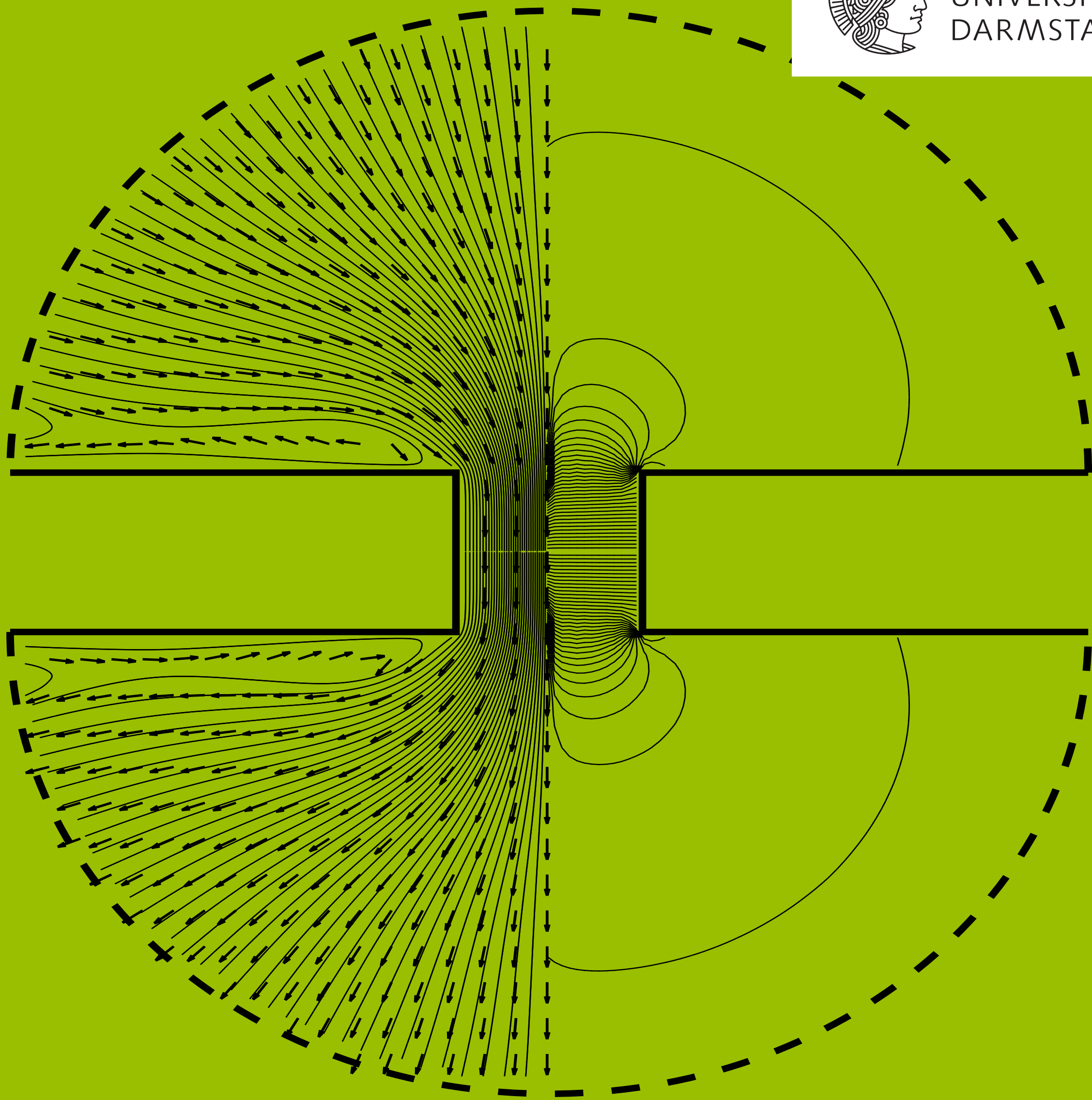
Biannual Report

Department of Mathematics
Research Group Numerical Analysis and Scientific Computing
2017 and 2018



TECHNISCHE UNIVERSITÄT DARMSTADT

On the cover page the velocity and pressure profile in the vicinity of one opening of a perforated wall within a visco-acoustic model is illustrated. It is obtained in the project "Impedance conditions for visco-acoustic models" (see page 18).

General Remark

This document contains a subset of the information of the Biannual Report of the Department of Mathematics at TU Darmstadt for 2017 and 2018. It has simply been obtained by extracting all the information provided by our Research Group Numerical Analysis and Scientific Computing from the complete report. All empty chapters have been removed. This is only meant to be supplementary, because it is hard to filter out information from the complete document.

Research Group Numerical Analysis and Scientific Computing

April 2020

Contents

1 Research Group Numerical Analysis and Scientific Computing

The research focus of the group for *Numerical Analysis and Scientific Computing* lies in the development, analysis, and implementation of novel, efficient, accurate, and reliable numerical methods for the solution of complex problems of practical interest. This includes the derivation and simplification of models, their analysis, the construction of appropriate numerical schemes for their simulation, the analysis of these numerical methods, the derivation of a-posteriori error estimates, the adaptive solution, and the consideration of related optimization and inverse problems.

The long-term goal of the group is to contribute to the fundamental research topics in the area of numerical mathematics and scientific computing, but also to provide software and expertise for the tackling of specific problems in engineering and the natural sciences. The group is currently engaged in projects in various application areas, e.g., in computational medicine and biology, in simulation and optimal control of gas and water supply networks, in inverse problems for fluid dynamics and non-destructive testing, in modeling and simulation of radiative transfer phenomena, in acoustic and optical tomography, in multiscale modeling and numerical approximation of soft matter systems, in simulation of transient acoustic and electromagnetic phenomena, in modeling and simulation in energy science and in modeling and simulation of compressible single- and multi-phase flows.

Particular research directions in the area of numerical mathematics that are pursued along these applications are, e.g., the development and numerical analysis of novel discretization schemes, the design and analysis of *a posteriori* error estimates, the uncertainty quantification for problems with variable inputs, and the structure preserving model reduction as well as the design and the analysis of model-adaptive schemes.

The research group *Numerical Analysis and Scientific Computing* has been and is engaged among others in various coordinated research activities, e.g., in the Graduate Schools (Excellence Initiative) GSC 233 Computational Engineering and GSC 1070 Energy Science and Engineering, the Transregional Collaborative Research Centers (Transregio/SFB) TRR 154 Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks and TRR 146 Multiscale Simulation Methods for Soft Matter Systems, the International Research Training Group IGK 1529 Mathematical Fluid Dynamics, the German Research Foundation (DFG) Priority Program SPP 1748 Reliable Simulation Techniques in Solid Mechanics — Development of Non-Standard Discretisation Methods, Mechanical and Mathematical Analysis, and the Funding Program "Future-oriented Technologies and Concepts for an Energy-efficient and Resource-saving Water Management - ERWAS" of the Federal Ministry of Education and Research (BMBF) (`http://www.bmbf.nawam-erwas.de/en`). In addition, the group has various industry partners, including cooperations with Robert Bosch GmbH Stuttgart, BASF Ludwigshafen, and Infineon München.

Members of the research group

Professors

Herbert Egger, Christoph Erath, Jan Giesselmann, Martin Kiehl, Jens Lang

Retired professors

Peter Spellucci

Postdocs

Jürgen Dölz, Pia Domschke, Sofia Eriksson, Alf Gerisch, Michelle Lass, Hadi Minbashian, Christopher Müller, Kersten Schmidt, Adrien Semin, Sebastian Ullmann, Mirjam Walloth

Research Associates

Anke Böttcher, David Frenzel, Hrishikesh Joshi, Thomas Kugler, Axel Lukassen, Pascal Mindt, Bogdan Radu, Moritz Schneider, Lucas Schöbel-Kröhn, Robert Schorr, Tobias Seitz, Christopher Spannring, Philipp Steinbach, Elisa Strauch, Zhen Sun, Gabriel Teschner, Lisa Wagner, Dimitrios Zacharenakis

Secretaries

Elke Dehnert, Dagmar Thies

Projects of the research group

Project: Numerical approximation of phase field models in elastic bodies

Phase field transformations occur in different nature contexts. Phases can, for instance, differ in aggregate state or material properties. In this project we study partial differential equations describing phase transitions in solid elastic bodies. We show that solutions of the phase field equations, namely the Allen-Cahn and the hybrid model, are connected to an associated free energy. The idea of the gradient flow is to describe the time derivative of the order parameter indicating the particular phase as the gradient flow of the free energy. Convergence and asymptotic stability of numerical schemes are investigated.

Contact: Anke Böttcher, Herbert Egger

References

[1] A. Böttcher and H. Egger. Energy stable discretization of Allen-Cahn type problems modeling the motion of phase boundaries. *arXiv:1703.02778*, 2017.

Project: Adaptive dynamical multiscale methods

The aim of this project is the development of an integrated, dynamic multiscale approach for the numerical solution of the compressible instationary Euler equations on network structures. These methods will be used for the description of the stochastic behavior of practically relevant outputs relative to randomized parameters in hyperbolic differential equations (quantification of uncertainty), the construction of reduced order models and an adaptive multilevel optimization for gas networks.
In the first project period, modelling aspects and the development of adaptive discretizations were of primary importance. Adaptive spatial and temporal discretizations are controlled and combined with models from a newly established model hierarchy such that an efficient simulation of gas networks over the whole time horizon relative to a prescribed tolerance becomes available.
In the second project period, the influence of dynamic market fluctuations, which can be described by randomized initial and boundary values, on objective functions and scopes for the optimal control of gas networks in the framework of an uncertainty quantification will be investigated. Therefore, adaptive stochastic collocation methods with multilevel-like strategies for the reduction of the variance will be used. The integrated application of multilevel methods in space, time, and model as well as stochastic components lead to a reduction of computing time if resolution hierarchies in the corresponding approximations (space, time, model, stochastics) are employed. The stochastic collocation is realised by means of anisotropic sparse Smolyak grids. The inherent sampling strategy allows for the use of reduced, structure-preserving models in order to further reduce the computing time even perspectively for large scaled networks. It is the goal to combine adaptive grid and model refinements with adaptive collocation methods to improve the multilevel methods and to achieve rigorous quality requirements for expectation and variances of solution functionals for the uncertainty quantification at reduced computing time.

Support: Project B01 within DFG TRR 154

Contact: Pascal Mindt, Elisa Strauch, Pia Domschke, Jens Lang

References

[1] P. Domschke, B. Hiller, J. Lang, and C. Tischendorf. Modellierung von Gasnetzwerken: Eine Übersicht. Preprint 2717, Fachbereich Mathematik, TU Darmstadt, 2017.

[2] J. Lang and P. Mindt. Entropy-preserving coupling conditions for one-dimensional Euler systems at junctions. *Networks & Heterogeneous Media*, 13(1):177, 2018.

[3] P. Mindt, J. Lang, and P. Domschke. Entropy-preserving coupling of hierarchical gas models. arXiv:1812.05927, 2018.

Project: Mathematical modelling and numerical methods for time-dependent PDE problems arising in mathematical biology

Biological processes like the invasion of tissue by cancer cells, the adhesion-driven reorganization of tissue, and the cascade of steps in fracture healing can be modeled as time-dependent PDEs. We develop structured-population models for the dedicated modelling of cellular surface-bound processes at the tissue scale and justify continuous non-local adhesion models from a spatial stochastic random walk. For the reliable, efficient and accurate simulation of these models, dedicated numerical schemes are required. We focus on general methods for taxis-diffusion-reaction systems and on particular schemes for the evaluation of the spatially nonlocal terms in models of cellular adhesion. In our approach, we follow the method of lines with finite volumes in space and linearly-implicit methods in time.

Partner: Mark A. J. Chaplain (University of St. Andrews, UK); Kevin J. Painter (Heriot-Watt University, Edinburgh, UK); Dumitru Trucu (University of Dundee, UK); Andreas Buttenschön (University of British Columbia, Canada); Thomas Hillen (University of Alberta, Canada)

Contact: Alf Gerisch, Pia Domschke

References

[1] A. Buttenschön, T. Hillen, A. Gerisch, and K. Painter. A space-jump derivation for non-local models of cell-cell adhesion and non-local chemotaxis. *J. Math. Biol.*, 76:429–456, 2018.

[2] P. Domschke, D. Trucu, A. Gerisch, and M. A. J. Chaplain. Structured models of cell migration incorporating molecular binding processes. *Journal of Mathematical Biology*, 75(6-7):1517–1561, 2017.

[3] A. Hodgkinson, M. A. J. Chaplain, P. Domschke, and D. Trucu. Computational approaches and analysis for a spatio-structural-temporal invasive carcinoma model. *Bulletin of Mathematical Biology*, 80(4):701–737, 2018.

Project: Adaptive refinement strategies for the simulation of gas flow in networks using a model hierarchy

A model hierarchy that is based on the one-dimensional isothermal Euler equations of fluid dynamics is used for the simulation and optimisation of natural gas flow through a pipeline network. Adaptive refinement strategies have the aim of bringing the simulation error below a prescribed tolerance while keeping the computational costs low. While spatial and temporal stepsize adaptivity is well studied in the literature, model adaptivity is a new field of research. The problem of finding an optimal refinement strategy that combines these three types of adaptivity is a generalisation of the unbounded knapsack problem. A refinement strategy that is currently used in gas flow simulation software is compared to two novel greedy-like strategies. Both a theoretical experiment and a realistic gas flow simulation show that the novel strategies significantly outperform the current refinement strategy with respect to the computational cost incurred.

Partner: Volker Mehrmann, Jeroen Stolwijk (TU Berlin)

Support: DFG TRR 154

Contact: Pia Domschke, Jens Lang

References

[1] P. Domschke, A. Dua, J. J. Stolwijk, J. Lang, and V. Mehrmann. Adaptive refinement strategies for the simulation of gas flow in networks using a model hierarchy. *Electronic Transactions on Numerical Analysis*, 48:97–113, 2018.

Project: Optimal control for instationary gas transport

The stable operation of gas networks requires the modeling, simulation, and optimization of gas transport on networks. In this project, we investigate the optimal control of instationary gas transport on pipeline networks with continuous and discrete controls. The mathematical formulation of such problems leads to PDE-constrained optimization problems with control and state-constraints and discrete decisions. For the numerical solution, we consider continuous minimization algorithms based on gradient information leading to locally optimal controls, as well as a first-discretize-then-optimize approach resulting in mixed integer nonlinear programs whose solutions are global optima for the considered problem.

Partner: Robert Burlacu, Alexander Martin, Matthias Sirvent, Lars Schewe (Universität Erlangen-Nürnberg); Martin Groß (University of Waterloo, Canada); Martin Skutella (TU Berlin); Marc Pfetsch, Winnifried Wollner (AG Optimierung, TU Darmstadt)

Support: DFG TRR 154

Contact: Herbert Egger

References

[1] R. Burlacu, H. Egger, M. Groß, A. Martin, M. E. Pfetsch, L. Schewe, M. Sirvent, and M. Skutella. Maximizing the storage capacity of gas networks: a global MINLP approach. *Optimization and Engineering*, pages 1–31, 2018.

[2] H. Egger, T. Kugler, and W. Wollner. Numerical optimal control of instationary gas transport with control and state constraints. *TRR154 Report No. 214*, 2017.

Project: Analysis and numerical solution of coupled volume-surface reaction-diffusion systems with application to cell biology

We consider the numerical solution of coupled volume-surface reaction-diffusion systems having a detailed balance equilibrium. Based on the conservation of mass, an appropriate quadratic entropy functional is identified and an entropy-entropy dissipation inequality is proven. This allows us to show exponential convergence to equilibrium by the entropy method. We then investigate the discretization of the system by a finite element method and an implicit time stepping scheme including the domain approximation by polyhedral meshes. Mass conservation and exponential convergence to equilibrium are established on the discrete level by arguments similar to those on the continuous level, and we obtain estimates of optimal order for the discretization error which hold uniformly in time. Some numerical tests are presented to illustrate these theoretical results. The analysis and the numerical approximation are discussed in detail for a simple model problem. The basic arguments, however, apply also in a more general context. This is demonstrated by the investigation of a particular volume-surface reaction-diffusion system arising as a mathematical model for asymmetric stem cell division.

Partner: Klemens Fellner, Bao Quoc Tang (TU Graz); Jan-Frederik Pietschmann (TU Chemnitz)

Support: DFG IGK 1529

Contact: Herbert Egger

References

[1] H. Egger, K. Fellner, J.-F. Pietschmann, and B. Q. Tang. A finite element method for volume-surface reaction-diffusion systems. *Appl. Math. Comput.*, 336:351–367, 2018.

Project: Energy stable discretization for compressible flow on networks

The transport of gas in pipeline networks is described by the Euler equations of gas dynamics. The friction at the pipe walls leads to a strong damping of oscillations and exponential stability of the evolution. The goal of this project is to devise and analyze new numerical schemes that preserve these properties during the discretization process.

Support: DFG TRR 154

Contact: Herbert Egger

References

[1] H. Egger. A robust conservative mixed finite element method for isentropic compressible flow on pipe networks. *SIAM J. Sci. Comput.*, 40:A108–A129, 2017.

[2] H. Egger, T. Kugler, and B. Liljegren-Sailer. Stability preserving approximations of a semilinear hyperbolic gas transport model. arXiv:1812.03726, 2018.

[3] H. Egger, T. Kugler, and V. Shashkov. An inexact Petrov-Galerkin approximation for gas transport in pipeline networks. arXiv:1811.05215, 2018.

Project: Structure preserving approximation of nonlinear evolution problems

Nonlinear evolution problems are often governed by energy conservation or dissipation which describe basic principles of thermodynamics. The goal of this project is to devise numerical discretization strategies that allow to guarantee corresponding properties after discretization in space and time.

Partner: Volker Mehrmann, Riccardo Morandin (TU Berlin)

Support: DFG TRR 154, GSC 233

Contact: Herbert Egger, Vsevolod Shashkov

References

[1] H. Egger. Energy stable Galerkin approximation of Hamiltonian and gradient systems. arXiv:1812.04253, 2018.

[2] H. Egger. Structure preserving approximation of dissipative evolution problems. arXiv:1804.08648, 2018.

Project: Spinodal decomposition of polymer-solvent systems

The goal of the project is to obtain stable and consistent descriptions of flow dynamics on multiple scales in a class of systems exhibiting highly complex non-equilibrium dynamics, namely phase-separating polymer solutions. This is done by combining (i) the derivation, analysis, and simulation of macroscopic two-fluid models describing the dynamics of viscoelastic phase separation, (ii) the mesoscopic simulation of viscoelastic phase separation by extension of a coupled Lattice-Boltzmann / Molecular Dynamics method, and (iii) the calibration of the macroscopic models to results from mesoscopic simulations by means of parameter estimation and inverse problems methodology.

Partner: Mária Lukácová-Medvidová, Paul Strasser (Universität Mainz); Burkhard Dünweg, Dominic Spiller (Max-Planck-Institut für Polymerforschung Mainz)

Support: DFG TRR 146

Contact: Herbert Egger, Oliver Habrich

Project: Numerical methods for radiative transfer

Radiative transfer is modelled by the linear Boltzmann equation, i.e., an integro-partial differential equation in 7 dimensional phase space. In this project, we investigate efficient numerical methods for the simulation of radiative transfer phenomena, e.g., the propagation of heavy ions through biological tissue or the transfer of heat by radiation.

Partner: Matthias Schlottbom (University of Twente, The Netherlands); Simon Arridge, Samuel Powell (UCL London, UK)

Support: DFG GSC 233

Contact: Herbert Egger

References

[1] H. Egger and M. Schlottbom. A perfectly matched layer approach for radiative transfer in highly scattering regimes. arXiv:1802.08305, 2018.

Project: Optimal convergence rates for adaptive algorithms

We analyze different adaptive mesh refinement strategies and prove optimal convergence rates. In particular, we are interested in optimal convergence rates for finite volume schemes for general elliptic PDEs. Furthermore, we consider the finite element scheme with an SUPG stabilisation for convection dominated problems and prove convergence with optimal rates of an adaptive algorithm. The third part of this project investigates several a posteriori estimates of $h - h/2$ type for a finite element discretization with an analysis of the adaptive strategy with respect to optimal convergence rates.

Partner: Dirk Praetorius (TU Wien)

Contact: Christoph Erath

References

[1] C. Erath, G. Gantner, and D. Praetorius. Optimal convergence behavior of adaptive FEM driven by simple $(h-h/2)$-type error estimators. arXiv:1805.00715, 2018.

[2] C. Erath and D. Praetorius. Céa-type quasi-optimality and convergence rates for (adaptive) vertex-centered FVM. In *Finite Volumes for Complex Applications VIII - Hyperbolic, Elliptic and Parabolic Problems*, volume 199, pages 210–223. Springer International Publishing, 2017.

[3] C. Erath and D. Praetorius. Adaptive vertex-centered finite volume methods for general second-order linear elliptic PDEs. *IMA J. Numer. Anal.*, published online, 2018.

[4] C. Erath and D. Praetorius. Optimal adaptivity for the SUPG finite element method. arXiv:1806.11000, 2018.

Project: WENO schemes in optimal control of nonlinear hyperbolic conservation laws

Many problems in natural science can be modeled with hyperbolic differential equations such as traffic modeling and fluid mechanics. The main difficulty of these equations is that solutions may become discontinuous even if the initial data and boundary conditions are smooth. In many applications we are interested in optimizing a given objective through optimal control. The main issue is that the control-to-state mapping is not differentiable with respect to common variational concepts. However, it can be shown that the control-to-state mapping is shift-differentiable. This concept implies the Fréchet-differentiability of objective functionals and yields adjoint-based formulas for their derivative. We investigate the numerical treatment of these optimal control problems by using weighted essentially non-oscillatory (WENO) schemes. We derive the discretization of the adjoint scheme by the first-optimize-then discretize approach. Furthermore, the consistency of the adjoint discretization is analyzed and numerical examples are presented.

Partner: Stefan Ulbrich (TU Darmstadt)

Support: Graduate School of Computational Engineering, DFG

Contact: David Frenzel, Jens Lang

Project: Multiscale structure-functional modeling of musculoskeletal mineralized tissues

Musculoskeletal mineralized tissues (MMTs) are natural examples of materials that show unique and highly variable combinations of stiffness and strength. One of the striking features of MMTs is that the diversity of elastic functions is achieved by only one common building unit, that is the mineralized collagen fibril, but with variable structural arrangements at several levels of hierarchical organization. A profound understanding of the structure-function relations in MMTs requires both experimental assessment of heterogeneous elastic and structural parameters and theoretical modeling of the elastic deformation behavior. Multi-scale and multi-modal assessment of MMTs will be used to probe not only the microarchitecture, but also anisotropic linear elastic properties from the nanoscale to the macroscale. By combining experimental data obtained from MMTs at various length scales with numerical homogenization approaches in continuum mechanics, we hypothesize to gain new insight into self-assembly mechanisms, construction rules and physiological boundary conditions of MMTs.

Within this joint project, we focus on the development as well as efficient and reliable implementation of numerical homogenization techniques. Together with the groups in Berlin and Paris we devise new mathematical models in order to aid the understanding of MMTs. The experimental assessment of MMTs is performed in Berlin and with external cooperation partners.

Partner: Raimondo Penta (University of Glasgow, UK); Kay Raum (Charité-Universitätsmedizin Berlin); Quentin Grimal (Biomedical Imaging Lab, UPMC Paris, France)

Support: DFG grants GE1894/3 and Ra1380/7 within DFG SPP 1420

Contact: Alf Gerisch, Jens Lang

References

[1] A. Gerisch, R. Penta, and J. Lang, editors. *Multiscale Models in Mechano and Tumor Biology: Modeling, Homogenization, and Applications*, volume 122 of *Lecture Notes in Computational Science and Engineering*. Springer, Cham, 2018.

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Project: Cross-diffusion in models from mathematical biology

Cross-diffusion terms are nowadays widely used in reaction-diffusion equations encountered in models from mathematical biology and in various engineering applications. In this project we study the underlying model equations of such systems and investigate analytically their properties with an emphasis on pattern formation and positivity preservation. We also investigate and apply suitable numerical simulation techniques for applications from mathematical biology.

Partner: Anotida Madzvamuse (University of Sussex, UK); Raquel Barreira (Polytechnic Institute of Setubal, Portugal)

Contact: Alf Gerisch

References

[1] A. Madzvamuse, A. Gerisch, and R. Barreira. Cross-diffusion in reaction-diffusion models: analysis, numerics and applications. In P. Quintela, P. Barrali, D. Gómez, et al., editors, *Progress in Industrial Mathematics at ECMI 2016*, pages 385–392. Springer, Cham, 2017.

Project: Uncertainty quantification in hyperbolic conservation laws

We study random systems of hyperbolic conservations laws, where the initial data as well as the flux function might be random. The goal of this project is to provide a posteriori error estimates for intrusive (stochastic Galerkin) as well as non-intrusive (stochastic collocation) methods. A key aspect of this analysis is to try to distinguishing between errors caused by space-time discretization and errors caused by stochastic discretization. These error estimators are a crucial ingredient in the construction of space-time-stochastic adaptive schemes.

Partner: Fabian Meyer, Christian Rohde (Universität Stuttgart)

Contact: Jan Giesselmann

References

[1] F. Meyer, J. Giesselmann, and C. Rohde. A posteriori error analysis for random scalar conservation laws using the stochastic Galerkin method. arXiv:1709.04351, 2017.

[2] F. Meyer, J. Giesselmann, and C. Rohde. A posteriori error analysis and adaptive non-intrusive numerical schemes for systems of random conservation laws. arXiv:1902.05375, 2019.

Project: A posteriori analysis for post-processed solutions

Smoothness increasing accuracy conserving (SIAC) filters are an efficient post-processing tool for discontinuous Galerkin numerical solutions in a wide variety of problems (elliptic as well as hyperbolic). The SIAC methodology is based on mollifying the numerical solution in such a way that the superconvergence-properties inherent in Galerkin methods lead to a super-convergent post-processed solution. Classically, SIAC post-processors have been employed for the construction of error indicators, i.e. the difference between the numerical solution and its post-processed version was used as an approximation of the discretization error. However, since the post-processed solution is in many cases much more accurate than the original numerical solution it seems desirable to construct meshes which are optimal with respect to the error of the post-processed solution. Our goal is to enable the construction of such meshes by providing reliable and locally efficient error estimators for post-processed solutions for elliptic problems. It turns out that classical, residual-based techniques for deriving error estimators lead to inefficient estimators for post-processed solutions. This is due to the fact that the post-processed solutions do not satisfy Galerkin orthogonality. Thus, we propose a simple and cheap modification of the post-processing which re-establishes Galerkin-orthogonality and reduces the error of the post-processed solution.

Partner: Andreas Dedner (University of Warwick); Jennifer K. Ryan (University of East Anglia); Tristan Pryer (University of Reading)

Contact: Jan Giesselmann

Project: Robust a posteriori error estimates for compressible multiphase flows

We are interested in a posteriori error analysis of finite element schemes for a one-dimensional model problem for liquid-vapour flows in Lagrangian coordinates. This system describes the phase-boundary as a thin layer and it can be seen as a simplified version of the Euler-Korteweg model. In particular, we are interested in the link between a posteriori error estimates and stability properties of the continuous equations. For the equations at hand, there are at least two stability frameworks that are applicable: Firstly, the relative entropy and, secondly, estimates employing eigenvalues of the linearized operator. Error estimators based on the relative entropy have been derived previously but suffer from high sensitivity when the capillarity number decreases. Thus, we pursue an idea which is based on the similarity of the equations at hand and the Allen-Cahn equation. Indeed, the equations at hand can be viewed as an Hamiltonian system induced by the energy for which the Allen-Cahn equation is a gradient flow. For the Allen-Cahn equation robust estimates (with respect to capillarity) have been obtained as long as the linearized system has well behaved eigenvalues and we work on extending these results to the Hamiltonian case.

Partner: Rüdiger Müller (WIAS Berlin)

Contact: Jan Giesselmann

References

[1] S. Bartels, R. Müller, and C. Ortner. Robust a priori and a posteriori error analysis for the approximation of Allen-Cahn and Ginzburg-Landau equations past topological changes. *SIAM J. Numer. Anal.*, 49(1):110–134, 2011.

[2] J. Giesselmann and T. Pryer. Reduced relative entropy techniques for a posteriori analysis of multiphase problems in elastodynamics. *IMA J. Numer. Anal.*, 36(4):1685–1714, 2016.

Project: A posteriori analysis for hyperbolic conservation laws on networks

We are interested in gas flows on networks which are modeled as one-dimensional isothermal Euler equations. At the nodes of the network conservation of mass and continuity of enthalpy are required. The goal of this project is to provide a posteriori error estimates for Runge Kutta discontinuous Galerkin schemes by extending similar results for one-dimensional problems with periodic boundary conditions. Those results are based on Lipschitz-continuous reconstructions of the numerical solution and the relative entropy framework. The latter is a stability framework for systems of hyperbolic conservation laws which allows us to relate residuals and discretization errors. Thus, a main contribution of this work is to extend the relative entropy framework to hyperbolic balance laws on networks. It turns out the most crucial step in this endeavor is to control the relative entropy fluxes at the nodes, which can be done for certain entropy compatible coupling conditions [1].

Partner: Raul Borsche (TU Kaiserslautern)

Contact: Jan Giesselmann

References

[1] G. A. Reigstad. Numerical network models and entropy principles for isothermal junction flow. *Netw. Heterog. Media*, 9(1):65–95, 2014.

Project: Moment methods for kinetic equations

We are interested in numerical methods for the linearized Boltzmann equation. In particular, we study moment methods, i.e. a spectral approximation using Hermite polynomials in velocity space. The construction of entropy stable schemes for initial boundary value problems is not trivial but has been achieved recently. We study the convergence of these schemes, i.e. under suitable assumptions on the regularity of the exact solution, we have provided an explicit convergence rate for the Hermite approximation and have confirmed it by numerical experiments.

Partner: Neeraj Sarna, Manuel Torrilhon (RWTH Aachen)

Contact: Jan Giesselmann

References

[1] N. Sarna, J. Giesselmann, and M. Torrilhon. Convergence analysis of the Grad's Hermite approximation to the Boltzmann equation. arXiv:1809.08213, 2018.

Project: Spatial model adaptation of compressible chemically reacting flows based on a posteriori error estimates

A numerically challenging and notoriously computationally expensive application is the numerical simulation of multi-component chemically reacting flows. One reason for it being so challenging is the interaction between convection and reaction, which in many cases have different time scales. The governing equations of chemically reacting flows can be simplified by assuming chemical equilibrium and then it is possible to replace the full system with the equilibrium system on a part of the computational domain without introducing significant errors. The domain decomposition is carried out by employing a posteriori error estimates developed for hyperbolic systems of partial differential equations with stiff source terms. The error estimate, derived based on the relative entropy framework, provides a computable upper bound for the distance between the numerical solution and the exact solution. The error estimate accounts for both the modeling and the discretization error, careful control of the two allows for real-time model and mesh adaptation.

Support: DFG Gi 1131/1-1

Contact: Hrishikesh Joshi, Jan Giesselmann

References

[1] J. Giesselmann and T. Pryer. A posteriori analysis for dynamic model adaptation problems in convection dominated problems. *Math. Models Methods Appl. Sci.*, 27:2381–2432, 2017.

Project: Galerkin methods for simulation, calibration, and control of partial differential equations on networks

This project is part of the Transregional Collaborative Research Centre TRR 154 *Mathematical modelling, simulation and optimization of gas networks*, and deals with the construction and analysis of numerical methods for singularly perturbed hyperbolic problems with parabolic limit. The main goal is to devise efficient asymptotic preserving numerical schemes, which inherit basic physical principles as conservation of mass, balance of momentum, and stability of the entropy. To model the flow of a gas mixture in a network of pipes we consider the one-dimensional Euler equations with friction. Our methods are used to further calibrate the simulation models by utilizing additional measurements. Furthermore, we consider optimal control problems, where for example compressor stations are controled to reach a desired state in the network.

Partner: Björn Liljegren-Sailer, Nicole Marheineke (Universität Trier), Volker Mehrmann (TU Berlin); Nicolai Strogies (WIAS Berlin); Winnifried Wollner (AG Optimierung, TU Darmstadt)

Support: Project C04 within DFG TRR 154

Contact: Herbert Egger, Thomas Kugler

References

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[3] H. Egger, T. Kugler, B. Liljegren-Sailer, N. Marheineke, and V. Mehrmann. On structure-preserving model reduction for damped wave propagation in transport networks. *SIAM Journal on Scientific Computing*, 40:A331–A365, 2018.

[4] H. Egger, T. Kugler, and V. Shashkov. An inexact Petrov-Galerkin approximation for gas transport in pipeline networks. arXiv:1811.05215, 2018.

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[6] H. Egger, T. Kugler, and W. Wollner. Numerical optimal control of instationary gas transport with control and state constraints. *TRR154 Report No. 214*, 2017.

Project: Space-time adaptive linearly implicit peer methods for parabolic problems

In this project a linearly implicit peer method is combined with a multilevel finite element method for the discretization of parabolic partial differential equations. Following the

Rothe method it is first discretized in time and then in space. A spatial error estimator based on the hierarchical basis approach is derived. It is shown to be a reliable and efficient estimator up to some small perturbations. The efficiency index of the estimator is shown to be close to the ideal value one for two one-dimensional test problems. Finally we compare the performance of the overall method, based on second, third, and fourth order peer methods with that of some Rosenbrock methods. We conclude that the presented peer methods offer an attractive alternative to Rosenbrock methods in this context.

Contact: Jens Lang, Alf Gerisch

References

[1] D. Schröder, A. Gerisch, and J. Lang. Space-time adaptive linearly implicit peer methods for parabolic problems. *J. Comp. Appl. Math.*, 316:330–344, 2017.

Project: Fully adaptive multilevel stochastic collocation method for randomized elliptic PDEs

We propose and analyse a new adaptive multilevel stochastic collocation method for randomized elliptic PDEs. A hierarchical sequence of adaptive mesh refinements for the spatial approximation is combined with adaptive anisotropic sparse Smolyak grids in the stochastic space in such a way as to minimize computational cost. We provide a rigorous analysis for the convergence and computational complexity of the adaptive multilevel algorithm.

Partner: Robert Scheichl (Universität Heidelberg)

Contact: Jens Lang

References

[1] J. Lang and R. Scheichl. Adaptive multilevel stochastic collocation method for randomized elliptic PDEs. Technical Report Technische Universität Darmstadt, Department of Mathematics, Preprint 2718, 2017.

Project: Simulation of reactive flows by projection onto time- and space-variable quasi-steady states

The simulation of a reactive flow leads to a partial differential equation, which usually contains a large number of unknown variables. Furthermore, the time scales of the different chemical reactions cover several orders of magnitude. In addition to the size the obtained partial differential equation is also very stiff and solving the partial differential equation is very time consuming. However, the fastest chemical reactions have small timescales and eventually reach their equilibrium in a period of time shorter than the timestep of the solver. In this case we can replace these chemical reactions by an algebraic equation. This approach leads to simulation of the chemical reaction system on a lower dimensional manifold describing the partial equilibrium of the fast reactions. Though, the state of the system can differ in time and space, the reaction rates depend on the state. For this reason the manifold changes in time and space. The goal of the project is to develop a model, which dynamically switches in space and time between the description of the chemical reactions via the kinetic model and the partial thermodynamic equilibrium.

Contact: Axel Lukassen, Martin Kiehl

References

[1] A. Lukassen and M. Kiehl. Reduction of round-off errors in chemical kinetics. *Combustion Theory and Modelling*, 21(2):183–204, 2017.

[2] A. A. Lukassen. *Simulation of chemical systems with fast chemistry*. PhD thesis, TU Darmstadt, 2018.

Project: Data assimilation for compressible flows

In this project, we investigate data assimilation (DA) techniques for compressible flows from a numerical analysis point of view. DA aims at bridging the gap between experimental approaches and numerical simulations for studying the behavior of an evolutionary system. In fact, DA techniques have long been used as the main tool for combining observational data and outputs of numerical models to provide a more realistic estimate of the evolving state of a dynamical system. In this project, we are going to provide solid mathematical ground for some DA techniques including 4D-Var when applied to compressible flow models and, in general, hyperbolic conservation laws (HCLs). However, given that solutions of HCLs are known to produce shock discontinuities in finite time, we face some difficulties in the numerical analysis of DA techniques for HCLs. In this project, we aim at alleviating these difficulties by applying some smooth reconstructions of numerical solutions which paves the path for mathematical analysis of DA techniques without adding artificial viscosity.

Contact: Jan Giesselmann, Hadi Minbashian

References

[1] J. Giesselmann, C. Makridakis, and T. Pryer. A posteriori analysis of discontinuous Galerkin schemes for systems of hyperbolic conservation laws. *SIAM J. Numer. Anal.*, 53(3):1280–1303, 2015.

Project: Efficient iterative methods for stochastic Galerkin finite element discretizations of Stokes flow with random data

When mathematical models are utilized to investigate physical phenomena, input data of the models are often not known precisely. In real-world applications, this is a result of measurement errors, production tolerances or a lack of knowledge in general. The field of uncertainty quantification (UQ) tackles this issue by quantifying the influence of data uncertainties on the model's solution. In this project, a particular approach is followed to solve forward UQ problems, namely the stochastic Galerkin method. Although its application can yield exponential convergence rates, large coupled systems of equations have to be solved in the process. In order to do this efficiently, sophisticated iterative methods and preconditioners are required. The goal of this project is to apply and extend existing methods specifically tailored to Stokes flow problems with random data.

Support: Graduate School Computational Engineering, DFG

Contact: Christopher Müller, Jens Lang, Sebastian Ullmann

References

[1] C. Müller. *Iterative Solvers for Stochastic Galerkin Discretizations of Stokes Flow with Random Data*. Dr. Hut Verlag, 2018.

[2] C. Müller, S. Ullmann, and J. Lang. A Bramble-Pasciak conjugate gradient method for discrete Stokes equations with random viscosity. arXiv:1801.01838, 2018.

[3] C. Müller, S. Ullmann, and J. Lang. A Bramble-Pasciak conjugate gradient method for discrete Stokes problems with lognormal random viscosity. In M. Schäfer, M. Behr, M. Mehl, and B. Wohlmuth, editors, *Recent Advances in Computational Engineering*, pages 63–87. Springer International Publishing, Cham, 2018.

Project: Mixed finite elements for acoustic and electromagnetic wave propagation

The study of wave propagation is an important topic in the field of engineering and it finds applications in various fields such as in antenna design, radar detection, noise cancellation, fiber optics, signal filtering, seismic prospection and many others. Therefore, the efficient and accurate simulation of wave phenomena is of big relevance from a practical point of view. Our goal is to design efficient mixed finite element approximations by means of mass lumping, which involves replacing the mass matrix by a block-diagonal approximation. This allows to efficiently apply explicit time stepping schemes. We look at different types of discretizations and provide thorough error analysis.

Support: Graduate School Computational Engineering, DFG

Contact: Herbert Egger, Bogdan Radu

References

[1] H. Egger and B. Radu. A mass-lumped mixed fem for acoustic wave propagation with inhomogeneous coefficients. *PAMM*, 18:1–2, 2018.

[2] H. Egger and B. Radu. A mass-lumped mixed finite element method for acoustic wave propagation. arXiv:1803.04238, 2018.

[3] H. Egger and B. Radu. A mass-lumped mixed finite element method for Maxwell's equations. arXiv:1810.06243, 2018.

[4] H. Egger and B. Radu. A second order multipoint flux mixed finite element method on hybrid meshes. arXiv:1812.03938, 2018.

[5] H. Egger and B. Radu. Super-convergence and post-processing for mixed finite element approximations of the wave equation. *Numer. Math.*, (2):427–447, 2018.

Project: Coupling of dynamical systems with convolution quadrature methods

Integrated circuits with smaller and smaller conducting structures lead to drastically faster processor generators in the last years. With the miniaturization there is more coupling of the signals between different conductors that is not anymore described by circuits. In this project we aim for coupled modelling of the dynamical behaviour of circuits and discretized 3D electromagnetic field equations through ports. We follow the convolution quadrature approach that leads to a model reduction based on precomputations for the electromagnetic field equations in frequency domains with a series of frequencies and to much reduced effort of the coupled dynamical simulation.

Support: Graduate School Computational Engineering, DFG

Contact: Herbert Egger, Kersten Schmidt, Vsevolod Shashkov

References

[1] H. Egger, V. Shashkov, and K. Schmidt. Multistep and Runge-Kutta convolution quadrature methods for coupled dynamical systems. arXiv:1811.09817, 2018.

Project: Interaction between boundary layers and domain singularities

In this project singularly perturbed partial differential equations including microperforated layers with emphasis on corner singularities shall be analyzed. Singularly perturbed partial differential equations are characterized by microscopic solution behaviour, especially boundary layers. Such a solution behaviour is caused by small (material) parameters in front of the leading order differential operator, like small viscosities, or equivalently large parameters in front of lower order terms as for highly conductive media in electromagnetism. Also, geometrically small features like for thin layers or sheets that may even possess a microstructure lead to boundary layers in the solution. Solution representations taking into account the interaction of boundary layers and domain singularities can be used to construct efficient numerical schemes.

Partner: Bérangère Delourme (University of Paris 13, France); Monique Dauge (University of Rennes 1, France); Ralf Hiptmair (ETH Zürich)

Contact: Adrien Semin, Kersten Schmidt

References

[1] A. Semin, B. Delourme, and K. Schmidt. On the homogenization of the Helmholtz problem with thin perforated walls of finite length. *ESAIM Math. Model. Numer. Anal.*, 52(1):29–67, 2018.

Project: Impedance conditions for visco-acoustic models

The acoustic damping in gas turbines and aero-engines relies to a great extent on acoustic liners that consist of a cavity and a perforated face sheet. The prediction of the impedance of the liners by direct numerical simulation is nowadays not feasible due to the hundreds to thousands of repetitions of tiny holes. We aim to obtain impedance conditions in viscous gases, especially for multiperforated acoustic absorbers, based on higher order asymptotic expansions and matched asymptotic expansion techniques.

Partner: Friedrich Bake (DLR Berlin); Anastasia Thöns-Zueva (TU Berlin)

Contact: Kersten Schmidt, Adrien Semin

References

[1] K. Schmidt, A. Semin, A. Thöns-Zueva, and F. Bake. On impedance conditions for circular multiperforated acoustic liners. *J. Math. Industry*, 8(1):15, 2018.

[2] A. Semin and K. Schmidt. On the homogenization of the acoustic wave propagation in perforated ducts of finite length for an inviscid and a viscous model. *Proc. R. Soc. Lond. A*, 474(2210), 2018.

Project: Model reduction techniques for biomechanical devices

Biomechanical devices like stents are used to recover the blood flow in arteria when they are blocked due to a disease. With optimized stent designs they remain comfortablely at position and guarantee a permanent blood flow for longer times. The modeling of the mechanical properties is challenging due to their structure as a network of struts and their interaction with the blood vessel as a contact problem. We aim for a model reduction based on homogenization of systems of differential equations on edges of a periodic graph.

Partner: Josip Tambača, Luka Grubišić, Matko Ljulj, Marko Hajba (University of Zagreb, Croatia)

Support: German Academic Exchange Service in the "Programm für projektbezogenen Personenaustausch mit Kroatien" (Project-ID 57334847), Graduate School Computational Engineering

Contact: Kersten Schmidt, Adrien Semin, Herbert Egger

Project: Shape optimization in acoustic-structure interaction

Acoustic-structure interaction is an emerging field in industry and mathematical modelling, with important applications in reducing the noise emitted by machines, vehicles, constructions, etc. In particular in the car industry, there is a huge interest to optimize and tailor the sound amplitudes within the car by changing the shape of parts of the elastic structure. We are interested in the minimization of the sound pressure by variation of the shape of the structure. For this we derive the shape derivative for the acoustic-structure interaction modelled by the Helmholtz equation for the acoustic part, the equations of linear elasticity and coupling conditions and consider a closed optimization process in 3D using a high-order finite element discretization on hexahedral meshes.

Partner: Antoine Laurain (University of São Paulo, Brazil); Philipp Kliewe (TU Berlin)

Contact: Kersten Schmidt

Project: Superconvergent IMEX Peer methods with variable step sizes

The spatial discretization of certain time-dependent PDEs (e.g. advection-reaction-diffusion systems) yields large systems of ODEs where the right-hand side admits a splitting into a stiff and non-stiff part. We construct time integrators that combine the favorable stability properties of implicit methods and the low computational costs of explicit schemes. In order to guarantee consistency and, thus, convergence, the implicit and explicit integrator must fit together. A natural way to construct these implicit-explicit (IMEX) Peer methods is to start with an appropriate implicit scheme and extrapolate it in a suitable manner. We follow the approach developed by Lang and Hundsdorfer in [1]. Peer methods have the advantage that all stage values have the same order and, hence, order reduction for stiff systems is avoided. Further, there remain enough free parameters such that additional properties can be guaranteed. This includes optimal zero-stability, A-stability of the implicit part and, in particular, superconvergence. In [2], we derive necessary and sufficient conditions on the coefficient matrices to construct new superconvergent IMEX schemes for $s = 2, 3, 4$ stages. When solving dynamical systems with sub-processes evolving on many different time scales, efficiency is greatly enhanced by automatic time step variation. Therefore, we investigate the theory, construction and application of IMEX Peer methods that are superconvergent even for variable step sizes. To construct schemes that keep their higher order for variable step sizes and exhibit favorable linear stability properties, we adapt our approach for constant step sizes and, eventually, derive additional necessary and sufficient conditions on the nodes and coefficient matrices. New superconvergent IMEX Peer methods which maintain the superconvergence property independently of step size changes are constructed for $s = 2, 3, 4$ stages.

Partner: Willem Hundsdorfer (CWI Amsterdam, The Netherlands); Rüdiger Weiner (Universität Halle-Wittenberg)

Contact: Moritz Schneider, Jens Lang

References

[1] J. Lang and W. Hundsdorfer. Extrapolation-based implicit-explicit Peer methods with optimised stability regions. *J. Comp. Phys.*, 337:203–215, 2017.

[2] M. Schneider, J. Lang, and W. Hundsdorfer. Extrapolation-based super-convergent implicit-explicit Peer methods with A-stable implicit part. *J. Comp. Phys.*, 367:121–133, 2018.

Project: Chemotaxis models on network structures

Chemotaxis describes the movement of cells and organisms caused by their reaction to chemical gradients. Since the first mathematical investigation of chemotactic phenomena by Keller and Segel, a variety of PDE models has been developed in order to reproduce the main features of population dynamics governed by chemotaxis. This project is concerned with some of these models in a network setting. Existence and uniqueness of global solutions has been considered for the minimal Keller-Segel model on a network. A finite element method that inherits the conservation of mass and positivity from the continuous model was developed and analyzed. Convergence of the method was obtained under general assumptions and convergence rates were deduced for smooth solutions.

Contact: Herbert Egger, Lucas Schöbel-Kröhn

References

[1] H. Egger and L. Schöbel-Kröhn. Chemotaxis on networks: Analysis and numerical approximation. arXiv:1805.00925, 2018.

Project: Numerical methods for a parabolic-elliptic interface problem

In this project, we want to find and analyze a suitable discretization method for a coupled system of partial differential equations consisting of the model problem for transport in porous media, which is a (possibly convection dominated) parabolic time-dependent diffusion-convection-reaction equation on a bounded domain and a diffusion process on the complement of the domain, modeled by the Laplace equation, which are coupled at the boundary. To approximate such problems the coupling of a method for the interior problem and the boundary element method (BEM) is of particular interest. Because of the possible convection domination, one would use such methods as an upwind stabilized Finite Volume Method (FVM) or a comparably stabilized Finite Element Method called Streamline Upwind Petrov Galerkin (SUPG). There are several methods to couple an interior method with BEM, depending on the formulation of the exterior problem and the transmission conditions between the interior and the exterior problem, one such method is the non-symmetric coupling, which has not been analyzed for the time-dependent case and thus is the main focus of this research project.

Support: Graduate School Computational Engineering, DFG

Contact: Robert Schorr, Christoph Erath

References

[1] H. Egger, C. Erath, and R. Schorr. On the non-symmetric coupling method for parabolic-elliptic interface problems. *SIAM J. Numer. Anal.*, 56(6):3510–3533, 2018.

[2] C. Erath and R. Schorr. Stable non-symmetric coupling of the finite volume and the boundary element method for convection-dominated parabolic-elliptic interface problems. *Preprint, arXiv:1805.05142*, 2018.

[3] C. Erath and R. Schorr. A simple boundary approximation for the non-symmetric coupling of finite element method and boundary element method for parabolic-elliptic interface problems. In *Numerical Mathematics and Advanced Applications ENUMATH 2017*, pages 993–1001. Springer International Publishing, 2019.

Project: Structure preserving simulation in nonlinear electromagnetics

The main aim of this project is to develop novel discretization schemes that preserve the inherent structure of underlying physical models for systems involving electromagnetics, i.e., conservation and/or dissipation of energy. Typical applications to be studied are electric machines, models of magnetohydrodynamics, and electronic devices leading to field-circuit coupled problems.

Partner: Herbert De Gersem, Sebastian Schöps (Institut für Theorie Elektromagnetischer Felder, TU Darmstadt)

Support: DFG GSC 233

Contact: Herbert Egger, Vsevolod Shashkov

References

[1] H. Egger, V. Shashkov, and K. Schmidt. Multistep and Runge-Kutta convolution quadrature methods for coupled dynamical systems. arXiv:1811.09817, 2018.

Project: Weighted reduced basis methods for parabolic partial differential equations with random input data

This project focuses on model order reduction for parabolic partial differential equations with parametrized random input data. The outcome of the model problem is the solution of the partial differential equation and a quantity of interest, which is determined by a functional that maps the solution to a real number. Due to the randomness of the input data, the expected value of the solution and the output is approximated by a Monte Carlo estimator. This work develops efficient reduced spaces by means of a weighted reduced basis method in order to decrease the expected solution errors compared to a non-weighted reduced basis method.

Support: Graduate School Computational Engineering, DFG

Contact: Christopher Spannring, Jens Lang, Sebastian Ullmann

References

[1] C. Spannring. *Weighted reduced basis methods for parabolic PDEs with random input data*. PhD thesis, TU Darmstadt, 2018.

[2] C. Spannring, S. Ullmann, and J. Lang. A weighted reduced basis method for parabolic PDEs with random data. In M. Schäfer, M. Behr, M. Mehl, and B. Wohlmuth, editors, *Recent Advances in Computational Engineering*, pages 145–161, Cham, 2018. Springer International Publishing.

Project: Simulation, optimization and uncertainty quantification for borehole thermal energy storage systems based on adaptive finite elements

Borehole thermal energy storage systems present an increasingly common solution for energy storage, especially in conjunction with renewable energies like solar power. In order to design such facilities and estimate their storage capabilities and efficiency, numerical simulations based on partial differential equations are inevitable. These simulations can be very challenging because of the great disparity in the magnitude of the simulated objects and the highly transient operation scenarios.

This project aims to build upon currently existing models [1] to efficiently simulate the behaviour of borehole thermal energy storage systems by means of adaptive finite elements. This is done with the adaptive PDE solver KARDOS. The model can be extended to include randomness, which allows for an uncertainty quantification. This is done with stochastic collocation based on deterministic PDE solutions to interpolate the stochastic solution and its properties over a domain of random variables. In future work, we also plan to optimize the layout and the performance of borehole thermal energy storage systems.

Partner: Ingo Sass, Daniel Schulte (Institut für Angewandte Geowissenschaften, TU Darmstadt)

Support: Darmstadt Graduate School of Excellence Energy Science and Engineering, GSC 1070

Contact: Philipp Steinbach, Jens Lang

References

[1] D. O. Schulte, W. Rühaak, B. Welsch, and I. Sass. Basimo - borehole heat exchanger array simulation and optimization tool. *Energy Procedia*, 97:210–217, 2016.

[2] P. Steinbach. Adaptive Finite-Elemente-Verfahren für Erdwärmesondenspeicher. Masterarbeit, Technische Universität Darmstadt, 2018.

Project: Adaptive moving finite element method for steady low-Mach-number compressible combustion

Recently, the renewable energies are increasingly recommended to be used in industry and their applications also exhibit a high rate of growth. Nevertheless, the corresponding contributions to the overall demand of energy are far from satisfactory. Hence, in a long-term future, the majority of energy will still be obtained by conventional processes through using coal, oil and gas as fuels and thus the premixed combustion remains important to industry with consideration of reducing the thermal formation of nitric oxides that constitutes a major portion of the pollutants and results in acid rain smog problems. While the computational fluid problem is still one of the most complicated tasks in the engineering field, the complexity of a reactive flow gets further increased not only because of the mixing process, like the mixing between fuel and oxidizer, but also the sophisticated mechanisms of chemical reactions. Herein, the time scales of the different elementary reactions always cover several orders of magnitude that makes computation very time comsuming. Moreover, nearly all the coefficients of the mass and heat transport processes are temperature and even pressure dependent. Hence, an adaptive discretization method is commonly recognized as an effective approach to solve such a complex system.

Contact: Zhen Sun, Jens Lang

References

[1] Z. Sun. *Adaptive Moving Finite Element Method for Steady Low-Mach-Number Compressible Combustion Problems*. PhD thesis, Technische Universität Darmstadt, 2018.

Project: Wall shear stress measurements using magnetic resonance imaging

The flow of blood in human vessels is of great interest in medicine. A very important physical quantity is the wall-shear stress (WSS) and its distribution along the wall, that can be computed from the geometry and the velocity therein. The goal of this project is to use both the magnetic resonance imaging (MRI) and a fluid dynamical model to provide accurate values of the WSS. In a first step the inverse problem of reconstructing the smooth flow domain and the velocity profile inside the flow domain from the MRI measurements is analyzed and solved. Now the focus is on the data assimilation problem to enhance the reconstructed velocity by utilizing knowledge of the governing fluid dynamics. From a mathematical point of view there arise a couple of problems like finding a proper model containing boundary conditions and minimizing the computational effort in the resulting optimization problem. The cardiology group of the Klinik für Radiologie (Universität Freiburg) will provide the MRI data, the Fachgebiet Strömungslehre und Aerodynamik (TU Darmstadt) will assess the accuracy of the developed algorithms by comparing the results with laser Doppler velocimetry (LDA) and CFD simulations for some selected test cases.

Partner: Andreas Bauer, Cameron Tropea (TU Darmstadt); Axel Krafft, Nina Shokina, Waltraud Buchenberg, Jürgen Hennig (Universität Freiburg)

Support: DFG Eg-331/1-1

Contact: Gabriel Teschner, Herbert Egger

References

[1] H. Egger and B. Hofmann. Tikhonov regularization in Hilbert scales under conditional stability assumptions. *Inverse Problems*, 34:115015, 2018.

[2] H. Egger, T. Seitz, and C. Tropea. Enhancement of flow measurements using fluid-dynamic constraints. *J. Comp. Phys.*, 344:558–574, 2017.

[3] H. Egger and G. Teschner. On the stable estimation of flow geometry and wall shear stress from magnetic resonance images. arXiv:1812.09848, 2018.

Project: Stochastic Galerkin reduced basis methods

We study stochastic Galerkin reduced basis methods for elliptic boundary value problems with parametrized random and deterministic inputs. For a given value of the deterministic parameter, a stochastic Galerkin finite element method can estimate the corresponding expected value and variance of a linear output at the cost of a single solution of a large block-structured linear algebraic system of equations. Reduced basis methods can lower the computational burden when statistical outputs are required for a high number of deterministic parameter queries. We aim at bounds for the error associated with the reduced-order estimates of the expected value and the variance.

Support: Graduate School Computational Engineering, DFG

Contact: Jens Lang

References

[1] S. Ullmann and J. Lang. Stochastic Galerkin reduced basis methods for parametrized linear elliptic PDEs. arXiv:1812.08519, 2018.

Project: Model reduction for incompressible flow

We study model order reduction based on proper orthogonal decomposition (POD) for unsteady incompressible Navier-Stokes problems, assuming that the snapshots are given by spatially adapted finite element solutions. We investigate two approaches: Firstly, a weak incompressibility constraint is imposed with respect to a pressure reference space. Secondly, the velocity reduced space is enriched with supremizers computed on a velocity reference space. In the presence of inhomogeneous Dirichlet conditions, suitable lifting functions must be provided.

Partner: Michael Hinze, Carmen Gräßle (Universität Hamburg)

Support: Graduate School Computational Engineering, DFG

Contact: Jens Lang

References

[1] C. Gräßle, M. Hinze, J. Lang, and S. Ullmann. POD model order reduction with space-adapted snapshots for incompressible flows. arXiv:1810.03892, 2018.

Project: EWAVE

EWAVE is part of the cooperation project ERWAS founded by the BMBF. The goal is to develop an innovative energy-management system which is currently tested at the Rheinisch-Westfälische Wasserwerkgesellschaft (RWW). A management system allows to compute optimal operation plans for the constructions of the water production, the water preparation and the water distribution. Additionally, the system can decide whether self-generated energy or energy purchased from energy supply companies is used. Mathematically, we develop numerical discretization methods which provide accuracy with higher order in time, are able to handle stiff source terms, and are compatible with adjoint based optimization.

Partner: Alexander Martin, Günter Leugering (Universität Erlangen-Nürnberg); Gerd Steinebach (Hochschule Bonn-Rhein-Sieg); Oliver Kolb (Universität Mannheim); Michael Plath (RWW Rheinisch-Westfälische Wasserwerkgesellschaft mbH); Olaf Kremsier (GreyLogix Aqua); Andreas Pirsing (Siemens AG, Siemens Industry Automation); Roland Rosen (Siemens AG, Siemens Corporate Technology)

Contact: Lisa Wagner, Jens Lang

References

[1] L. Wagner. *Second-Order Implicit Methods for Conservation Laws with Applications in Water Supply Networks*. PhD thesis, Technische Universität Darmstadt, 2017.

Project: Residual-type a posteriori error estimator for a quasi-static Signorini contact problem

This project deals with the construction and the analysis of a residual-type a posteriori estimator for a quasi-static Signorini problem. In order to obtain an efficient, reliable and localized estimator, an error notion which measures the error in the displacements, the velocities and a suitable approximation of the contact forces is introduced. Further, the local properties of the solution are exploited such that the spatial estimator has no contributions related to the non-linearities in the interior of the actual time-dependent contact zone but gives rise to an appropriate refinement of the free boundary zone. The estimator splits in temporal and spatial contributions which can be used for the adaptation of the time step as well as the mesh size. To illustrate the performance of the estimator, the theoretical results are accompanied by numerical studies.

Contact: Mirjam Walloth

References

[1] M. Walloth. Residual-type a posteriori error estimator for a quasi-static Signorini contact problem. Preprint 2721, Fachbereich Mathematik, TU Darmstadt, 2018.

Project: Structure preserving adaptive enriched Galerkin methods for pressure-driven 3D fracture phase-field models (subproject of priority program 1748)

The project is concerned with the development of innovative enriched Galerkin methods for the reliable simulation of pressure-driven fracture problems. Within this project, convergent adaptive mesh-refinement schemes based on new efficient error estimators for the variational inequality associated with the fracture irreversibility will be developed.

Partner: Katrin Mang, Thomas Wick (Universität Hannover); Winnifried Wollner (AG Optimierung, TU Darmstadt)

Support: DFG Priority Program 1748

Contact: Mirjam Walloth

References

[1] M. Walloth. Residual-type A Posteriori Estimators for a Singularly Perturbed Reaction-Diffusion Variational Inequality – Reliability, Efficiency and Robustness. arXiv:1812.01957, 2018.

Project: Numerical methods for multi-phase flows with topological changes

The aim of this research project is the investigation of systems modeling compressible flows of one substance that is present as both liquid and vapor. Two phase flows are important in processes of practical interest such as combustion, cryogenics, and cloud formation, where the scales of interest are rather large. Understanding their modeling, which is usually based on averaged models, motivates us to develop tools for the simulation of small scale models. In this case, a posteriori analysis is crucial in determining how reliable a numerical scheme is and it allows for error control of the exact and the numerical solutions. While the former are considered to be weak-entropic solutions, the latter cannot be strong solutions since they are given in the context of a Discontinuous Galerkin (DG) framework. At the same time, exact solutions are not smooth in general. We introduce sufficiently regular intermediate functions called reconstructions that are considered as strong solutions of a perturbed system and then by employing a variant of the relative entropy technique we overcome the obstacle of the non-convexity of the energy. Thereby, we obtain an a posteriori estimator for the difference between the reconstruction and the numerical solution. This means, we explicitly bound the difference between the exact and the numerical solutions.

Contact: Dimitrios Zacharenakis, Jan Giesselmann

References

[1] J. Giesselmann and T. Pryer. Reduced relative entropy techniques for a posteriori analysis of multiphase problems in elastodynamics. *IMA J. Numer. Anal.*, 36:1685–1714, 2016.

[2] J. Giesselmann and D. Zacharenakis. A Posteriori Analysis for the Euler-Korteweg Model. In *Theory, Numerics and Applications of Hyperbolic Problems I*, pages 631–642. Springer International Publishing, 2018.

2 Collaborative Research Projects and Cooperations

The department is involved in a number of interdisciplinary research projects including excellence projects, collaborative research centres and priority programs. This section gives a brief overview of these activities.

2.1 Collaborative Research Centre Transregio TRR 146

Multiscale modeling is a central topic in theoretical condensed matter physics and materials science. One prominent class of materials, whose properties can rarely be understood on one length scale and one time scale alone, is soft matter. The properties of soft materials are determined by an intricate interplay of energy and entropy, and minute changes of molecular interactions may lead to massive changes of macroscopic system properties.
In a joint effort of physicists, chemists, applied mathematicians, and computer scientists, the Collaborative Research Center TRR 146 investigates some of the most pressing problems in multiscale modeling, viz.

- Dynamics: In the past, multiscale coarse-graining approaches have to a large extent focused on static equilibrium properties. However, a thorough understanding of the coarse-grained dynamical system properties is necessary if one wants to apply multiscale concepts to the study of transport and nonequilibrium processes.

- Coarse-graining and mixed resolution: In many applications, selected small (e.g., functional) regions of a material must be treated in great detail, whereas the large bulk can be modeled at a coarse-grained level. Simulation schemes are desirable, where fine-grained and coarse-grained regions can dynamically be assigned to the current state of the system. In this context, we will also have to re-analyze fundamental aspects of coarse-graining from a mathematical point of view.

- Bridging the particle-continuum gap: So far, only few successful attempts have been made to combine particle models of soft matter with continuum models in a nontrivial fashion. Multiscale schemes for particle models have mostly been developed in the soft matter community, whereas schemes for treating continuum models with variable resolution are developed in the applied mathematics community. In the CRC-TR, we will bring these two communities together to advance the field as a whole.

Problems addressed in the TRR 146 require a massive interdisciplinary effort at the level of fundamental science and algorithmic development. The TRR 146 brings together scientists with complementary expertise in a wide range of modeling methods. Also one professor of the Department of Mathematics (Egger) is in the group of principal investigators.

2.2 Collaborative Research Centre Transregio TRR 154

The Collaborative Research Centre Transregio TRR 154 “Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks” was established in 2014 and is after successful evaluation in its second funding period. The energy transition ("Energiewende") in Germany and its success are currently in the focus of public interest. This transition is of central significance to society, politics, and science, since Germany, like many other industrial nations, finds itself in a situation of dramatically increased dependence on a reliable, secure, and affordable energy supply. At the same time, the request for clean, environment- and climate-friendly energy generation is as large as never before. In order to achieve that and, in parallel, to master the nuclear power phase-out, natural gas as an energy source will play a pivotal role in the coming decades. Within this time span, a sufficient amount of natural gas will be available; it will be readily accessible, tradable, and storable. Nevertheless, the focus on an efficient natural gas supply implies a multiplicity of problems concerning gas transport and network technology as well as the consideration of market-regulatory conditions, and also the coupling with other energy sources. As an example, we mention that gas carriers must provide evidence that, within given technical capacities, all contracts which come into existence on the market are physically and technically satisfiable.

The aim of the TRR 154 is to offer answers to these challenges by using methods of mathematical modelling, simulation, and optimization and, in turn, to provide solutions of increased quality. Novel mathematical findings are required in different areas such as mathematical modelling, numerical analysis, simulation and integer, continuous, and stochastic optimization as well as equilibrium problems in order to achieve this aim. As examples, we mention the modelling and analysis of complex networks of hyperbolic balance equations including switches and the development of a mixed-integer optimization theory together with its algorithmic realisation for such networks including the handling of data uncertainty. Furthermore, efficient hierarchical numerical approximation techniques for the resulting algebraically coupled PDEs need to be developed and a sophisticated error control, taking the interaction with the mixed-integer optimization algorithms into account, is required.

The Department of Mathematics at TU Darmstadt is involved with Dr. Domschke and Professors Egger, Lang, Pfetsch, Schwartz, Ulbrich, and Wollner in the collaborative research centre Transregio TRR 154. Furthermore, groups at Universität Erlangen-Nürnberg (speaker), HU Berlin, TU Berlin, Universität Duisburg-Essen, and WIAS – Leibniz-Institut im Forschungsverbund Berlin e.V. are part of TRR 154.

The homepage of TRR 154 is `trr154.fau.de`.

2.3 Graduate School of Computational Engineering

Computational Engineering (CE) denotes computer based modeling, analysis, simulation, and optimization. It is a cost-effective, efficient and complementary approach to study engineering applications and to engineer new technical solutions when experimental investigations are too complex, risky, or costly. CE enables the creation of scalable models to support research, development, design, construction, evaluation, production, and operation of engineering applications which address key issues in future technology developments for the economy and society in areas such as energy, health, safety, and mobility.

However, such engineering applications are becoming increasingly complex. Consequently, the theory and methodologies required to investigate corresponding systems become challenging.

With the Graduate School of Computational Engineering, TU Darmstadt was able to further strengthen its role in CE. The school enables highly talented PhD students to develop their scientific skills in a focused way, and to cooperate under optimal conditions in a highly stimulating interdisciplinary environment based on the interaction of Computer Science, Mathematics, and Engineering Sciences. Partnerships with well established research organizations as well as cooperation with industry increase the impact of the Graduate School. Building on the well established interdepartmental expertise at TU Darmstadt, the Graduate School focusses on the following key research areas: modeling and simulation of coupled multi-physics problems, simulation based optimization, and hierarchical multi-scale modeling and simulation. The research efforts in the above fields are accompanied by corresponding developments of methods of visualization, simulated reality, high-performance computing, verification and validation, as well as software engineering and lifecycle research. The PhD students work together within research foci comprising one or more of the above topics. The joint research on specially defined use cases will further strengthen the interdisciplinary skills and cooperation.

Eight professors of the Department of Mathematics are Principal Investigators within the Graduate School Computational Engineering (Aurzada, Bothe, Egger, Giesselmann, Lang, Pfetsch, Ulbrich, Wollner) with expertise in Probability Theory and Stochastic Analysis, Mathematical Modeling and Analysis, Numerical Analysis and Scientific Computing, Numerics of Partial Differential Equations, Discrete Optimization, and Nonlinear Optimization and Optimal Control. Five more members of the department are Research Group Leaders (Disser, Erath, Marschall, Schwartz, Ullmann) with scientific focus on Online Optimization, Numerical Analysis, Two-Phase and Interfacial Flows, Discrete-Nonlinear Optimization, and Uncertainty Quantification. Together they supervise more than 12 interdisciplinary PhD projects within the Graduate School in close cooperation with a co-supervisor from Engineering or Computer Science. The field of Computational Electromagnetics is represented by one research assistant (Dölz), who is also a member of the Darmstadt Mathematical School.

2.4 Graduate School of Energy Science and Engineering

The mission of the Darmstadt Graduate School of Energy Science and Engineering is to educate tomorrow's leading Energy Engineers in a multidisciplinary field of expertise needed to identify and master the most demanding scientific, engineering, economic and social challenges in an interdisciplinary approach. The main challenge is viewed to be a continuous transition from the carbon-based, non-renewable primary energy sources of today to renewable and environmentally friendly energy resources of tomorrow.

The optimal strategy to meet this challenge is, on the one hand, to improve conventional energy technologies and render them progressively more efficient to meet the ever more stringent demands on pollutant emissions and, on the other hand, to simultaneously develop innovative, advanced renewable energy technologies which must be brought to a competitive technological readiness level and provide safe, reliable and cost-effective solutions.

Two professors of the Department of Mathematics are Principal Investigators within the Graduate School Energy Science and Engineering (Lang, Ulbrich) with expertise in Numerical Analysis, Nonlinear Optimization and Optimal Control.

2.5 International Research Training Group IRTG 1529

The International Research Training Group "Mathematical Fluid Dynamics"(IRTG 1529) is funded by the German Research Foundation (DFG) and the Japan Society for the Promotion of Science (JSPS). It is associated with TU Darmstadt and with two universities located in Tokyo, Waseda University and University of Tokyo.

The research of the program focuses on analytical, numerical and stochastic aspects as well as on modeling, optimization and aerodynamics of fluid dynamics. It distinguishes itself through joint teaching and supervision. The core program consists of interdisciplinary lectures and seminars and includes research and study periods in Tokyo. Presently, there are 12 PhD students and 2 Postdocs on the Darmstadt side and a similar amount on the Japanese side.

The principal investigators in Darmstadt are Volker Betz, Dieter Bothe, Herbert Egger, Reinhard Farwig, Matthias Hieber, Ulrich Kohlenbach, Maria Lukáčová, Cameron Tropea and Stefan Ulbrich. The participating colleagues in Tokyo are Tadahisa Funaki, Yoshikazu Giga, Yosuke Hasegawa, Akitoshi Kawamura, Hideo Kozono, Hirofumi Notsu, Yoshihiro Shibata, Masahiro Yamamoto, Masao Yamazaki and Keita Yokoyama.

IRTG 1529 is organizing seminars, short courses, workshops and conferences on a regular basis in Darmstadt and Tokyo. The list of speakers in 2017 and 2018 includes leading experts of the field, e.g., P. Constantin, R. Danchin, G.P. Galdi, Y. Giga, F. Flandoli, H. Koch, H. Kozono, T. Ogawa, F. Otto, F. Lin, J. Prüss, G. Seregin, G. Simonett, R. Takada, E. Titi and Z. Xin.

Highlights of the program were several conferences or bigger workshops in 2017 and 2018, e.g., the "International Workshops on Mathematical Fluid Dynamics" at Waseda University, Tokyo, in March 2017 and January 2018 and in Darmstadt in May 2018.

2.6 Scientific and Industrial Cooperations

In the following we list all scientific and industrial projects by names of the researcher of our department in alphabetic order, by names of partners in universities and industry, and the title of the project.

Jürgen Dölz

- Prof. Dr. Helmut Harbrecht (Universität Basel): Software cooperation on boundary element methods.
- Prof. Dr. Michael Multerer (USI Lugano, Switzerland): Software cooperation on boundary element methods.
- Group of Prof. Dr. Sebastian Schöps (Institut für Theorie Elektromagnetsicher Felder, TU Darmstadt): Software cooperation on boundary element methods.

Pia Domschke

– Prof. Dr. Mark A. J. Chaplain (University of St. Andrews, UK), Dr. Dumitru Trucu (University of Dundee, UK), Dr. Alf Gerisch (TU Darmstadt): Mathematical Modelling of Cancer Invasion.

– Jun.-Prof. Dr. Oliver Kolb (Universität Mannheim): Simulation and optimization of gas and water supply networks.

Herbert Egger

– Prof. Dr. Simon Arridge, Dr. Samuel Powell (UCL London, UK), Prof. Dr. Matthias Schlottbom (University of Twente, The Netherlands): Numerical methods for radiative transfer.

– Prof. Dr. Jan-Frederik Pietschmann (TU Chemnitz), Prof. Dr. Matthias Schlottbom (University of Twente, The Netherlands): Parameter estimation for nonlinear inverse problems.

– Prof. Dr. Bernd Hofmann (TU Chemnitz): Conditional stability and regularization of inverse problems.

– Prof. Dr. Volker Mehrmann (TU Berlin): Structure preserving approximation of Hamiltonian systems.

– Prof. Dr. Andreas Hildebrandt (Universität Mainz), Prof. Dr. Günther Of (TU Graz): Numerical approximation of non-local diffusion processes.

– Prof. Dr. Martin Schmidt (Universität Trier): Global optimal control of linear dynamical systems.

Christoph Erath

– Prof. Dr. Dirk Praetorius (TU Wien): Optimal convergence of adaptive mesh refinement schemes.

– Prof. Dr. Olaf Steinbach (TU Graz): Coupling FEM-BEM.

Alf Gerisch

– Prof. Dr. Mark A. J. Chaplain (University of St. Andrews, UK), Dr. Dumitru Trucu (University of Dundee, UK), Dr. Pia Domschke (TU Darmstadt), Prof. Dr. Kevin J. Painter (Heriot-Watt University, Edinburgh, UK), Prof. Dr. Thomas Hillen (University of Alberta, Canada), Dr. Andreas Buttenschön (UBC Vancouver, Canada): Mathematical Modelling of Cancer Invasion.

– Prof. Dr. Kai Raum (Charité Universitätsmedizin Berlin), Prof. Dr. Quentin Grimal (Biomedical Imaging Lab, UPMC Paris, France), Dr. Raimondo Penta (University of Glasgow, UK): Multiscale structure-functional modelling of musculoskeletal mineralized tissues.

– Prof. Dr. Jens Lang (TU Darmstadt), Prof. Dr. Rüdiger Weiner, Dr. Helmut Podhaisky (Universität Halle-Wittenberg): Peer methods and their application in the Finite Element system KARDOS.

– Prof. Dr. Anotida Madzvamuse (University of Sussex, UK), Dr. Raquel Barreira (Polytechnic Institute of Setubal, Portugal): Cross-diffusion in models from mathematical biology.

Jan Giesselmann

– Group of Prof. Dr. Christian Rohde (Universität Stuttgart): Uncertainty quantification in hyperbolic conservation laws.

– Prof. Dr. Andreas Dedner (University of Warwick, UK), Prof. Dr. Jennifer Ryan (University of East Anglia, UK), Prof. Dr. Tristan Pryer (University of Reading, UK): Reconstruction techniques for energy-based a posteriori error estimates.

– Dr. Rüdiger Müller (WIAS Berlin): Robust a posteriori error estimates for compressible multiphase flows.

– Dr. Raul Borsche (TU Kaiserslautern): A posteriori analysis for hyperbolic conservation laws on networks.

– Group of Prof. Dr. Manuel Torrilhon (RWTH Aachen): Moment methods for kinetic equations.

Jens Lang

– Prof. Dr. Willem Hundsdorfer (CWI Amsterdam, The Netherlands): IMEX Peer methods.

– Prof. Dr. Weizhang Huang (University of Kansas, USA), Lennard Kamenski (WIAS Berlin): Anisotropic mesh methods.

– Prof. Dr. Rüdiger Weiner (Universität Halle-Wittenberg): IMEX Peer methods.

– Prof. Dr. Michael Hinze, Carmen Gräßle (Universität Hamburg): Model reduction for incompressible flow.

– Prof. Dr. Robert Scheichl (Universität Heidelberg): Uncertainty quantification.

– Prof. Dr. Volker Mehrmann (TU Berlin): Model hierarchy for gas networks.

– Prof. Dr. Malte Braack (Universität Kiel): Adaptive moving FEM for compressible combustion.

– Dr. Rainald Ehrig (ZIB): Kardos programming.

Kersten Schmidt

– Group of Prof. Dr. Reinhold Schneider (TU Berlin): High-order finite element modelling in Quantum Physics.

– Group of Prof. Dr. Volker Mehrmann (TU Berlin): Parametric and nonlinear eigenvalue problems.

- Groups of Prof. Dr. Luka Grubišić and Prof. Dr. Josip Tambača (University of Zagreb, Croatia): Nonlinear eigenvalue problems and model reduction techniques for biomechanical devices.

- Prof. Dr. Patrick Joly (INRIA Paris-Saclay, France), Prof. Dr. Monique Dauge (University of Rennes 1, France), Dr. Bérangère Delourme (University of Paris 13, France), Dr. Sébastien Tordeux (INRIA Bordeaux South-West, France): Impedance boundary conditions for PDEs with boundary layers.

- Prof. Dr. Ralf Hiptmair (ETH Zürich): Modelling in electromagnetics and boundary element methods.

- Prof. Dr. Antoine Laurain (University of São Paulo, Brazil): Shape optimization.

Sebastian Ullmann

- Prof. Dr. Michael Hinze, Carmen Gräßle (Universität Hamburg): Model reduction for incompressible flow.

Mirjam Walloth

- Prof. Dr. Thomas Wick (Universität Hannover), Prof. Dr. Winnifried Wollner (AG Optimierung, TU Darmstadt), Katrin Mang (Universität Hannover): Adaptive numerical simulation of quasi-static fracture phase-field models.

- Prof. Dr. Andreas Veeser (University of Milano, Italy): A posteriori error estimators for contact problems.

- Prof. Dr. Rolf Krause (USI Lugano, Switzerland): Adaptive finite element discretization methods for the numerical simulation of static and dynamic contact problems.

3 Publications

3.1 Co-Editors of Publications

3.1.1 Editors of Journals

Alf Gerisch

– *PLOS ONE* (Academic Editor)

Jens Lang

– *Applied Numerical Mathematics* (Editor)

3.1.2 Editors of Proceedings

Alf Gerisch

– *Multiscale Models in Mechano and Tumor Biology: Modeling, Homogenization, and Applications. Lecture Notes in Computational Science and Engineering, volume 122, Springer, Cham, 2018* (jointly with Raimondo Penta and Jens Lang)

3.2 Monographs and Books

[1] A. Gerisch, R. Penta, and J. Lang, editors. *Multiscale Models in Mechano and Tumor Biology: Modeling, Homogenization, and Applications*, volume 122 of *Lecture Notes in Computational Science and Engineering*. Springer, Cham, 2018.

[2] C. Müller. *Iterative Solvers for Stochastic Galerkin Discretizations of Stokes Flow with Random Data*. Dr. Hut Verlag, 2018.

[3] Z. Sun. *Adaptive Moving Finite Element Method for Steady Low-Mach-Number Compressible Combustion Problems*. Dr. Hut Verlag, 2018.

3.3 Publications in Journals and Proceedings

3.3.1 Journals

[1] A. Buttenschön, T. Hillen, A. Gerisch, and K. Painter. A space-jump derivation for non-local models of cell-cell adhesion and non-local chemotaxis. *J. Math. Biol.*, 76:429–456, 2018.

[2] P. Domschke, A. Dua, J. J. Stolwijk, J. Lang, and V. Mehrmann. Adaptive refinement strategies for the simulation of gas flow in networks using a model hierarchy. *Electronic Transactions on Numerical Analysis*, 48:97–113, 2018.

[3] P. Domschke, D. Trucu, A. Gerisch, and M. A. J. Chaplain. Structured models of cell migration incorporating molecular binding processes. *Journal of Mathematical Biology*, 75(6-7):1517–1561, 2017.

[4] L. Drescher, H. Heumann, and K. Schmidt. A high order galerkin method for integrals over contour lines with an application to plasma physics. *SIAM Numer. Math.*, 55(6):2592–2615, 2017.

[5] H. Egger, C. Erath, and R. Schorr. On the non-symmetric coupling method for parabolic-elliptic interface problems. *SIAM J. Numer. Anal.*, 56(6):3510–3533, 2018.

[6] H. Egger and T. Kugler. Damped wave systems on networks: Exponential stability and uniform approximations. *Numer. Math.*, 138:839–867, 2018.

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[12] C. Erath and D. Praetorius. Adaptive vertex-centered finite volume methods for general second-order linear elliptic pdes. *IMA J. Numer.Anal.*, published online, 2018.

[13] C. Erath and R. Schorr. An adaptive non-symmetric finite volume and boundary element coupling method for a fluid mechanics interface problem. *SIAM J. Sci. Comput.*, 39(3):A741–A760, 2017.

[14] S. Eriksson. Asymptotic expansion techniques for singularly perturbed boundary integral equations. *Journal of Scientific Computing*, 75(2):906–940, 2018.

[15] A. Hodgkinson, M. A. J. Chaplain, P. Domschke, and D. Trucu. Computational approaches and analysis for a spatio-structural-temporal invasive carcinoma model. *Bulletin of Mathematical Biology*, 80(4):701–737, 2018.

[16] J. Lang and W. Hundsdorfer. Extrapolation-based implicit-explicit Peer methods with optimised stability regions. *J. Comp. Phys.*, 337:203–215, 2017.

[17] J. Lang and P. Mindt. Entropy-preserving coupling conditions for one-dimensional Euler systems at junctions. *Netw. Heterog. Media*, 13:177–190, 2018.

[18] A. A. Lukassen and M. Kiehl. Operator splitting for chemical reaction systems with fast chemistry. *Journal of Computational and Applied Mathematics*, 344:495–511, 2018.

[19] A. A. Lukassen and M. Kiehl. Parameter estimation with model order reduction for elliptic differential equations. *Inverse Problems in Science and Engineering*, 26(4):479–497, 2018.

[20] F. Meyer, J. Giesselmann, and C. Rohde. A posteriori error analysis for random scalar conservation laws using the stochastic galerkin method. *IMA J. Numer. Anal.*, 2019.

[21] S. Nicaise and A. Semin. Density and trace results in generalized fractal networks. *ESAIM: Mathematical Modelling and Numerical Analysis*, 52(3):1023–1049, 2018.

[22] R. Penta and A. Gerisch. The asymptotic homogenization elasticity tensor properties for composites with material discontinuities. *Continuum Mechanics and Thermodynamics*, 29:187–206, 2017.

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[29] M. Walloth. A reliable, efficient and localized error estimator for a discontinuous Galerkin method for the Signorini problem. *Appl. Numer. Math.*, 135:276–296, 2019.

3.3.2 Proceedings and Chapters in Collections

[1] H. Egger and T. Kugler. An asymptotic preserving mixed finite element method for wave propagation in pipelines. In *Theory, Numerics and Applications of Hyperbolic Problems I*, pages 515–527. Springer International Publishing, Cham, 2017.

[2] H. Egger and B. Radu. A mass-lumped mixed fem for acoustic wave propagation with inhomogeneous coefficients. *PAMM*, 18:1–2, 2018.

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et al., editors, *Progress in Industrial Mathematics at ECMI 2016*, pages 385–392. Springer International Publishing, Cham, 2017.

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[12] M. Walloth. Localized and efficient estimators for obstacle problems in the context of standard residual estimators. *PAMM*, 17:767–768, 2017.

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3.4 Preprints

[1] P. Domschke, B. Hiller, J. Lang, and C. Tischendorf. Modellierung von Gasnetzwerken: Eine Übersicht. Preprint 2717, Fachbereich Mathematik, TU Darmstadt, 2017.

[2] H. Egger, T. Kugler, and B. Liljegren-Sailer. Stability preserving approximations of a semilinear hyperbolic gas transport model. arXiv:1812.03726, 2018.

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[13] C. Erath and R. Schorr. Stable non-symmetric coupling of the finite volume and the boundary element method for convection-dominated parabolic-elliptic interface problems. arXiv:1805.05142, 2018.

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3.5 Reviewing and Refereeing

Jürgen Dölz: SIAM Journal on Scientific Computing

Herbert Egger: Mathematical Reviews; Applied Mathematics and Computer Science, Applied Numerical Mathematics, Applied Mathematics and Computation, Computational and Applied Mathematics with Applications, BIT Numerical Mathematics, Computational and Applied Mathematics, Computers and Mathematics with Applications, ESAIM: Control Optimisation and Calculus of Variations, ESAIM:Mathematical Modelling and Numerical Analysis, Inverse Problems, Journal Applied Mathematics and Computing, Journal Inverse and Ill-posed Problems, Journal Mathematical Analysis and Applications, Mathematical and Compuational Applications, Mathematical Methods in the Applied Sciences, Numerische Mathematik, SIAM Journal on Numerical Analysis, SIAM Journal on Scientific Computing

Christoph Erath: Mathematical Reviews; SIAM Journal Scientific Computing, Computers and Mathematics with Applications, Applied Mathematics and Computation, Monthly

Weather Review, Science China Mathematics, Finite Volumes for Complex Applications 8

Alf Gerisch: Biomechanics and Modeling in Mechanobiology, European Journal of Applied Mathematics, Journal of Theoretical Biology, Numerical Algorithms, Numerical Methods for Partial Differential Equations, The Fund for Scientific Research (FNRS, Belgium), Research Foundation - Flanders (FWO, Belgium), Netherlands Organisation for Scientific Research (NWO, The Netherlands)

Jan Giesselmann: Mathematical Reviews; Computational Methods in Applied Mathematics, Computational and Applied Mathematics, Networks and Heterogeneous Media, SIAM Journal on Numerical Analysis, Zeitschrift für Angewandte Mathematik und Physik

Jens Lang: Applied Numerical Mathematics, Combustion Theory and Modelling, Journal of Physics A: Mathematical and General, Inverse Problems, Computing and Visualization in Science, International Journal of Hyperthermia, International Journal for Numerical Methods in Fluids, Transactions on Mathematical Software, Journal of Computational Physics, Computational and Applied Mathematics, IMA Journal of Numerical Analysis, Mathematics of Computation, SIAM Journal Numerical Analysis, SIAM Journal Scientific Computing

Kersten Schmidt: Advances in Computational Mathematics, Computers and Structures, SIAM Journal on Applied Mathematics, Zeitschrift für Angewandte Mathematik und Physik

Sebastian Ullmann: Advances in Computational Mathematics, Applied Numerical Mathematics, Computational and Applied Mathematics, ESAIM: M2AN: Mathematical Modelling and Numerical Analysis, SIAM/ASA Journal on Uncertainty Quantification

Mirjam Walloth: IMA Journal of Numerical Analysis, ESAIM: M2AN: Mathematical Modelling and Numerical Analysis, SIAM Journal on Numerical Analysis

3.6 Software

ANACONDA: *Solving Hyperbolic Partial Differential Algebraic Equations on Networks*
ANACONDA is a software package to solve hyperbolic partial differential algebraic equations on networks. Particularly, it is designed to solve simulation and optimal control tasks for gas and water supply networks.

Contributor at TU Darmstadt: Pia Domschke, Jens Lang, Lisa Wagner, and formerly Oliver Kolb (now at Universität Mannheim)

FastCOIN: *Fast adaptive stochastic COllocation INfrastructure*
FastCOIN is a software package that implements an adaptive, anisotropic stochastic collocation approach on sparse grids for the quantification of uncertainty in PDEs or other models with random parameters described by finitely many random variables. This includes, in particular, finite-dimensional parametrizations of correlated random

fields. Similar to a Monte Carlo simulation, this approach decouples and, hence, parallelizes the stochastic problem into a set of deterministic problems. FastCOIN is able to resolve a stochastic parameter space of dimensions up to $20-50$.

Contributor at TU Darmstadt: Jens Lang, Alf Gerisch, Sebastian Ullmann, and formerly Bettina Schieche (now at COMSOL)

KARDOS: *Solving Time-Dependent Partial Differential Equations*
KARDOS is a software package to solve partial differential equations in one, two and three space dimension adaptively in space and time. Linearly implicit one-step methods of Rosenbrock type or two-step PEER-methods are coupled with standard Finite Elements of various orders. Extensions that we are working on include: incorporation of computational fluid dynamics, optimisation and moving finite elements.

Contributor at TU Darmstadt: Jens Lang, Alf Gerisch, Zhen Sun

CONCEPTS: *High-order and generalized finite element library*
The numerical C++ library provides finite element methods of higher order, generalized finite element methods and boundary element methods in common object-oriented structures. We developed hp-adaptive finite element methods on curved quadrilateral and hexadredal meshes with locally varying and anisotropic polynomial orders for Poisson and Helmholtz problems, problems in elektromagnetics, quantum physics, viscous acoustics (based on Navier-Stokes equations), elasticity and coupling of those models. The matrices can be assembled and linear systems solved in parallel where we also give access to external direct solvers. There is is a number of time integration schemes for dynamical modelling. CONCEPTS has got a large class documentation and various tutorials are available.
For more information, see `https://wiki.math.ethz.ch/Concepts`

Contributor at TU Darmstadt: Kersten Schmidt, Adrien Semin, Vsevolod Shashkov

donlp2: *Solving general smooth nonlinear optimization problems, last revision January 2015*
donlp2 is a software for the solution of general nonlinear programming problems. Different versions exist concerning the programming language (strict f77, f90, C99), the user interface and some options (for example elimination of redundant linear equality constraints and an interfacing known as “reverse communication”). donlp2 is free for research, whereas commercial use requires licensing by TU Darmstadt. During the report period 21 academic (free) licenses were given. There were 7 commercial requests, but due to misconceptions concerning the royalty fee from the partners side these were not satisfied. For more information, see `www.mathematik.tu-darmstadt.de/fbereiche/numerik/staff/spellucci/DONLP2/`

Contributor at TU Darmstadt: Peter Spellucci

numawww: *Interactive computing exercises for numerical methods and continuous optimization*
Numawww is a cgi/html-based computing device for general numerical methods and methods of continuous optimization. In operation since 1996 it has been continuously further developed. It may be used for exercises during a numerical methods

course, as a self teaching aid or even as a small scale computing device, requiring minimal knowledge of programming which is presented inside the system itself. It is accessible from anywhere in the world. During 2017 there were 33620 visits from 44 countries viewing 163132 pages and in 2018 29442 visits from 39 countries viewing 166548 pages. Any application comes with predefined test cases which can be used without programming knowledge at all. Presently only the English version receives further development, but the German version will be maintained. In the current report period some minor improvements were done, but presently a major revision making it even more comfortably to use is under development. For more information, see `numawww.mathematik.tu-darmstadt.de`

Contributor at TU Darmstadt: Peter Spellucci

TriangularTaylorHood: *Triangular Taylor Hood finite elements, version 1.5.0.0*
This Matlab toolbox solves PDE problems with mixed P2/P1 (Taylor Hood) finite elements. The capabilities of the toolbox are demonstrated with an unsteady thermally driven flow in a tall cavity, as described in `http://dx.doi.org/10.1002/fld.395` (Christon et al., 2002). Source code and license: `https://de.mathworks.com/matlabcentral/fileexchange/49169-triangular-taylor-hood-finite-elements`

Contributor at TU Darmstadt: Sebastian Ullmann

4 Theses

4.1 Habilitations

2018

Schmidt, Kersten, *Asymptotic and numerical analysis of impedance and absorbing boundary conditions* (Umhabilitation von TU Berlin)

4.2 PhD Dissertations

2017

Seitz, Tobias, *Geometry identification and data enhancement for distributed flow measurements* (Herbert Egger)

Wagner, Lisa Sabine, *Second-Order Implicit Methods for Conservation Laws with Applications in Water Supply Networks* (Jens Lang)

2018

Alex, Jerome, *The periodic Steiner problem* (Herbert Egger)

Lukassen, Axel Ariaan, *Simulation von chemischen Reaktionssystemen mit schnellen chemischen Reaktionen* (Martin Kiehl)

Mindt, Pascal, *Hierarchical Gas Model Coupling on Networks* (Jens Lang)

Müller, Christopher, *Iterative solvers for stochastic Galerkin discretizations of Stokes flow with random data* (Jens Lang)

Spannring, Christopher, *A weighted reduced basis method for parabolic PDEs with random input data* (Jens Lang)

Sun, Zhen, *Adaptive Moving Finite Element Method for Steady Low-Mach-Number Compressible Combustion Problems* (Jens Lang)

4.3 Master Theses

2017

Barg, Angelika, *Ziel-orientierte Adaptivität für eine stochastische Galerkin-Finite-Elemente-Methode* (Sebastian Ullmann)

Göbel, Rebecca, *Numerische Verfahren für Chemotaxis Modelle* (Herbert Egger)

Köster, Thorben, *Runge-Kutta-Verfahren mit optimaler Stabilität für unstetige, räumliche Diskretisierungen* (Jens Lang)

Strauch, Elisa, *Stochastische finite Elemente zur Berechnung von Spannungen in der oberen Erdkruste* (Sebastian Ullmann)

2018

Cuca, Aleksandar, *Numerische Untersuchung von Blowup in einem Keller-Segel System* (Jens Lang)

Habrich, Oliver André, *Numerical Approximation and Parameter Identification for the Cahn-Hilliard Equation* (Herbert Egger)

Kiel, Steffen, *Das Vorgehen von Bayes für Inverse Probleme* (Jens Lang)

Müller, Fabian, *Numerical quadrature on irregular domains and application in the Finite Cell Method* (Herbert Egger)

Steinbach, Philipp, *Adaptive Finite Elemente Verfahren für Erdwärmesonderspeicher* (Jens Lang)

4.4 Bachelor Theses

2017

Kaiser, Kim Doreen, *Exponentielle Konvergenz der zusammengesetzten Trapezregel und ihre Anwendung* (Alf Gerisch)

Kiel, Steffen, *The Nyström method for Fredholm integral equations of the second kind* (Christoph Erath)

Kosara, Thomas, *Fast Fourier Transform zur effizienten Berechnung von Matrix-Vektor-Produkten mit zirkulanten Matrizen* (Alf Gerisch)

Kunkel, Teresa, *Simulation von Ionentransport durch biologisches Gewebe* (Herbert Egger)

Philippi, Nora Marie, *Splitting Methods for Transport Equations* (Christoph Erath)

Strelow, Erik Laurin, *Spektralmethoden und Zeitintegration höherer Ordnung* (Alf Gerisch)

2018

Accorsini, Lisamarie, *Integralapproximation auf einem periodischen Gitter* (Alf Gerisch)

Klopp, Adrian, *Simulation and control of epidemics of influenza-like diseases* (Martin Kiehl)

5 Presentations

5.1 Talks and Visits

5.1.1 Invited Talks and Addresses

Pia Domschke

10/10/2018 *Error-controlled adaptive simulation of large gas networks*
2nd Conference Mathematics of Gas Transport (MoG2), Berlin

Herbert Egger

31/03/2017 *A scatter correction algorithm for computed tomography in semi-transparent media*
100 Years Radon Workshop, RICAM Linz

03/04/2017 *On compressible flow in pipeline networks: Variational principles and numerical approximation*
Seminar in Applied Mathematics, Eindhoven University of Technology, The Netherlands

06/04/2017 *On compressible flow in pipeline networks: Variational principles and numerical approximation*
Seminar 4TU, University of Twente, The Netherlands

28/06/2017 *Accelerated image reconstrucion algorithms in fluorescence optical tomography*
PASC, Lugano, Switzerland

03/11/2017 *A mixed finite element approximation for the isentropic Euler equations*
Seminar in Mathematics, Universität Basel

15/12/2017 *Inverse problems for partial differential equations*
TRR 146 Lecture Series, Universität Mainz

07/05/2018 *Structure preserving numerical approximation of dissipative evolution problems*
Workshop on Mathematical Fluid Dynamics, Bad Boll

25/07/2018 *Optimal control of instationary gas transport*
IFIP, Essen

26/07/2018 *Tikhonov regularization under conditional stability*
IFIP, Essen

31/07/2018 *Variational methods for radiative transfer*
Seminar in Applied Mathematics, Universität Innsbruck

18/10/2018 *Structure preserving numerical approximation of dissipative evolution problems*
IGPM Seminar, RWTH Aachen

30/11/2018 *Estimation of geometry and flow characteristics from magnetic resonance measurements*
Analysis, Control and Inverse Problems for PDEs, Naples, Italy

Christoph Erath

07/06/2018 *Efficient solving of a time-dependent interface problem*
Universität Innsbruck

Sofia Eriksson

01/06/2017 *A dual consistent finite difference method*
Workshop "Numerical methods for PDEs and their applications", Uppsala University, Sweden

Alf Gerisch

21/02/2017 *A nonlocal model for adhesion in cancer invasion: modelling and numerics*
Workshop *Mathematical Models for Cell Migration and Dispersal*, TU Kaiserslautern

01/12/2017 *Nonlocal PDE models for cellular adhesion with application in cancer invasion*
International Conference *Current Trends in Theoretical and Computational Differential Equations with Applications*, South Asian University, New Delhi, India

06/12/2017 *Nonlocal PDE models for cellular adhesion with application in cancer invasion*
Mathematics Colloquium, Indian Institute of Technology (IIT) Roorkee, India

07/03/2018 *A comparison of integro-PDE models of cellular adhesion derived from a space-jump process*
Gemeinsame Jahrestagung der DMV und der GDM 2018, Paderborn

25/10/2018 *Attraction and Repulsion in Biological Tissues: Challenges for Models, Analysis, and Numerics*
ZIH Colloquium, TU Dresden

Martin Kiehl

25/02/2017 *Die Mathematik im Puzzlestein – Warum Mathematiker ein Leben lang spielen?*
Mathematikolympiade Hessen, Darmstadt

11/03/2017 *Mathematische Modellierung mit Funktionen.*
Tag der Mathematik, Reinheim

24/03/2017 *Mathematische Modellierung mit Schülern beim Zentrum für Mathematik.*
Forum für Begabung, Hochschule Darmstadt

10/03/2018 *Wie gewinnt man mit Mathematik eine Goldmedaille im Skifliegen?*
MINT Tagung für junge Lehrer, Hochschule Darmstadt

10/03/2018 *Von Galileo und Kepler zu Newton – Spass an Physik durch Mathematik*
MINT Tagung für junge Lehrer, Hochschule Darmstadt

Jens Lang

08/05/2017 *Adaptivity in numerical methods for ODEs and PDEs*
University of Bath, UK

18/05/2017 *Adaptive modelling, simulation and optimization of complex water and gas flow in supply networks*
University of Bath, UK

19/07/2017 *Reduced-order models with space-adapted snapshots*
Quantification of Uncertainty: Improving Efficiency and Technology, Trieste, Italy

12/09/2017 *Rosenbrock-Wanner-methods: construction and mission*
International Conference on Scientific Computation and Differential Equations (SciCADE) 2017, Bath, UK

01/03/2018 *Adaptivity in numerical methods for ODEs and PDEs*
Isaac Newton Institute Cambridge, UK

06/03/2018 *Adaptive multilevel stochastic collocation method for randomized elliptic PDEs*
Isaac Newton Institute Cambridge, UK

16/06/2018 *Adaptivity in numerical methods for ODEs and PDEs: Towards the simulation of a full heartbeat*
Universität Innsbruck

26/07/2018 *Reduced-order models with space-adapted snapshots*
World Congress of Computational Mechanics 2018, New York, USA

05/09/2018 *IMEX-Peer methods based on extrapolation*
Conference on the Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-15) 2018, Halle (Saale)

Christopher Müller

28/11/2018 *What is...? Reduced order modeling*
What is...? Seminar, Fachbereich Mathematik, TU Darmstadt

Kersten Schmidt

23/04/2018 *Asymptotic and numerical analysis of absorbing and impedance boundary conditions*
Department of Mathematics, University of Zagreb

06/07/2018 *A high order Galerkin method for the approximation of contour integrals*
Rhein-Main Arbeitskreis, Darmstadt

11/07/2018 *Einfach Randbedingungen – asymptotische und numerische Analysis von absorbierenden und Impedanzrandbedingungen*
Fachbereich Mathematik, TU Darmstadt

Tobias Seitz

15/12/2017 *Data enhancement for distributed flow measurements*
TRR 146 Lecture Series, Universität Mainz

Adrien Semin

09/05/2018 *Asymptotic and numerical analysis of absorbing and impedance boundary conditions*
Universität Halle-Wittenberg, Halle (Saale)

24/10/2018 *What are... PML and ABC?*
What is? Seminar, Fachbereich Mathematik, TU Darmstadt

Gabriel Teschner

13/06/2018 *What is...? Spannungsbasierte Modellierung*
What is...? Seminar, Fachbereich Mathematik, TU Darmstadt

Mirjam Walloth

07/07/2017 *Residual-type a posteriori estimators for continuous and discontinuous Galerkin methods for Signorini problems.*
Rhein-Main Arbeitskreis, Mannheim

12/10/2017 *Adaptive finite elements for contact problems based on efficient and reliable residual-type a posteriori estimators.*
7th GACM Colloquium on Computational Mechanics, Stuttgart

23/01/2018 *Residual-type a posteriori estimator for a quasi-static contact problem.*
Mathematisches Institut, Universität Freiburg

5.1.2 Contributed Talks

Jürgen Dölz

06/10/2018 *On the best approximation of the hierarchical matrix product*
16th Workshop on Fast Boundary Element Methods in Industrial Applications, Hirschegg

12/10/2018 *On the best approximation of the hierarchical matrix product*
2nd Workshop of the Agility Group on Numerical Analysis of the International Association of Applied Mathematics and Mechanics (GAMM), Augsburg

Herbert Egger

25/09/2017 *A mixed finite element approximation for the isentropic compressible Euler equations*
30th Chemnitz FEM Symposium, Strobl

02/11/2017 *A mixed finite element approximation for the isentropic compressible Euler equations*
GAMM Workshop on Numerical Analysis, Aachen

21/05/2018 *Tikhonov regularization under conditional stability*
Inverse Problems: Modeling and Simulation, Malta

12/07/2018 *A hybrid mixed discontinuous Galerkin method for compressible flow on networks*
International Conference on Spectral and High Order Methods, London, UK

05/09/2018 *Structure preserving approximation of evolution problems with dissipation*
Conference on the Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-15) 2018, Halle (Saale)

27/09/2018 *Mass-lumped mixed finite element methods for Maxwell's equations*
12th International Conference on Scientific Computing in Electrical Engineering, Taormina, Italy

11/10/2018 *Structure preserving numerical approximation of dissipative evolution problems*
GAMM Workshop on Numerical Analysis, Augsburg

Christoph Erath

12/06/2017 *Céa-type quasi-optimality and convergence rates for (adaptive) vertex-centered FVM*
Finite Volumes for Complex Applications VIII (FVCA 8), Lille, France

25/09/2017 *Adaptive vertex-centered finite volume methods (Petrov-Galerkin) with convergence rates for general second-order linear elliptic PDE*
30th Chemnitz FEM Symposium, Strobl

26/09/2017 *Adaptive coupling of finite volume and boundary element methods: non-symmetric and three-field FVM-BEM*
30th Chemnitz FEM Symposium, Strobl

13/10/2017 *A non-symmetric FEM-BEM coupling method for a parabolic-elliptic interface problem*
15. Söllerhaus Workshop on Fast BEM in Industrial Applications, Hirschegg

20/03/2018 *Non symmetric FEM-BEM coupling for solving a time-dependent interface problem*
89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), München

26/06/2018 *Non symmetric FEM-BEM coupling for solving a time-dependent interface problem*
Symposium of the International Association for Boundary Element Methods 2018, Paris, France

02/07/2018 *Was sind/waren meine bisherigen Forschungsarbeiten?*
Research Meeting for Cooperation, Graz

Sofia Eriksson

19/01/2017 *Coupling of the cell-centered finite volume method and the boundary element method for time-dependent problems of advection-diffusion type*
Seminar der AG Numerik, TU Darmstadt

02/10/2017 *A dual consistent finite difference method*
University of East Anglia, Norwich, UK

David Frenzel

30/10/2017 *Optimal control of hyperbolic conservation laws*
CE Research Colloquium, TU Darmstadt

27/06/2018 *WENO schemes in optimal control of hyperbolic conservation laws (Poster)*
XVII International Conference on Hyperbolic Problems Theory, Numerics, Applications (Hyp2018), Pennsylvania State College, USA

30/10/2018 *WENO schemes in optimal control of nonlinear hyperbolic conservation laws*
Seminar der AG Numerik, TU Darmstadt

18/12/2018 *WENO schemes in optimal control of nonlinear hyperbolic conservation laws*
CE Research Colloquium, TU Darmstadt

Alf Gerisch

26/07/2018 *Insight into a nonlocal PDE model of cellular adhesion by microscale space-jump process modelling*
European Conference on Mathematical and Theoretical Biology (ECMTB) 2018, Lisbon, Portugal

04/09/2018 *FFT-based evaluation of nonlocal terms in PDE systems*
Conference on the Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-15) 2018, Halle (Saale)

Thomas Kugler

21/03/2018 *Optimal control of instationary gas transport*
89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), München

05/06/2018 *Structure preserving model reduction for wave propagation with nonlinear damping*
Seminar der AG Numerik, TU Darmstadt

27/06/2018 *Structure preserving model reduction for wave propagation with nonlinear damping*
XVII International Conference on Hyperbolic Problems Theory, Numerics, Applications (Hyp2018), Pennsylvania State College, USA

Jens Lang

26/09/2017 *On the stability and conditioning of anisotropic Finite-Element-Runge-Kutta methods*
30th Chemnitz FEM Symposium, Strobl

Axel Ariaan Lukassen

09/03/2017 *Parameter estimation with reduced basis methods for elliptic differential equations*
88th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), Weimar

22/03/2018 *Operator splitting for stiff differential equations*
89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), München

23/10/2018 *Simulation von chemischen Reaktionssystemen mit unterschiedlichen Zeitskalen*
Doctoral examination, Darmstadt

Christopher Müller

21/03/2017 *Stochastic Galerkin methods for incompressible flows (Poster)*
7th Retreat of the GSC CE 2017, Seeheim

19/07/2017 *Conjugate gradient methods for stochastic Galerkin finite element matrices with saddle point structure (Poster)*
Quantification of Uncertainty: Improving Efficiency and Technology, Trieste, Italy

29/09/2017 *Efficient iterative methods for discrete Stokes equations with random viscosity*
4th International Conference on Computational Engineering (ICCE), Darmstadt

04/12/2017 *Iterative solvers for stochastic Galerkin finite element discretizations of Stokes flow with lognormal random data*
CE Research Colloquium, TU Darmstadt

16/04/2018 *Efficient iterative methods for discrete Stokes equations with random viscosity (Poster)*
SIAM Conference on Uncertainty Quantification 2018, Garden Grove, California, USA

18/06/2018 *Iterative solvers for stochastic Galerkin discretizations of Stokes flow with random data*
Doctoral examination, TU Darmstadt

Bogdan Radu

23/03/2017 *Mixed finite element methods for the acoustic wave equation*
CE Research Colloquium, TU Darmstadt

20/11/2017 *A mixed finite element method for wave propagation with mass lumping*
Seminar der AG Numerik, TU Darmstadt

21/03/2018 *A Mixed FEM with mass lumping for acoustic wave propagation*
89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), München

26/06/2018 *A Mixed FEM with mass lumping for acoustic wave propagation*
XVII International Conference on Hyperbolic Problems Theory, Numerics, Applications (Hyp2018), Pennsylvania State College, USA

Kersten Schmidt

22/03/2018 *High-oder adaptive mortar finite element discretization for PDE eigenvalue problems in quantum chemistry*
89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), München

26/07/2018 *Multiharmonic analysis for nonlinear acoustics with small excitation amplitude*
Conference on Mathematics of Wave Phenomena, Karlsruhe

Moritz Schneider

11/09/2017 *Superconvergent IMEX Peer methods*
International Conference on Scientific Computation and Differential Equations (SciCADE) 2017, Bath, UK

15/05/2018 *Superconvergent IMEX Peer methods*
Seminar der AG Numerik, TU Darmstadt

06/09/2018 *Superconvergent IMEX Peer methods with A-stable implicit part*
Conference on the Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-15) 2018, Halle (Saale)

Lucas Schöbel-Kröhn

13/11/2017 *Analysis and numerical approximation of chemotaxis on networks*
Seminar der AG Numerik, TU Darmstadt

25/01/2018 *Analysis and numerical approximation of chemotaxis on networks*
Seminar of the International Research Training Group 1529, TU Darmstadt

24/07/2018 *Degenerate parabolic equations modelling gas transport on networks*
IFIP TC 7 Conference on System Modelling and Optimization, Essen

Robert Schorr

12/06/2017 *Comparison of adaptive non-symmetric and three-field FVM-BEM coupling*
Finite Volumes for Complex Applications VIII (FVCA 8), Lille, France

25/09/2017 *Non-symmetric coupling of Finite Element Method and Boundary Element Method for parabolic-elliptic interface problems*
European Conference on Numerical Mathematics and Advanced Applications (ENUMATH), Voss, Norway

23/10/2017 *Non-symmetric coupling of Finite Element Method and Boundary Element Method for parabolic-elliptic interface problems*
CE Research Colloquium, TU Darmstadt

20/03/2018 *Stable non-symmetric coupling of the finite volume and the boundary element method for convection-dominated parabolic-elliptic interface problems*
89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), München

26/06/2018 *Stable non-symmetric coupling with the boundary element method for convection-dominated parabolic-elliptic interface problems*
Symposium of the International Association for Boundary Element Methods, Paris, France

27/08/2018 *Stable non-symmetric coupling with the boundary element method for convection-dominated parabolic-elliptic interface problems*
CE Research Colloquium, TU Darmstadt

Tobias Seitz

21/03/2017 *Identification and optimization of flow and transport phenomena (Poster)*
7th Retreat of the GSC CE, Seeheim

Adrien Semin

09/03/2018 *Asymptotic modeling of the wave-propagation over acoustic liners*
Seminar der AG Numerik, TU Darmstadt

26/08/2018 *Asymptotic modelling of the wave propagation in presence of an array of Helmholtz resonators*
Conference on Mathematics of Wave Phenomena, Karlsruhe

Vsevolod Shashkov

22/11/2018 *Convolution quadrature methods for coupled nonlinear-linear dynamical systems*
Seminar der AG Numerik, TU Darmstadt

Christopher Spannring

21/03/2017 *Reduced basis methods for PDE problems with random data (Poster)*
7th Retreat of the GSC CE 2017, Seeheim

19/07/2017 *Weighted reduced basis methods for parabolic PDEs with random data (Poster)*
Quantification of Uncertainty: Improving Efficiency and Technology, Trieste, Italy

19/09/2017 *A weighted reduced basis method for parabolic PDEs with random data*
Reduced Basis Summer School 2017, Goslar

29/09/2017 *A weighted reduced basis method for parabolic PDEs with random data*
4th International Conference on Computational Engineering (ICCE), Darmstadt

20/11/2017 *Weighted reduced basis method for parabolic PDEs with random data*
CE Research Colloquium, TU Darmstadt

16/04/2018 *A weighted reduced basis method for parabolic PDEs with random data*
SIAM Conference on Uncertainty Quantification 2018, Garden Grove, California, USA

28/06/2018 *Weighted reduced basis methods for parabolic PDEs with random input data*
Doctoral examination, TU Darmstadt

Philipp Steinbach

10/07/2018 *Adaptive Finite-Elemente-Verfahren für Erdwärmesondenspeicher*
Seminar der AG Numerik, TU Darmstadt

28/11/2018 *Adaptive Finite-Elemente-Verfahren für Erdwärmesondenspeicher (Poster)*
Geothermiekongress 2018, Essen

Elisa Strauch

09/01/2018 *A multi-level Monte Carlo finite element method for stresses along paths*
Seminar der AG Numerik, TU Darmstadt

12/03/2018 *A multi-level Monte Carlo method for stresses along paths (Poster)*
3rd Workshop of the Agility Group on Uncertainty Quantification of the International Association of Applied Mathematics and Mechanics (GAMM), TU Dortmund

Gabriel Teschner

16/01/2018 *Fast iterative solvers for fluid flow problems discretized by finite elements*
Seminar der AG Numerik, TU Darmstadt

27/09/2018 *Estimation of flow geometry and wall shear stress from magnetic resonance imaging*
Chemnitz Symposium on Inverse Problems 2018, TU Chemnitz

Sebastian Ullmann

01/03/2017 *Adaptive reduced-order modeling for flows under uncertainty*
SIAM Conference on Computational Science and Engineering, Atlanta, Georgia, USA

08/09/2017 *CFD under uncertainty: combining model order reduction with spatial adaptivity*
Workshop on Frontiers of Uncertainty Quantification in Engineering, München

28/09/2017 *Model order reduction and spatial adaptivity for incompressible flows with random data*
4th International Conference on Computational Engineering (ICCE), Darmstadt

05/03/2018 *Stochastic Galerkin reduced basis methods for parametrized random elliptic PDEs (Poster)*
UNQW03, Isaac Newton Institute, Cambridge, UK

12/04/2018 *Stochastic Galerkin reduced basis methods for parametrized random elliptic PDEs (Poster)*
Model Reduction of Parametrized Systems, Nantes, France

16/04/2018 *Stochastic Galerkin reduced basis methods for parametrized random elliptic PDEs (Poster)*
SIAM Conference on Uncertainty Quantification 2018, Garden Grove, California, USA

29/05/2018 *Stochastic Galerkin reduced basis methods for parametrized random elliptic PDEs*
Uncertainty quantification for complex systems: theory and methodologies, Isaac Newton Institute, Cambridge, UK

06/09/2018 *Model order reduction for space-adaptive simulations of unsteady incompressible flows*
Conference on the Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-15) 2018, Halle (Saale)

Mirjam Walloth

12/01/2017 *A reliable, efficient and localized error estimator for a discontinuous Galerkin method for the Signorini problem*
Seminar der AG Numerik, TU Darmstadt

09/03/2017 *A reliable, efficient and localized error estimator for a discontinuous Galerkin method for the Signorini problem*
88th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), Weimar

21/03/2018 *A posteriori error estimation in space and time for contact problems in linear viscoelasticity*
89th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), München

14/09/2018 *Reliable, efficient and robust a posteriori estimators for the variational inequality in fracture phase-field models*
Jahrestreffen des SPP 1748, Dresden

Dimitrios Zacharenakis

01/10/2018 *A posteriori error estimates for a discontinuous Galerkin approximation of the Navier-Stokes-Korteweg model (Poster)*
Fall School on Hyperbolic Conservation Laws and Mathematical Fluid Dynamics, Universität Würzburg

11/12/2018 *A posteriori error estimates for a discontinuous Galerkin approximation of the Navier-Stokes-Korteweg model*
Seminar der AG Numerik, TU Darmstadt

5.1.3 Visits

Herbert Egger, University of Twente, TU Eindhoven, The Netherlands, April 2017

Herbert Egger, RWTH Aachen, October 2018

Herbert Egger, Universität Innsbruck, October 2018

Alf Gerisch, Indian Institute of Technology (IIT) Roorkee, India, November–December 2017

Jens Lang, University of Bath, UK, April–May 2017

Jens Lang, University of Southern Denmark, Odense, Denmark, June 2017

Jens Lang, Isaac Newton Institute, University of Cambridge, UK, March–April 2018

Sebastian Ullmann, Isaac Newton Institute, University of Cambridge, UK, May–June 2018

5.2 Organization and Program Commitees of Conferences and Workshops

Mirjam Walloth

– Current Trends and Open Problems in Computational Solid Mechanics (jointly with Fadi Aldakheel, Thomas Wick, Winnifried Wollner, Peter Wriggers), Oct 8–9, 2018, Universität Hannover

6 Workshops and Visitors at the Department

6.1 Visitors at the Department

Dr. Raimondo Penta (University of Glasgow, UK), June 2018.

Rasa Giniunaite (University of Oxford, UK), August 2018.

Prof. Dr. Ram Jiwari (Indian Institute of Technology Roorkee, India), June-July 2017.

Carmen Gräßle (Universität Hamburg), June 2017, January-February 2018, April 2018.

6.2 Workshops and Conferences at the Department

- Mathematische Modellierungswoche, October 15–20, 2017, Fuldatal (organized by Martin Kiehl, TU Darmstadt and Tobias Braumann, Zentrum für Mathematik, Bensheim)
- Mathematische Modellierungswoche, October 7–12, 2018, Fuldatal (organized by Martin Kiehl, TU Darmstadt and Tobias Braumann, Zentrum für Mathematik, Bensheim)

7 Other scientific and organisational activities

7.1 Memberships in Scientific Boards and Committees

Martin Kiehl

- Vorsitzender des Aufsichtsrats, Zentrum für Mathematik, Bensheim

Jens Lang

- Member of Board of Deans of the DFG Graduate School of Excellence Computational Engineering, TU Darmstadt, since 2008
- Member of Scientific Steering Committee of Profile Area Thermo-Fluids & Interfaces, TU Darmstadt, since 2017
- Member of Scientific Committee of the Conference on the Numerical Solution of Differential and Differential-Algebraic Equations to be held at the Martin-Luther University Halle-Wittenberg every three years

7.2 Awards

Awards

Mirjam Walloth: Ruth Moufang-Postdoktorandinnen-Förderpreis (Fachbereich Mathematik, TU Darmstadt), June 02, 2017

The department of mathematics is involved in various activities for schools, secondary school students, and public relations. In addition to printed information material, the department of mathematics presents itself to the public on its web pages. These were fundamentally revised in 2017 and provide useful information about all aspects of the study as well as an attractive insight into the department. The information is available in German and in English.

Math on Demand In April 2015, the mathematics department of TU Darmstadt launched the programme *Math on Demand* for mathematically interested secondary school students and mathematics teachers. The purpose of this programme is to stimulate their interest in mathematics beyond the traditional classroom. On demand, scientists from the mathematics department offer lectures or workshops, which are intended to illustrate the variety and importance of mathematics in everyday life, and to give a first insight in some recent developments in the tremendous opportunities for careers in mathematics and about the mathematics programme at TU Darmstadt.

By now ten scientists (F. Aurzada, P. Domschke, R. Haller-Dintelmann, A. Knof, B. Kümmerer, M. Otto, A.-M. von Pippich, U. Reif, A. Schwartz, B. Seyfferth) offer lectures covering a wide range of topics. In 2017 and 2018, 17 lectures or workshops were held for a variety of audiences from the Rhine-Main metropolitan area and its surroundings. Further information is available on the webpage `https://www.mathematik.tu-darmstadt.de/studium/orientierung_und_beratung/veranstaltungen_fuer_studieninteressierte/math_on_demand.en.jsp`

Summer school "Faszination Mathematik" for secondary school students

The following is a list of further public relations activities.

Activities for secondary school students and prospective students

- Presentation of the department with a booth and several talks at the job and study information fair HoBIT, Hochschul- und Berufsinformationstage, three days every January: about 20.000 participants; with a booth staffed by professors, academic staff and students and scientific talks from the fields of Analysis, Logic, and Stochastics in 2017 and from the fields of Algebra, Logic and Geometry in 2018.

- Presentation of the department and its study programmes at the university information day, TUDay, every May: with talks by the student advisor, sample lectures and tutorial classes, meetings with students of the department; about 80 participants over the course of the day (lectures from the fields of Algebra and Analysis in 2017 and two lectures from the field of Optimization in 2018).

- Annual organization of an afternoon with several talks about mathematics for secondary school students, "Darmstädter Schülerinnen- und Schülernachmittag zur Mathematik" (organization: Prof. Kohler; in 2017 with talks from the fields of Algebra, Geometry, Didactics and Stochastics and in 2018 from the fields of Analysis, Numerical Analysis and Scientific Computing and Stochastics).

- Annual participation at the information days for female students, “Schnuppertage für Schülerinnen”, with participation at the central event for female students with interest in STEM/MINT programmes and an on-site presentation of the department including a talk by the student advisor, a sample lecture and talks with female mathematicians, about 30 participants in each year (organized by the department’s gender equaltity officers; lectures from the field of Stochastics in 2017 and from the field of Optimization in 2018)

- Support of the annual organization of the Mathematikolympiade Hessen (third level) in cooperation with the Center for Mathematics Bensheim for all grades (about 20 participants per grade each year) (Prof. Kiehl, academic staff and students).
  In the recent years, the department had the opportunity to host the finals.
  Mathematical afternoon lectures were delivered by Prof. Kiehl and Prof. von Pippich (2017) and Prof. Reif and Prof. Bokowski (2018).

- Organization of the Mathematical Modeling Week for secondary school students in grade 12 in cooperation with Center for Mathematics Bensheim each October (40 participants each year) (Prof. Kiehl).

- Involvement in the annual German Maths Contest (Bundeswettbewerb Mathematik) (Prof. (em.) Alber, Prof. Roch)

- In connection with the project course “Teaching in Mathematics: Problem Solving” (Prof. Bruder, StR Krauth, OStR Klein and participating students, winter semester 2016/17), diverse mathematical “Knobelstraßen” for secondary schools were developed and conducted at several schools in Darmstadt and Frankfurt.

Other activities

- In cooperation with the “Hochschuldidaktische Arbeitsstelle (HDA)” (Center of University Didactics) at the TU Darmstadt Prof. Kümmerer and Sandra Lang produced an image film (in German) to report on the innovative multidisciplinary lecture course “Mathematik als gemeinsame Sprache der Naturwissenschaften” (Mathematics: The Common Language of Natural Sciences). This lecture course addresses all teacher students who study at least one of the subjects mathematics, physics, chemistry, biology, or informatics. It is a building block of the recently founded “Vernetzungsbereich” (interlinking area), which is established as a part of the MINTplus initiative of the TU Darmstadt to profile the teachers education at our university. It is financially supported by the German Bundesministerium für Bildung und Forschung as part of the “Qualitiätsoffensive Lehrerbildung”. The common mathematical language provides a link between different natural sciences and fosters crossover cooperations in school teaching.

- A short film (in German) was produced by Prof. Kümmerer in cooperation with the “Hochschuldidaktische Arbeitsstelle (HDA)” (Center of University Didactics) at the TU Darmstadt, which gives didactic hints on the use of blackboards in lecture courses (`https://www.einfachlehren.tu-darmstadt.de/themensammlung/details_12352.de.jsp`

- On the occasion of the 450th anniversary of the former Court and present University and State Library of Darmstadt, an exhibition “Geheimnis – Herrschaft – Wissen” (Mystery – Dominion – Knowledge) with particularly valuable treasures from the library’s holdings was arranged. In cooperation with B. Gebert (University Library Darmstadt), Prof. V. Huth (Institut für Personengeschichte, Bensheim), Prof. Kümmerer (TU Darmstadt, Department of Mathematics), Prof. Schenk (TU Darmstadt, Department of History) handwritings and prints from the collection of the Hessian landgraves on astronomy, astrology, and medicine, but also on secret sciences such as alchemy were presented at the University Library from from 18 July to 22 October 2017.
- Talk titled “Unendliche Weiten; und wie man darin ein Optimum sucht. Numerische Methoden für unendlichdimensionale Optimierungsprobleme”, Lecture in the series “Was steckt dahinter?” (June 6, 2018, Prof. Wollner)
- Talk titled “Stille Post - Wie wir Nachrichten zuverlässig übertragen können”, lecture for children organized by the Bürgerstiftung Darmstadt (November 11, 2018, Prof. Wollner)
- Talk titled ”Das Rucksackproblem: Wie Mathematiker Koffer packen”, lecture for secondary school students at the “Tags der Mathematik 2018”, Merck KGaA, Darmstadt (March 3, 2018, Christopher Hojny)
- Talk titled ”Lineare und ganzzahlige Optimierung”, at Goethe Gymnasium, Bensheim (June 6, 2018, Prof. Pfetsch)
- Talk titled ”Unendliche Summe”, visit from the Bertolt Brecht Gymnasium Darmstadt (October 24, 2018, Prof. Haller-Dintelmann)
- Talk titled ”Wie gewinnt man eine Goldmedaille im Skifliegen? Parameteroptimierung in dynamischen Systemen”, visit from the Georg-August-Zinn-Schule Reichelsheim (September 26, 2018, Prof. Kiehl)
- Annual Graduation Event: celebration with friends and family of the graduated students (organisation: Prof. Aurzada and staff).

Technische Universität Darmstadt
Fachbereich Mathematik
AG Numerik und Wissenschaftliches Rechnen
Dolivostr. 15
D-64293 Darmstadt

Building: S4|10
Homepage: `http://num.mathematik.tu-darmstadt.de`
Fax: +49-(0)6151 16-23164
E-mail: {egger,erath,giesselmann,kiehl,lang}@mathematik.tu-darmstadt.de