons, *Tech. Report 2019-12, Seminar for Applied Mathematics, ETH Zürich, Switzerland*, 2019.

Title: Exponential ReLU DNN expression of analytic and Gevrey regular functions on intervals, analytic and radially symmetric functions in high dimension

Researchers: Joost A. A. Opschoor [(1)]
Philipp C. Petersen [(2)]
Christoph Schwab [(1)]
Jakob Zech [(3)]

Institute: [(1)] Seminar for Applied Mathematics
ETH Zürich
[(2)] Faculty of Mathematics
University of Vienna
[(3)] Department of Aeronautics and Astronautics
MIT

Description:

In [4], we establish approximation rate bounds for emulations of real-valued functions on intervals by deep neural networks (DNNs for short). The approximation results are given for DNNs based on the ReLU activation function. The approximation error is measured with respect to Sobolev norms. The proofs build on the approximation of (piecewise) polynomials by ReLU networks, based on the ReLU DNN approximation of the multiplication operator introduced in [5]. It is shown that ReLU DNNs allow for essentially the same approximation rates as nonlinear, variable-order, free-knot (or so-called "*hp*-adaptive") spline approximations and spectral approximations, for a wide range of Sobolev and Besov spaces. In particular, exponential convergence rates in terms of the DNN size for piecewise Gevrey functions with point singularities are established. Combined with recent results on ReLU DNN approximation of rational, oscillatory, and high-dimensional functions, this corroborates that continuous, piecewise affine ReLU DNNs afford algebraic and exponential convergence rate bounds which are comparable to "best in class" schemes for several important function classes of high and infinite smoothness. Using composition of DNNs, we also prove that radial-like functions obtained as compositions of the above with the Euclidean norm and, possibly, anisotropic affine changes of coordinates can be emulated at exponential rate without the curse of dimensionality.

In [3], we consider the approximation of analytic maps $u : [-1, 1]^d \to \mathbb{R}$ by deep ReLU neural networks, for a possibly large input dimension $d \in \mathbb{N}$. As in previous work [2], we assume quantitative control of the domain of holomorphy of u. In [3], we assume that u admits a holomorphic extension to a Bernstein polyellipse $\mathcal{E}_{\rho_1} \times \ldots \times \mathcal{E}_{\rho_d} \subset \mathbb{C}^d$ with semiaxis sums $\rho_i > 1$, containing $[-1, 1]^d$. This assumption is not restrictive, as such $\rho_i > 1$ exist for all analytic maps $u : [-1, 1]^d \to \mathbb{R}$. We establish exponential convergence in terms of the neural network size N, as the error in Lipschitz norm $W^{1,\infty}([-1, 1]^d)$ is

shown to decay as $O(\exp(-bN^{1/(d+1)}))$ for a constant $b > 0$ determined by $\{\rho_j\}_{j=1}^d$. In addition, we discuss deep neural networks with a so-called "rectified power unit" (RePU) activation function, $x \mapsto \max\{x, 0\}^r$ for $x \in \mathbb{R}$, $r \in \mathbb{N}$, $r \geq 2$. RePU networks can exactly emulate polynomials ([1]), and can therefore approximate u with convergence of the order $O(\exp(-cN^{1/d}))$ for $c > 0$ depending on $\{\rho_j\}_{j=1}^d$.

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6

High-performance Hardware

Information Technology Services

The IT Services of ETH are currently operating two large Linux clusters, **Euler** in Lugano and **Leonhard** in Zurich. Both are named after Swiss mathematician Leonhard Euler.

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.

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 consisted of 448 compute nodes (HP BL460c Gen8), each equipped with 24 cores (two 12-core Intel Xeon E5-2697v2) and between 64 and 256 GB of memory. All compute nodes were 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.).

Euler I was decommissioned at the end of 2018 to make room for Euler V (see details below).

A second phase (Euler II) was installed in 2015. It consists of 768 compute nodes (HP BL460c Gen9), each equipped with 24 cores (two 12-core Intel Xeon E5-2680v3) and between 64 and 512 GB of memory. Euler II also contains four huge-memory nodes with 64 cores (four 16-core Intel Xeon E7-8867v3) 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 (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.

A fourth phase (Euler IV) was installed at the beginning of 2018. It consists of 288 compute nodes (HPE XL230k Gen10), each equipped with 36 cores (two Intel Xeon Gold 6150) and 192 GB of memory. These nodes are connected together using a new 100 Gb/s InfiniBand EDR network and to rest of Euler via 10G/40G Ethernet.

A fifth phase (Euler V) was installed at the end of 2018. It consists of 352 compute nodes (HPE BL460c Gen10), each equipped with 24 cores (two 12-core Intel Xeon Gold 5118) and 96 GB of memory. These nodes re-use the InfiniBand and Ethernet networks of Euler I. At

the same time, 5 new huge-memory nodes were added to Euler, each equipped with 48 cores (two 24-core AMD Epyc 7451) and 2048 GB of memory.

Euler contains two storage systems: a 1.8 PB Lustre parallel file system (DDN ES14KX) for scratch and medium-term storage; and a 1.2 PB NAS (NetApp) for home directories, applications and long-term project storage.

Leonhard

Leonhard was originally divided into two fully independent clusters with their own networks and storage systems: Leonhard **Open** for applications dealing with open research data, and Leonhard **Med** for applications dealing with confidential bio-medical data. Both clusters are based on the same hardware components and use the same software stack (operating system, management tools, libraries and applications).

The first phase of Leonhard was installed at the beginning of 2017. It consists of 36 regular compute nodes (HPE XL170r Gen9), each equipped with 36 cores (two 18-core Intel Xeon E5-2697v4) and either 128 or 512 GB of memory; and 12 GPU-accelerated nodes, each equipped with 20 cores (two 10-core Intel Xeon E5-2650v4), 8 GPUs (Nvidia GTX-1080) and 256 GB of memory.

A second phase was installed between the end of 2017 and the beginning of 2018. It consists of 48 regular compute nodes (HPE XL230k Gen10), each equipped with 36 cores (two 18-core Intel Xeon Gold 6140) and either 128, 512 or 768 GB of memory; 10 GPU nodes, each with 20 cores (two 10-core Intel Xeon E5-2630v4), 8 GPUs (Nvidia GTX-1080) and 256 GB of memory; and 50 GPU nodes with the same specifications but Nvidia GTX-1080 Ti GPUs.

A third phase was installed between the end of 2018 and the first half of 2019. It consists of 5 huge-memory nodes similar to those installed in Euler; 10 GPU nodes similar to those of the 2nd phase; 20 new GPU nodes, each with 36 cores (two 18-core Intel Xeon Gold 6240), 8 GPUs (Nvidia RTX-2080 Ti) and 384 GB of memory; 4 high-end GPU systems (Nvidia DGX-1), each with 40 cores (two 20-core Intel Xeon E5-2698v4), 8 GPUs (Nvidia Tesla V100 with SXM2 interconnect) and 512 GB of memory.

Leonhard originally contained two parallel storage systems (DDN GS14K) with 2.0 PB of usable space in Leonhard Open and 1.5 PB in Leonhard Med. In the 1st half of 2019, these two systems were converted from IBM Spectrum Scale (aka GPFS) into a unified, 3.5 PB Lustre system. This conversion enables multi-tenancy on the storage side, while providing a significant performance boost.

To enable multi-tenancy on the network side, the InfiniBand network of Leonhard Open was converted to 100G Ethernet in the 1st half of 2019. Since the 48 most recent regular nodes of Leonhard (HPE XL230k Gen10) were not compatible with 100G Ethernet, they were moved to Euler and replaced with a different model (HPE XL170r Gen10). The InfiniBand network of Leonhard Med will be converted to 100G Ethernet in the 2nd half of 2019. Once this conversion is complete, Leonhard will be a true multi-tenant cluster. The old Leonhard Open and Leonhard Med will simply be two separate tenants (with different levels of security) in this new cluster.

7

Publications*

*only CSE-related articles
in refereed journals

Group of K. Boulouchos selected publications

1. G.K. Giannakopoulos, C.E. Frouzakis, P.F. Fischer, A.G. Tomboulides, K. Boulouchos, LES of the Gas-Exchange Process Inside an Internal Combustion Engine Using a High-Order Method *Flow, Turbulence and Combustion*, 198, 1–20, 2019

2. G.K. Giannakopoulos, C.E. Frouzakis, S. Mohan, A.G. Tomboulides, M. Matalon, Consumption and displacement speeds of stretched premixed flames – Theory and simulations *Combustion and Flame*, 208, 164–181, 2019 N

3. G. Xu, M. Kotzagianni, P. Kyrtatos, Y.M. Wright, K. Boulouchos Experimental and numerical investigations of the unscavenged prechamber combustion in a rapid compression and expansion machine under engine-like conditions, *Combustion and Flame*, 204, 68–84, 2019

4. M. Banholzer, W. Vera-Tudela, C. Traxinger. M. Pfitzner. Y.M. Wright. K. Boulouchos, Numerical investigation of the flow characteristics of underexpanded methane jets, Physics of Fluids, 31, 056105, 2019

Group name: Computer-assisted Applications in Medicine (CAiM), D-ITET, ETH Zurich
Group of Prof. Orcun Goksel

List of publications: Selected publications from 2018/2019

Y Gong, O Goksel: *"Weighted Mean Curvature"*, Signal Processing 164:329-339, 2019.

V Vishnevskiy, R Rau, O Goksel: *"Deep Variational Networks with Exponential Weighting for Learning Computed Tomography"*, In MICCAI: 310-318, Shenzhen, 2019.

F Ozdemir, P Fuernstahl, O Goksel: *"Learn the New, Keep the Old: Extending Pretrained Models with New Anatomy and Images"*, In MICCAI: 361-369, Granada, Spain, 2018.

A AlBahou, C Tanner, O Goksel: *"ScatGAN for Reconstruction of Ultrasound Scatterers using Generative Adversarial Networks"*, In IEEE Int Symp Biomed Imaging: 1674-7, Venice, 2019.

A Gomariz, W Li, E Ozkan, C Tanner, O Goksel: *"Siamese Networks with Location Prior for Landmark Tracking in Liver Ultrasound Sequences"*, In IEEE ISBI: 1757-1760, Venice, 2019.

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M Ciganovic, F Ozdemir, M Farshad, O Goksel: *"Deep learning techniques for bone surface delineation in ultrasound"*, In SPIE Medical Imaging: 10955-33, San Diego, 2019.

F Pean, C Tanner, C Gerber, P Fuernstahl, O Goksel: *"A comprehensive and volumetric musculoskeletal model for the dynamic simulation of the shoulder function"*, CMBBE 22, 2019.

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SJ Sanabria, MB Rominger, O Goksel: *"Speed-of-Sound Imaging Based on Reflector Delineation"*, IEEE Trans Biomedical Engineering 66(7):1949-1962, 2019.

E Ozkan O Goksel: *"Compliance Boundary Conditions for Patient-Specific Deformation Simulation Using the Finite Element Method"*, Biomed Physics & Eng Expr 4(2):025003, 2018.

CF Otesteanu, V Vishnevskiy, O Goksel: *"FEM Based Elasticity Reconstruction Using Ultrasound for Imaging Tissue Ablation"*, Int J Comp Asst Radiology Surgery 13:885-94, 2018.

SJ Sanabria, E Ozkan, MB Rominger, O Goksel: *"Spatial Domain Reconstruction for Imaging Speed-of-Sound with Pulse-Echo Ultrasound: Simulation and In-Vivo Study"*, Physics in Medicine and Biology 63:215015, 2018.

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A Gomariz, et al: *"Quantitative spatial analysis of hematopoiesis-regulating stromal cells in the bone marrow microenvironment by multiscale 3D microscopy"*, Nature Comm 9(2532), 2018.

A complete list of publications can be found at: www.caim.ee.ethz.ch/~ogoksel

Group R. Hiptmair: Publications 2017/2018

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C. Winkelmann, R. Casagrande, R. Hiptmair, P.-T. Müller, J. Ostrowski and T. W. Schläpfer (2018), Electro-thermal simulations with skin-layers and contacts, in *Scientific computing in electrical engineering*, Vol. 28 of *Math. Ind.*, Springer, Cham, pp. 43–52.

Institute/Group: Institute of Virtual Manufacturing

List of publications:

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Neuhauser, F.M.; Bachmann, G.; Hora, P.: Surface defect classification and detection on extruded aluminum profiles using convolutional neural networks. *International Journal of Material Forming 2019*

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

List of publications:

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The conveyor belt umbrella sampling (CBUS) scheme: Principle and application to the calculation of the absolute binding binding free energies of alkali cations to crown ethers.
J. Chem. Theory Comput., submitted (2019)

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 2018 and July 2019

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2. Choi, K., A. Droudian, R.M. Wyss, K.-P. Schlichting, and H.G. Park, Multifunctional wafer-scale graphene membranes for fast ultrafiltration and high permeation gas separation. Science Advances, 2018. **4**(11): p. eaau0476.
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4. Delgoshaie, A.H., P.W. Glynn, P. Jenny, and H.A. Tchelepi, A Flexible Temporal Velocity Model for Fast Contaminant Transport Simulations in Porous Media. Water Resources Research, 2018. **54**(10): p. 8500-8513.
5. Delgoshaie, A.H., P.W. Glynn, P. Jenny, and H.A. Tchelepi, The stochastic counterpart of conservation laws with heterogeneous conductivity fields: Application to deterministic problems and uncertainty quantification. Journal of Computational Physics: X, 2019. **2**: p. 100005.
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18. Meyer, D.W., A simple velocity random-walk model for macrodispersion in mildly to highly heterogeneous subsurface formations. Advances in Water Resources, 2018. **121**: p. 57-67.
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Computational Polymer Physics, D-MATL, ETH Zurich

Martin Kröger

www.complexfluids.ethz.ch

List of peer-reviewed publications

Z. Shen, H. Ye, M. Kröger, Y. Li,
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