Biannual Report

Department of Mathematics
Research Group Numerical Analysis and Scientific Computing
2019 and 2020

TECHNISCHE
UNIVERSITÄT
DARMSTADT

The cover illustration is by courtesy of Brice Loustau, postdoc at DAMS from Aug. 2018 to July 2020. It shows the Poincaré disk representing the hyperbolic plane tesselated with polygons which arise from the lift of a hyperbolic surface. The graphics illustrates the behaviour of harmonic maps between hyperbolic surfaces of the same genus.

General Remark

This document contains a subset of the information of the Biannual Report of the Department of Mathematics at TU Darmstadt for 2019 and 2020. 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 2022

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, and 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. 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

Neelabja Chatterjee, Jürgen Dölz, Pia Domschke, Alf Gerisch, Hadi Minbashian, Christopher Müller, Mania Sabouri, Kersten Schmidt, Adrien Semin, Mirjam Walloth

Research Associates

Anke Böttcher, David Frenzel, Oliver André Habrich, Hrishikesh Joshi, Thomas Kugler, Teresa Kunkel, Richard Franz Löscher, Axel Lukassen, Nora Marie Philippi, Bogdan Radu, Moritz Schneider, Lucas Schöbel-Kröhn, Vsevolod Shashkov, Philipp Steinbach, Elisa Strauch, Erik Laurin Strelow, Gabriel Teschner, Dimitrios Zacharenakis

Secretaries

Elke Dehnert, Dagmar Thies

Projects of the research group

Project: Convergence Analysis of Fractional Conservation Laws using Discontinuous Galerkin Method

Fractional conservation laws encompass a large number of applicable models, ubiquitous in natural, physical or biological processes. Standard examples include Black–Scholes model from finance or Burgers equation with *fractional Laplacian* source term. Fractional conservation laws can be viewed as natural nonlocal generalization of the viscous conservation law. There is a plethora of research work available, conducted to explore the construction and convergence of different numerical methods approximating the actual equation. One of them being a certain class of discontinuous Galerkin methods, which takes into account the effects of the convective term and the fractional term. The aim of this project is to discretize the fractional conservation law model using the discontinuous Galerkin method with forward Euler time discretization and obtain an *a priori* error estimate which will determine rate of convergence of the numerical solution to the smooth exact solution. This desired error estimate consists of contributions from two different quantities. First contribution is due to the error between the numerical solution and the appropriate projection of the exact solution on the finite element space of piecewise polynomials. We are going to estimate this quantity by using the *stability* of the scheme, with the help of properly chosen CFL condition. Second contribution has its origin in the error between the exact solution and the appropriate projection of it on the finite element space of piecewise polynomials. This quantity will be estimated using the regularity of the exact solution and an application of Bramble–Hilbert Lemma.

Contact: Jan Giesselmann, Neelabja Chatterjee

References

[1] N. Alibaud. Entropy formulation for fractal conservation laws. *J. Evol. Equ.*, 7(1):145–175, 2007.

[2] S. Cifani and E. R. Jakobsen. Entropy solution theory for fractional degenerate convection-diffusion equations. *Ann. Inst. H. Poincaré Anal. Non Linéaire*, 28(3):413–441, 2011.

[3] S. Cifani, E. R. Jakobsen, and K. H. Karlsen. The discontinuous Galerkin method for fractional degenerate convection-diffusion equations. *BIT*, 51(4):809–844, 2011.

[4] B. Cockburn and C.-W. Shu. The local discontinuous Galerkin method for time-dependent convection-diffusion systems. *SIAM J. Numer. Anal.*, 35(6):2440–2463, 1998.

[5] J. Droniou and C. Imbert. Fractal first-order partial differential equations. *Arch. Ration. Mech. Anal.*, 182(2):299–331, 2006.

[6] Q. Zhang and C.-W. Shu. Error estimates to smooth solutions of Runge-Kutta discontinuous Galerkin methods for scalar conservation laws. *SIAM J. Numer. Anal.*, 42(2):641–666, 2004.

Project: Uncertainty quantification for forward and inverse problems

We study the numerical solution of forward and inverse acoustic scattering problems by randomly shaped obstacles in three-dimensional space using a fast isogeometric boundary element method. We show that the knowledge of the deformation field's expectation and covariance at the surface of the scatterer are already sufficient to compute the surface Karhunen-Loève expansion. Multilevel quadrature methods are then used for the efficient approximation of quantities of interest, such as the scattered wave's expectation and variance. Computing the wave's Cauchy data at an artificial, fixed interface enclosing the random obstacle, we can also directly infer quantities of interest in free space. Adopting the Bayesian paradigm we also compute the expected shape and the variance of the scatterer from noisy measurements of the scattered wave at the artificial interface. Numerical results for the forward and inverse problem are given to demonstrate the feasibility of the proposed approach.

Partner: H. Harbrecht (Universität Basel); C. Jerez-Hanckes (Universidad Adolfo Ibanez, Santiago, Chile); M. Multerer (USI Lugano)

Contact: Jürgen Dölz

References

[1] J. Dölz, H. Harbrecht, C. Jerez-Hanckes, and M. Multerer. Isogeometric multilevel quadrature for forward and inverse random acoustic scattering. arXiv:2010.14613, 2020.

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 expectations and variances of solution functionals for the uncertainty quantification at reduced computing time.

Support: Project B01 within DFG TRR 154

Contact: Elisa Strauch, Pia Domschke, Jens Lang

References

[1] P. Domschke, O. Kolb, and J. Lang. Fast and reliable transient simulation and continuous optimization of large-scale gas networks. arXiv:2012.02737, 2020.

[2] J. Lang, P. Domschke, and E. Strauch. Adaptive single- and multilevel stochastic collocation methods for uncertain gas transport in large-scale networks. arXiv:2012.03565, 2020.

[3] P. Mindt, J. Lang, and P. Domschke. Entropy-preserving coupling of hierarchical gas models. *SIAM Journal on Mathematical Analysis*, 51:4754–4775, 2019.

Project: Model order reduction for inverse problems

We study the efficient numerical solution of linear inverse problems with operator valued data which arise, e.g., in seismic exploration, inverse scattering, or tomographic imaging. The high-dimensionality of the data space implies extremely high computational cost already for the evaluation of the forward operator, which makes a numerical solution of the inverse problem, e.g., by iterative regularization methods, practically infeasible. To overcome this obstacle, we develop a novel model reduction approach that takes advantage of the underlying tensor product structure of the problem and which allows to obtain low-dimensional certified reduced order models of quasi-optimal rank. A complete analysis of the proposed model reduction approach is given in a functional analytic setting and the efficient numerical construction of the reduced order models as well as of their application for the numerical solution of the inverse problem is discussed. In summary, the setup of a low-rank approximation can be achieved in an offline stage at essentially the same cost as a single evaluation of the forward operator, while the actual solution of the inverse problem in the online phase can be done with extremely high efficiency. The theoretical results are illustrated using a typical model problem in fluorescence optical tomography.

Partner: J. Dölz (Uni Bonn); M. Schlottbom (U Twente)

Support: DFG TRR 146, DFG TRR 154

Contact: Herbert Egger

References

[1] J. Dölz, H. Egger, and M. Schlottbom. A model reduction approach for inverse problems with operator valued data. arXiv:2004.11827, 2020.

Project: Domain decomposition with rotating geometries

Engineering problems sometimes involve static and rotating geometries, e.g., propellers and ambient space or stators and rotors. It is then natural to introduce a domain decomposition with different coordinate systems rotating relative to each other. A typical example of such problems arises in electric machines. We propose and analyze a mortar method based on finite element or isogeometric analysis discretization of the individual subdomains which are coupled by a Lagrange multiplier technique. Trigonometric polynomials (harmonics) are chosen for the space of Lagrange-multipliers to take into account the rotational symmetry. We study the numerical stability of such discretization schemes and, in particular, derive simple criteria guaranteeing the relevant inf-sup stability condition. The validity and sharpness of the theoretical results is demonstrated by numerical tests.

Partner: M. Haruntyunyan; M. Merkel; S. Schöps (TEMF, TU Darmstadt)

Support: GSC 233

Contact: Herbert Egger, Richard Löscher

References

[1] H. Egger, M. Harutyunyan, M. Merkel, and S. Schöps. On the stability of harmonic mortar methods with application to electric machines. arXiv:2005.12020, 2020. To appear in Proceedings of SCEE 2020.

Project: dGFEM-BEM coupling for the Helmholtz equation

As a model problem we consider the Helmholtz equation in an interior and the corresponding exterior domain. This problem can be considered as a scattering problem. Therefore, the coupling of two different numerical methods is of highest interest to simulate the possible different behaviour of the model problem in the different domains. In this project we consider a novel approach, namely the coupling of a discountinous Galerkin method with the boundary element method. We develop a rigorous analysis of our approach as well as some convincing numerical examples.

Partner: Jens Markus Melenk (TU Wien); Lorenzo Mascotto (University of Vienna); Ilaria Perugia (University of Vienna); Alexander Rieder (University of Vienna)

Contact: Christoph Erath

Project: Non-symmetric isogeometric FEM-BEM couplings

The project considers the coupling of the finite element and the boundary element method in an isogeometric framework to approximate either two-dimensional Laplace interface problems or boundary value problems consisting in two disjoint domains. We consider the finite element Method in the bounded domains to simulate possibly non-linear materials. The boundary element method is applied in unbounded or thin domains where the material behavior is linear. The isogeometric framework allows us to combine different design and analysis tools: first, we consider the same type of NURBS parameterizations for an exact geometry representation and second, we use the numerical analysis for the Galerkin approximation. Moreover, it facilitates to perform h- and p-refinements. Practical examples (e.g., magneto static field of engines) will show the effectiveness of our numerical coupling approach.

Partner: Mehdi Elasmi (TU Darmstadt); Stefan Kurz (TU Darmstadt)

Support: Graduate School Computational Engineering, DFG

Contact: Christoph Erath

References

[1] M. Elasmi, C. Erath, and S. Kurz. Non-symmetric isogeometric FEM-BEM couplings. arXiv:2007.09057, 2020.

Project: Mathematical modelling of 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, the healing of tissue wounds, 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, include cross-diffusion processes in different models, study the effect of multiple adhesion terms of different form in wound healing models, consider mechanochemial models of pattern formation, 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); Jonathan Sherratt (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. Voss-Böhme and A. Gerisch. Multi-scale analysis of contact-dependent interaction in tissue aggregation and invasion. In O. Wolkenhauer, editor, *Systems Medicine*, pages 156–168. Academic Press, Oxford, 2021, published online August 2020.

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

Project: Regularized moment methods for kinetic equations

Moment equations employing entropy closures are an interesting method for solving kinetic equations since they lead to equations that are very close to compressible fluid mechanics equations and posses a natural entropy structure. However, solving these equations numerically is rather delicate since the entropy closure makes it necessary to solve constrained minimization problems and numerical errors might make these problems unfeasible. This difficulty can be overcome using regularized minimization problems, as introduced in [1]. The goal of our research is to show convergence of solutions to the regularized moment system to solutions of the non-regularized moment system in case the regularization parameter goes to zero.

Partner: Martin Frank (KIT), Graham W. Alldredge (RWTH Aachen)

Contact: Jan Giesselmann

References

[1] G. W. Alldredge, M. Frank, and C. D. Hauck. A regularized entropy-based moment method for kinetic equations. *SIAM J. Appl. Math.*, 79(5):1627–1653, 2019.

Project: Reduced basis construction via snapshot calibration

Standard model reduction techniques using proper orthogonal decomposition of snapshot matrices are not very efficient when applied to hyperbolic partial differential equations due to slow singular value decay. Our goal is to induce a faster singular value decay by computing snapshots on a transformed spatial domain, or the so-called snapshot calibration/transformation. We are particularly interested in problems involving shock collision, shock rarefaction-fan collision, shock formation, etc. For such problems, we propose spatial transformation using monotonic feature matching. We consider discontinuities and kinks as features, and by carefully partitioning the parameter domain. We prove that our method results in a fast m-width decay of a so-called calibrated manifold. It turns out, that calibration induces dependence of the m-width on the accuracy of the full order model, which is in contrast to elliptic and parabolic problems that do not require calibration. Our method is "data-driven" in the sense that it uses only solution snapshots and not the underlying partial differential equation.

Partner: Martin Frank (KIT), Graham W. Alldredge (RWTH Aachen)

Contact: Jan Giesselmann

References

[1] N. Sarna, J. Giesselmann, and P. Benner. Data-driven snapshot calibration via monotonic feature matching. arXiv:2009.08414, 2020.

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, Aaron Brunk (Universität Mainz); Burkhard Dünweg, Dominic Spiller (Max-Planck-Institut für Ploymerforschung Mainz)

Support: DFG TRR 146

Contact: Herbert Egger, Oliver Habrich

References

[1] A. Böttcher and H. Egger. Structure preserving discretization of Allen-Cahn type problems modeling the motion of phase boundaries. *Vietnam J. Math.*, 48:847–863, 2020.

[2] A. Brunk, B. Dünweg, H. Egger, O. Habrich, M. Lukacova-Medvidova, and D. Spiller. Analysis of a viscoelastic phase separation model. arXiv:2012.04234, 2020.

[3] H. Egger, O. Habrich, and V. Shahskov. Energy stable Galerkin approximation of Hamiltonian and gradient systems. *Comput. Meth. Appl. Math.*, 2020. in press.

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

Simulation of some physical phenomena poses challenges as the interaction between different physics at a range of time and length scales needs to be resolved. One example is chemically reacting flows, where chemical reactions and convection interact. Computational resources can be better utilized by carrying out local mesh and model adaptation. The aim of this project is spatial model adaptation for hyperbolic balance laws based on a posteriori error estimates. We apply the proposed approach to compressible chemically reacting flows. In this example, the governing equations can be simplified by assuming chemical equilibrium which we denote as the simple system. We derive a posteriori error estimates using the relative entropy framework. The error estimates account for the modeling and the discretization errors, which can be used to perform the model and mesh adaptation. The model adaptation is done by decomposing the computational domain and locally choosing the full system where necessary and the simplified system where sufficient. The resulting system is numerically solved using discontinuous Galerkin method with multiresolution analysis on a hierarchy of nested grids with coarse data on a uniform grid. The component of the numerical solution on the nested grids is referred to as the details. The magnitude of the details decay as you increase the number of refinement levels when the numerical solution is locally smooth. We compare the mesh adaptation done based on the thresholding of the details and the residual. To this end we use *Multiwave*, which is a library designed for simulations of nonlinear hyperbolic balance laws.

Support: DFG Gi 1131/1-1 (up to 09.2020)

Partner: Siegfried Müller (RWTH Aachen), Aleksey Sikstel (Universität Erlangen-Nürnberg)

Contact: Jan Giesselmann, Hrishikesh Joshi

References

[1] N. Gerhard, F. Iacono, G. May, S. Müller, and R. Schäfer. A high-order discontinuous Galerkin discretization with multiwavelet-based grid adaptation for compressible flows. *J. Sci. Comput.*, 62:25–52, 2015.

[2] J. Giesselmann and H. Joshi. Model adaptation of balance laws based on a posteriori error estimates and surrogate fluxes. *Finite volumes for complex applications IX – methods, theoretical aspects, examples (FVCA 9)*, pages 375–383, 2020.

[3] 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.

[4] S. Müller and A. Sikstel. Multiwave. https://www.igpm.rwth-aachen.de/forschung/multiwave, Institut für Geometrie und Praktische Mathematik, RWTH Aachen, 2018.

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: Martin Kiehl

References

[1] A. Lukassen and M. Kiehl. Operator splitting for stiff chemical reaction systems. *J.Comput. Appl. Math.*, 344:495–511, 2018.

Project: Stability and structure preserving approximation of hyperbolic problems on networks

We study the exponential stability of damped wave propagation problems on one-dimensional networks which arise in in the modeling of gas-transport processes on acoustic time- and length scales. Exponential stability of the problems is proven and the structure-preserving discretization by mixed finite elements and implicit time-stepping schemes is investigated. In addition, the application of model order reduction schemes is discussed.

Partner: B. Liljegren-Sailer, N. Marheineke (Uni Trier); V. Mehrmann (TU Berlin)

Support: DFG TRR 154

Contact: T. Kugler, Herbert Egger

References

[1] H. Egger and T. Kugler. Uniform exponential stability of Galerkin approximations for damped wave systems. In *Advanced Finite Element Methods with Applications, Selected papers from the 30th Chemnitz Finite Element Symposium*. Springer, 2019.

[2] H. Egger, T. Kugler, and B.-L. Sailer. Stability preserving approximations of a semilinear hyperbolic gas transport model. Springer, 2019. in press.

[3] H. Egger, T. Kugler, and V. Shashkov. An inexact Petrov-Galerkin approximation for gas transport in pipeline networks. In *Proceedings of ICOSAHOM 2018*. Springer.

[4] T. Kugler. *Galerkin methods for simulation of wave propagation on a network of pipes*. PhD thesis, 2020.

Project: Boundary observers for flow in gas networks

We consider the flow of gas through networks, where measurements are available at certain vertices. Based on these nodal observations we set up an observer system in order to recover the original system state.
We model the gas flow through pipes by a system of semilinear hyperbolic partial differential equations based on Riemann invariants, which is an approximation of the isothermal Euler equations in the case of small velocities. For the observer system the algebraic node conditions are replaced by terms depending on the difference between the exact solution and the state of the observer system. We can show that the observer converges exponentially to the original system state.

Partner: Martin Gugat (Universität Erlangen-Nürnberg)

Support: Project C05 within DFG TRR 154

Contact: Jan Giesselmann, Teresa Kunkel

References

[1] M. Gugat and J. Giesselmann. Boundary feedback stabilization of a semilinear model for the flow in star-shaped gas networks. submitted to ESAIM: Control, Optimisation and Calculus of Variations, 2020.

Project: Relative energy estimates, asymptotic stability and structure preserving discretization for isentropic flow in gas networks

Gas transport in one-dimensional pipe networks can be described as an abstract dissipative Hamiltonian system, for which quantitative stability bounds can be derived by means of relative energy estimates. This allows us to conclude stability of solutions to subsonic flow problems with respect to perturbations in initial and boundary data as well as model parameters. In addition, we can prove convergence to the parabolic limit problem in the practically relevant high friction regime. Furthermore, the stability estimates are inherited almost verbatim by variational discretization schemes, like mixed finite elements in space and the implicit Euler method in time, leading to quantitative convergence rates and asymptotic stability in the limiting high friction regime. The results are first derived for the flow on a single pipe, but in the spirit of the port-Hamiltonian formalism, they naturally extend to pipe networks.

Support: Projects C04 and C05 within DFG TRR 154

Contact: Herbert Egger, Jan Giesselmann, Teresa Kunkel, Nora Philippi

References

[1] H. Egger and J. Giesselmann. Stability and asymptotic analysis for instationary gas transport via relative energy estimates. arXiv:2012.14135, 2020.

Project: Adaptive Multilevel Stochastic Collocation Strategy for Solving Elliptic PDEs with Random Data

We propose and analyse a fully adaptive strategy for solving elliptic PDEs with random data in this work. 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 the computational cost. The novel aspect of our strategy is that the hierarchy of spatial approximations is sample dependent so that the computational effort at each collocation point can be optimised individually. We outline a rigorous analysis for the convergence and computational complexity of the adaptive multilevel algorithm and we provide optimal choices for error tolerances at each level. Two numerical examples demonstrate the reliability of the error control and the significant decrease in the complexity that arises when compared to single level algorithms and multilevel algorithms that employ adaptivity solely in the spatial discretisation or in the collocation procedure.

Partner: Robert Scheichl (Universität Heidelberg); David Silvester (University of Manchester)

Contact: Jens Lang

References

[1] J. Lang, R. Scheichl, and D. Silvester. A fully adaptive multilevel stochastic collocation strategy for solving elliptic pdes with random data. *Journal of Computational Physics*, 419:109692, 2020.

Project: A Third-Order Weighted Essentially Non-Oscillatory Scheme in Optimal Control Problems Governed by Nonlinear Hyperbolic Conservation Laws

The weighted essentially non-oscillatory (WENO) methods are popular and effective spatial discretization methods for nonlinear hyperbolic partial differential equations. Although these methods are formally first-order accurate when a shock is present, they still have uniform high-order accuracy right up to the shock location. In this project, we propose a novel third-order numerical method for solving optimal control problems subject to scalar nonlinear hyperbolic conservation laws. It is based on the first-disretize-then-optimize approach and combines a discrete adjoint WENO scheme of third order with the classical strong stability preserving three-stage third-order Runge-Kutta method SSPRK3. We analyze its approximation properties and apply it to optimal control problems of tracking-type with non-smooth target states. Comparisons to common first-order methods such as the Lax-Friedrichs and Engquist-Osher method show its great potential to achieve a higher accuracy along with good resolution around discontinuities.

Contact: David Frenzel, Jens Lang

References

[1] D. Frenzel. *Weighted Essentially Non-Oscillatory Schemes in Optimal Control Problems Governed by Nonlinear Hyperbolic Conservation Laws*. PhD thesis, TU Darmstadt, 2020.

[2] D. Frenzel and J. Lang. A third-order weighted essentially non-oscillatory scheme in optimal control problems governed by nonlinear hyperbolic conservation laws. arXiv:2009.12392, 2020.

Project: POD model order reduction with space-adapted snapshots for flow problems

We consider 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 propose two approaches of deriving stable POD-Galerkin reduced-order models for this context. In the first approach, the pressure term and the continuity equation are eliminated by imposing a weak incompressibility constraint with respect to a pressure reference space. In the second approach, we derive an inf-sup stable velocity-pressure reduced-order model by enriching the velocity reduced space with supremizers computed on a velocity reference space. For problems with inhomogeneous Dirichlet conditions, we show how suitable lifting functions can be obtained from standard adaptive finite element computations. We provide a numerical comparison of the considered methods for a regularized lid-driven cavity problem.

Partner: Carmen Gräßle; Michael Hinze (Universität Koblenz-Landau)

Contact: Jens Lang, Sebastian Ullmann

References

[1] C. Gräßle, M. Hinze, J. Lang, and S. Ullmann. POD model order reduction with space-adapted snapshots for incompressible flows. *Advances in Computational Mathematics*, 45:2401–2428, 2019.

[2] C. Gräßle, M. Hinze, J. Lang, S. Ullmann, and J. Lang. Model order reduction for space-adaptive simulations of Navier-Stokes. volume 19 of *Proceedings of Applied Mathematrics and Mechanics*, doi:10.1002/pamm.201900435, 2019. Wiley-VCH Verlag GmbH & Co. KGaA Weinheim.

Project: Entropy-Preserving Coupling of Hierarchical Gas Models

This project is concerned with coupling conditions at junctions for transport models which differ in their fidelity to describe transient flow in gas pipelines. It also includes the integration of compressors between two pipes with possibly different models. A hierarchy of three one-dimensional gas transport models is built through the 3×3 polytropic Euler equations, the 2×2 isentropic Euler equations, and a simplified version of it for small velocities. To ensure entropy preservation, we make use of the novel entropy-preserving coupling conditions recently proposed by Lang and Mindt [1] and require the continuity of the total enthalpy at the junction and that the specific entropy for pipes with outgoing flow equals the convex combination of all entropies that belong to pipes with incoming flow. We prove the existence and uniqueness of solutions to generalized Riemann problems at a junction in the neighborhood of constant coupling functions and stationary states which belong to the subsonic region. This provides the basis for the well-posedness of certain Cauchy problems for initial data with sufficiently small total variation.

Partner: Pia Domschke (Frankfurt School of Finance & Management)

Contact: Jens Lang, Pascal Mindt

References

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

[2] P. Mindt, J. Lang, and P. Domschke. Entropy-preserving coupling of hierarchical gas models. *SIAM Journal on Mathematical Analysis*, 51:4754–4775, 2019.

Project: Modeling of Osteoarthritis

Understanding the pathophysiological processes of cartilage degradation requires adequate model systems to develop therapeutic strategies towards osteoarthritis (OA). Although different in vitro or in vivo models have been described, further comprehensive approaches are needed to study specific disease aspects. This study aimed to combine in vitro and in silico modeling based on a tissue-engineering approach using mesenchymal condensation to mimic cytokine-induced cellular and matrix-related changes during cartilage degradation. Thus, scaffold-free cartilage-like constructs (SFCCs) were produced based on self-organization of mesenchymal stromal cells (mesenchymal condensation) and (i) characterized regarding their cellular and matrix composition or secondly (ii) treated with interleukin-1β (IL-1β) and tumor necrosis factor α (TNFα) for 3 weeks to simulate OA-related matrix degradation. In addition, an existing mathematical model based on partial differential equations was optimized and transferred to the underlying settings to simulate the distribution of IL-1β, type II collagen degradation and cell number reduction. By combining in vitro and in silico methods, we aimed to develop a valid, efficient alternative approach to examine and predict disease progression and effects of new therapeutics.

Partner: Marie-Christin Weber, Alexandra Damerau, Moritz Pfeiffenberger, Timo Gaber, Frank Buttgereit, Annemarie Lang (Charite Berlin); Lisa Fischer, Sebastian Götschel, Rainald Ehrig (ZIB Berlin); Igor Ponomarev (Research Center of Medical Technology and Biotechnology, Bad Langensalza); Susanna Röblitz (University of Bergen)

Contact: Jens Lang

References

[1] M.-C. Weber, L. Fischer, A. Damerau, I. Ponomarev, M. Pfeiffenberger, T. Gaber, S. Götschel, J. Lang, S. Röblitz, F. Buttgereit, R. Ehrig, and A. Lang. Macroscale mesenchymal condensation to study cytokine-driven cellular and matrix-related changes during cartilage degradation. *Biofabrication*, 12:045016, 2020.

Project: Adaptive Moving Finite Element Method for Steady Low Mach Number Compressible Combustion Problems

This work surveys an r-adaptive moving mesh finite element method for the numerical solution of premixed laminar flame problems. Since the model of chemically reacting flow involves many different modes with diverse length scales, the computation of such a problem is often extremely time-consuming. Importantly, to capture the significant characteristics of the flame structure when using detailed chemistry, a much more stringent requirement on the spatial resolution of the interior layers of some intermediate species is necessary. Here, we propose a moving mesh method in which the mesh is obtained from the solution of so-called moving mesh partial differential equations. Such equations result from the variational formulation of a minimization problem for a given target functional that characterizes the inherent difficulty in the numerical approximation of the underlying physical equations. Adaptive mesh movement has emerged as an area of intense research in mesh adaptation in the last decade. With this approach points are only allowed to be shifted in space leaving the topology of the grid unchanged. In contrast to methods with local refinement, data structure hence is unchanged and load balancing is not an issue as grid points remain on the processor where they are. We will demonstrate the high potential of moving mesh methods for effectively optimizing the distribution of grid points to reach the required resolution for chemically reacting flows with extremely thin boundary layers.

Partner: Malte Braack (Christian-Albrechts-Universität Kiel)

Contact: Jens Lang, Zhen Sun

References

[1] Z. Sun, M. Braack, and J. Lang. An adaptive moving finite element method for steady low Mach number compressible combustion problems. *International Journal for Numerical Methods in Fluids*, 92:1081–1095, 2020.

Project: Fast and Reliable Transient Simulation and Continuous Optimization of Large-Scale Gas Networks

We are concerned with the simulation and optimization of large-scale gas pipeline systems in an error-controlled environment. The gas flow dynamics is locally approximated by sufficiently accurate physical models taken from a hierarchy of decreasing complexity and varying over time. Feasible work regions of compressor stations consisting of several turbo compressors are included by semiconvex approximations of aggregated characteristic fields. A discrete adjoint approach within a first-discretize-then-optimize strategy is proposed and a sequential quadratic programming with an active set strategy is applied to solve the nonlinear constrained optimization problems resulting from a validation of nominations. The method proposed here accelerates the computation of near-term forecasts of sudden changes in the gas management and allows for an economic control of intra-day gas flow schedules in large networks. Case studies for real gas pipeline systems show the remarkable performance of the new method.

Partner: Pia Domschke (Frankfurt School of Finance & Management); Oliver Kolb (Universität Mannheim)

Contact: Jens Lang

References

[1] P. Domschke, O. Kolb, and J. Lang. Fast and reliable transient simulation and continuous optimization of large-scale gas networks. arXiv:2012.02737, 2020.

Project: Discrete Adjoint Implicit Peer Methods in Optimal Control

It is well known that in the first-discretize-then-optimize approach in the control of ordinary differential equations the adjoint method may converge under additional order conditions only. For Peer two-step methods we derive such adjoint order conditions and pay special attention to the boundary steps. For s-stage methods, we prove convergence of order s for the state variables if the adjoint method satisfies the conditions for order $s-1$, at least. We remove some bottlenecks at the boundaries encountered in an earlier paper of Schröder et al. [2] and discuss the construction of 3-stage methods for the order pair (3,2) in detail including some matrix background for the combined forward and adjoint order conditions. The impact of nodes having equal differences is highlighted. It turns out that the most attractive methods are related to BDF. Three 3-stage methods are constructed which show the expected orders in numerical tests.

Partner: Bernhard A. Schmitt (Universität Marburg)

Contact: Jens Lang

References

[1] J. Lang and B. A. Schmitt. Discrete adjoint implicit peer methods in optimal control. arXiv:2002.12081, 2020.

[2] D. Schröder, J. Lang, and R. Weiner. Stability and consistency of discrete adjoint implicit peer methods. *Journal of Computational and Applied Mathematics*, 262:73–86, 2014.

Project: Analysis and numerical approximation of nonlinear evolution equations on network structures

We study nonlinear evolution problems on one-dimensional network structures. Typical applications involve, e.g., the transport of gas in pipeline systems, the movement of cells or bacteria in biological networks, or heat transfer in electronic circuits. The modeling of such systems is presented and the systematic analysis and numerical approximation is studied in a common framework.

Support: DFG TRR 154

Contact: Lucas Schöbel-Kröhn, Herbert Egger

References

[1] H. Egger and L. Schöbel-Kröhn. Chemotaxis on networks: analysis and numerical approximation. *ESAIM: Math. Model. Numer. Anal.*, 54:1339–1372, 2020.

[2] L. Schöbel-Kröhn. *Analysis and numerical approximation of nonlinear evolution equations on network structures*. PhD thesis, 2020.

Project: Reduced order models for parametric convection-diffusion-reaction equations with random data based on adaptive snapshots

This project is concerned with the efficient solution of convection-diffusion-reaction equations with sets of deterministic and stochastic input data. We are particularly interested in the multi-query context where the stochastic problem must be solved for a large number of values of the deterministic parameters. In order to solve this task we consider a two step approach: we compute snapshots of the solution using adaptively constructed stochastic Galerkin finite element discretizations and use these snapshots to set up a Galerkin reduced order model based on proper orthogonal decomposition or a greedy procedure. Using adaptive discretizations reduces the computational costs in the offline phase of the reduced order model but also has some important consequences for its functionality. We investigate these influences and derive an error etsimator for the reduced solution which reveals all error sources involved.

Contact: Christopher Müller, Jens Lang

References

[1] S. Ullmann, C. Müller, and J. Lang. Stochastic Galerkin reduced basis methods for parametrized linear elliptic partial differential equations. arXiv:1812.08519, 2020.

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 using the example of gas networks*, and deals with the construction, analysis and efficient realization of numerical methods for partial differential equations on networks. We derive thermodynamically consistent models for gas transport on pipe networks under consideration of coupling conditions at pipe junctions. The focus is on the transport of gas mixtures and non-isothermal models as the one-dimensional Euler equations with friction. A structure preserving discretization based on a variational formulation of corresponding problems allows an efficient numerical approximation using Galerkin schemes. Basic properties like conservation of mass and dissipation of energy are inherited. Furthermore, we investigate singularly perturbed problems on networks and derive asymptotic preserving schemes. Our Galerkin methods are then used in the context of inverse problems, more precisely for state and parameter estimation by measurements at vertices, as well as for the efficient realization of control strategies on gas networks.

Partner: Michael Hintermüller (HU Berlin)

Support: Project C04 within DFG TRR 154

Contact: Herbert Egger, Nora Philippi

References

[1] H. Egger and J. Giesselmann. Stability and asymptotic analysis for instationary gas transport via relative energy estimates. arXiv:2012.14135, 2020.

[2] H. Egger and N. Philippi. A hybrid discontinuous galerkin method for transport equations on networks. In *International Conference on Finite Volumes for Complex Applications*, pages 487–495. Springer, 2020.

[3] H. Egger and N. Philippi. On the transport limit of singularly perturbed convection–diffusion problems on networks. *Mathematical Methods in the Applied Sciences*, 2020.

Project: Mass lumping strategies for the efficient implementation of acoustic and electromagnetic wave propagation

The study of wave propagation is an important topic in the field of engineering and it finds application 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: GSC 233

Contact: Herbert Egger, Bogdan Radu

References

[1] H. Egger and B. Radu. A second order finite element method with mass lumping for wave equations in H(div). arXiv:1912.07057, 2019.

[2] H. Egger and B. Radu. A mass-lumped mixed finite element method for acoustic wave propagation. *Numer. Math.*, 145:239–269, 2020.

[3] H. Egger and B. Radu. A mass-lumped mixed finite element method for Maxwell's equations. In *Proceedings of SCEE 2018*. Springer, 2020. in press.

[4] H. Egger and B. Radu. A second order finite element method with mass lumping for Maxwell's equations on tetrahedra. *SIAM J. Numer. Analysis*, 2020. accepted.

[5] H. Egger and B. Radu. A second order multipoint flux mixed finite element method on hybrid meshes. *SIAM J. Numer. Anal.*, 58:1822–1844, 2020.

Project: Numerical approximation of poroelastic phenomena

We consider the systematic numerical approximation of Biot's quasistatic model for the consolidation of a poroelastic medium. Various discretization schemes have been analysed for this problem and inf-sup stable finite elements have been found suitable to avoid spurious pressure oscillations in the initial phase of the evolution. In this paper, we first clarify the role of the inf-sup condition for the well-posedness of the continuous problem and discuss the choice of appropriate initial conditions. We then develop an abstract error analysis that allows us to analyse some approximation schemes discussed in the literature in a unified manner. In addition, we propose and analyse the high-order time discretization by a scheme that can be interpreted as a variant of continuous-Galerkin or particular Runge-Kutta methods applied to a modified system. The scheme is designed to preserve both the underlying differential-algebraic structure and the energy-dissipation property of the problem. In summary, we obtain high-order Galerkin approximations with respect to space and time and derive order-optimal convergence rates. The numerical analysis is carried out in detail for the discretization of the two-field formulation by Taylor-Hood elements and a variant of a Runge-Kutta time discretization. Our arguments can however be extended to three- and four field formulations and other time discretization strategies.

Partner: M. Lymbery; J. Kraus (Universität Duisburg/Essen)

Support: GSC 233, TU Darmstadt

Contact: Mania Sabouri, Herbert Egger

References

[1] H. Egger and M. Sabouri. On the structure preserving high-order approximation of quasistatic poroelasticity. arXiv:1912.13086, 2019. Accepted.

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 domain 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, K. Schmidt, and V. Shashkov. Multistep and Runge-Kutta convolution quadrature methods for coupled dynamical systems. *Comput. Appl. Math.*, 2019.

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 leads 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, Anita Schulz (DLR Berlin)

Contact: Kersten Schmidt, Adrien Semin

References

[1] K. Schmidt and A. Semin. Surface homogenization of an array of Helmholtz resonators for a viscoacoustic model using two-scale convergence. arXiv:2003.11965, 2020.

[2] 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.

[3] 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 optimizing stent designs they remain comfortable 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

References

[1] M. Ljulj, K. Schmidt, A. Semin, and J. Tambača. Homogenization of the time-dependent heat equation on planar one-dimensional periodic structures. arXiv:1912.12989, 2019.

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 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

References

[1] P. Kliewe, A. Laurain, and K. Schmidt. Shape optimization in acoustic-structure interaction. In preparation.

Project: Contour integration methods for nonlinear eigenvalue problems

Nonlinear eigenvalue problems (NEVPs) arise in many modern physical calculations. For linear eigenvalue problems all or a number of largest or smallest eigenvalues can be computed together with well-known techniques. For NEVPs eigenvalues can be computed separately with techniques like Newton or linearization based algorithms. With contour integration methods, several hundred of eigenvalues of a nonlinear eigenvalue problem inside a closed region of the complex plane can be computed together. For this complex integrals contours are approximated by quadrature rules leading to small matrices from which the eigenvalues are extracted. We are interested to analyze contour integration methods for the efficient computation of the spectrum in electromagnetic devices, using the filter functions as tools and contours adapted to the presence of singular points like branch cuts.

Partner: Luka Grubišić (University of Zagreb, Croatia), Rolf Schuhmann (TU Berlin)

Contact: Kersten Schmidt

References

[1] P. Jorkowski, K. Schmidt, C. Schenker, L. Grubišić, and R. Schuhmann. Adapted contour integration for nonlinear eigenvalue problems in wave-guide coupled resonators. Submitted, 2020.

Project: Super-convergent 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, super-convergence. In [2], we derive necessary and sufficient conditions on the coefficient matrices to construct new super-convergent 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 super-convergent 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 super-convergent IMEX Peer methods which maintain the super-convergence property independent of step size changes are constructed for $s = 2, 3, 4$ stages in [3].

Partner: 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.

[3] M. Schneider, J. Lang, and R. Weiner. Super-convergent implicit-explicit peer methods with variable step sizes. *J. Comput. Appl. Math.*, 2019. Available online 26 September 2019, 112501.

Project: Well-balanced and asymptotic preserving IMEX Peer methods

Peer methods are a comprehensive class of time integrators offering numerous degrees of freedom in their coefficient matrices that can be used to ensure advantageous properties, e.g., A-stability or super-convergence. In [1], we show that the super-convergent implicit-explicit (IMEX) Peer methods recently designed in [2, 3] are well-balanced and asymptotic preserving by construction without additional constraints on the coefficients. These properties are relevant when solving (the space discretisation of) hyperbolic systems of balance laws, for example.

Contact: Moritz Schneider, Jens Lang

References

[1] M. Schneider and J. Lang. Well-Balanced and Asymptotic Preserving IMEX-Peer Methods. Numerical Mathematics and Advanced Applications ENUMATH 2019, doi:10.1007/978-3-030-55874-1, 2021. Springer International Publishing.

[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.

[3] M. Schneider, J. Lang, and R. Weiner. Super-convergent implicit-explicit peer methods with variable step sizes. *J. Comput. Appl. Math.*, 2019. Available online 26 September 2019, 112501.

Project: Structure preserving simulation in nonlinear evolution problems

The main aim of this project is to develop novel discretization schemes that preserve the inherent geometric structure of underlying physical models, e.g., conservation or dissipation of energy or the production of entropy. Such systems arise in a variety of applications, e.g., in nonlinear wave propagation problems, in acoustics or electromagnetics, but also in nonlinear partial differential equations describing phase transformation. Two classes of such systems are identified and appropriate variational space- and time discretization schemes are developed. The applicability of the new methods is demonstrated in several applications.

Partner: Prof. Bai-Xiang Xu (TU Darmstadt)

Support: DFG GSC 233, SPP 2256

Contact: Herbert Egger, Vsevolod Shashkov

References

[1] H. Egger. Structure preserving approximation of dissipative evolution problems. *Numer. Math.*, 143:85–106, 2019.

[2] H. Egger. Energy stable Galerkin approximation of Hamiltonian and gradient systems. *Comput. Meth. Appl. Math.*, 2020. in press.

[3] H. Egger, T. Kugler, and V. Shashkov. An inexact Petrov-Galerkin approximation for gas transport in pipeline networks. In *Proceedings of ICOSAHOM 2018*. Springer.

[4] H. Egger and V. Shashkov. On energy preserving high-order discretizations for nonlinear acoustics. In *Proceedings ENUMATH 2019*. Springer, 2019. in press.

[5] Y. Yang, P. Kühn, M. Yi, H. Egger, and B.-X. Xu. Non-isothermal phase-field modeling of heat-melt-microstructure-coupled processes during powder bed fusion. *JOM*, 72:1719–1733, 2020.

Project: Efficient discretization of memory kernels

This project is devoted to the numerical solution of Volterra integro-differential equations arising in a variety of problems, e.g., multiscale models, dispersive media, boundary element methods for wave propagation, or field-circuit coupled problems. The main challenge consists in the efficient evaluation of memory terms, represented as Volterra integral operators. For a problem with N time-steps, a naive realization leads to algorithms with $O(N^2)$ complexity and requiring $O(N)$ active memory. For the efficient realization, we consider a convolution quadrature approach having $O(N \log N)$ complexity and $O(\log N)$ active memory, and we present a further improvement leading to an algorithm with optimal $O(N)$ complexity. The latter is based on $\mathcal{H}^2$-matrix compression techniques, which we make suitable for a successive evaluation needed for evolutionary problems. We further discuss the application to typical model problems in electromagnetics.

Support: EXC GSC 233, DFG TRR 146

Partner: J. Dölz (Uni Bonn)

Contact: Herbert Egger, Vsevolod Shashkov

References

[1] J. Dölz, H. Egger, and V. Shashkov. Fast and oblivious evolutionary evaluation of volterra integral operators. *in preparation*.

[2] J. Dölz, H. Egger, and V. Shashkov. A convolution quadrature method for Maxwell's equations in dispersive media. In *Proceedings SCEE 2020*. Springer, 2020.

[3] H. Egger, K. Schmidt, and V. Shashkov. Multistep and Runge-Kutta convolution quadrature methods for coupled dynamical systems. *Comput. Appl. Math.*, 2019.

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

Borehole heat exchanger (BHE) arrays have become a common implement for extracting and/or storing heat energy from and into the soil. Building these facilities is expensive and their performance is subject to various sources of uncertainty, such as deviating borehole paths and unknown soil conditions. To examine this, we work on simulating BHE arrays and performing uncertainty quantifications, where we study the influence of geometries deviating from the planned layout and other sources of uncertainty.

We make use of a 3D simulation model for BHE arrays in a patch of soil with optional groundwater flow, designed as a system of partial differential equations (PDEs). Continuing our work from [2], the system is solved with a simulation toolkit, which was programmed as an extension for the finite element method solver KARDOS. The toolkit builds on previous work for the simulation tool BASIMO [1] and was validated with benchmarks calculated with the commercial software FEFLOW, which specializes in heat transfer in porous media among other things. For the uncertainty quantification, we utilize an adaptive, anisotropic stochastic collocation method, which uses solutions of the PDE system as samples.

In our research, we investigated the influence of deviating borehole paths on BHE arrays in a heat extraction application. We performed a case study for a specific facility and were able to generalize our findings to show that facilities of this type and operation are surprisingly robust to introduced sources of uncertainty disturbing the array geometry [3].

Partner: Ingo Sass, Daniel O. Schulte, Bastian Welsch (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, TU Darmstadt, 2018.

[3] P. Steinbach, D. O. Schulte, B. Welsch, I. Sass, and J. Lang. Quantification of bore path uncertainty in borehole heat exchanger arrays. arXiv:2103.00271, 2021.

Project: Probabilistic constraints in optimization problems on flow network

Optimization under uncertainties can be realized using probabilistic constraints so that inequality constraints are satisfied with a predefined probability level. In order to compute the probability in the constraints, we analyze two methods: the spheric radial decomposition and the kernel density estimation. The second approach provides approximations of probability density functions which we integrate to approximate the corresponding probability. We consider stationary and transient flow models with uncertain boundary data on networks. As constraint we consider the probability that the solution at specific nodes meet some given bounds. In both settings, we compute derivatives of the probabilistic constraints using the kernel density estimation and derive necessary optimality conditions for the approximated optimization problem. Both approaches are applied to a realistic stationary gas network and provide similar results. Further, we investigate a realistic transient setting, a water contamination problem, for which we extend both methods.

Partner: Michael Schuster; Martin Gugat (Universität Erlangen-Nürnberg)

Support: DFG TRR 154

Contact: Elisa Strauch, Jens Lang

References

[1] M. Schuster, E. Strauch, M. Gugat, and J. Lang. Probabilistic constrained optimization on flow networks. arXiv:2009.00352, 2020.

Project: Physics informed neural networks applied to gas pipeline systems

Physics informed neural networks emerged from the machine learning community and offer a new way to approximate solutions of partial differential equations. Based on them, we want to develop a reduced order model for gas pipeline systems. Because of the underlying transport equations which describe the gas flow, this task is not well suited for common reduced order methods like the reduced basis method. Further, we want to analyze the method mathematically and investigate how well-established ideas from other PDE solvers can be applied to physics informed neural networks.

Partner: Marc Pfetsch (TU Darmstadt)

Support: DFG TRR 154

Contact: Erik Laurin Strelow, Jens Lang

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. In a recent collaboration with the project partners from the cardiology group of the Klinik für Radiologie (Universität Freiburg), we have discovered, that this procedure already provides reasonable estimates of the wall-shear stress in the case of well registered geometry. However, due to lower signal respective contrast to noise ratio (SNR/CNR) in practice and due to the present boundary layers high sensitivity of the wall-shear stress estimates with respect to accurate geometry identification there is need of further development. Therefore, the focus is on the data assimilation problem to enhance both, the reconstructions of the geometry and the velocity by utilizing knowledge of the governing fluid dynamics. The investigations of the collaborators from the Fachgebiet Strömungslehre und Aerodynamik (TU Darmstadt) have revealed that a laminarization of typical physiologically pulsating flows, rendering the classical Navier-Stokes equation is a suitable fluid dynamical model. We have developed a framework based on a parametric description and a localization strategy, that allows attacking the reconstruction problem with methods of shape optimization and optimal control in a computationally feasible manner.

Partner: Andreas Bauer, Cameron Tropea (TU Darmstadt); Axel Krafft, Nina Shokina, 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. *Inverse Problems*, 35:095001, 2019.

[4] N. Shokina, G. Teschner, A. Bauer, C. Tropea, H. Egger, J. Hennig, and A. Krafft. Parametric sequential method for mri-based wall shear stress quantification. *IEEE Transactions on Medical Imaging*, 2020.

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 are developed.

Partner: Katrin Mang; Thomas Wick; Winnifried Wollner

Support: DFG Priority Program 1748
Contact: Mirjam Walloth

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 a complementary expertise in a wide range of modeling methods. Also one professor of the Department of Mathematics (Egger) is under 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 after successful evaluation is now 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 this 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 has been involved in the collaborative research centre Transregio TRR 154 with Dr. Domschke and Professors Giesselmann, Egger, Lang, Pfetsch, Schwartz and Ulbrich. Furthermore, groups at Universität Erlangen-Nürnberg (speaker), HU Berlin, TU Berlin, Universität Duisburg-Essen, and Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS) are part of TRR 154.

The homepage of TRR 154 is reachable at `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. Four more members of the department are Research Group Leaders (Disser, Erath, Marschall, Schwartz) with scientific focus on Online Optimization, Numerical Analysis, Two-Phase and Interfacial Flows, and Discrete-Nonlinear Optimization. Together they supervise more than 14 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 Priority Programme SPP 1748

Numerical simulation techniques are an essential component for the construction, design and optimization of cutting-edge technologies as for example innovative products, new materials as well as medical-technical applications and production processes. These important developments pose great demands on quality, reliability and capability of numerical methods, which are used for the simulation of these complex problems. Challenges are for example capture of incompressibility, anisotropy and discontinuities. Existing computer-based solution methods often provide approximations which cannot guarantee substantial, absolutely necessary stability criteria respectively fulfill them. Especially in the field of geometrical and material non-linearity such uncertainties appear. Typical problems are insufficient or even pathological stress approximations due to unsuitable approximation spaces as well as weak convergence behavior because of stiffening effects or mesh distortion. Similar problems arise in the framework of crack and contact problems. Here the resolution of the local discontinuities as well as their evolution plays a key role. The scientists of the DFG Priority Programme 1748 "Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretization Methods, Mechanical and Mathematical Analysis" have set themselves the goal to establish a new quality in the area of non-conventional discretization methods. Herein the work program of the SPP is founded:

1. The evolution of modern non-conventional discretization methods,
2. their mathematical analysis and
3. the exploration of their application limits on the basis of suitable benchmark problems

The SPP1748 is coordinated by Prof. Dr.-Ing. habil. Jörg Schröder (Universität Duisburg-Essen). The current second funding period started in 2018, comprising 11 scientific projects.
The Department of Mathematics participates with two PIs (Walloth, Wollner) during the second funding period.

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.

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. Jürgen Dölz (Universität Bonn): Fast and oblivious convolution quadrature.
- Prof. Dr. Maria Lukacova, Dr. Burkhard Dünweg (JGU Mainz): Modeling and Simulation of spinodal decomposition.

- Prof. Dr. Matthias Schlottbom (University of Twente, The Netherlands): Model order reduction for inverse problems.
- Prof. Dr. Sebastian Schöps (TU Darmstadt): Electromagnetic interface problems.
- Prof. Dr. Cameron Tropea (TU Darmstadt), Prof. Dr. Jürgen Hennig (UK Freiburg): Estimation of wall-shear stress in human arteries.
- Prof. Dr. Bai-Xiang Xu (TU Darmstadt): Phasefield modeling of additive manufaturing processes.
- Dr. Liljegren-Sailer (Universität Trier): Numerical approximation of gas transport models.

Christoph Erath

- Prof. Dr. Jens Markus Melenk (TU Wien) and Lorenzo Mascotto, PhD (University of Vienna) and Dr. Alexander Rieder (University of Vienna) and Prof. Ilaria Perugia, PhD (University of Vienna): dGFEM-BEM for Helmholtz problems.
- Prof. Dr. Stefan Kurz (TU Darmstadt) and Mehdi Elasmi (TU Darmstadt): Isogeometric FEM-BEM couplings.
- Prof. Dr. Herbert Egger (TU Darmstadt): Mixed FEM for parabolic problems.

Alf Gerisch

- Prof. Dr. Mark A. J. Chaplain (University of St. Andrews, UK), Dr. Dumitru Trucu (University of Dundee, UK), Dr. Pia Domschke (Frankfurt School of Finance & Management), 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. 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. Jonathan Sherratt (Heriot-Watt University, Edinburgh, UK): Mathematical modelling of wound healing.

Jan Giesselmann

- SFB Transregio 154: Mathematische Modellierung, Simulation und Optimierung am Beispiel von Gasnetzwerken, Speaker: Prof. Dr. Alexander Martin (Universität Erlangen-Nürnberg).
- Group of Prof. Dr. Christian Rohde (Universität Stuttgart): Uncertainty quantification in hyperbolic conservation laws.
- Prof. Dr. Martin Gugat (Universität Erlangen-Nürnberg): Boundary observers for hyperbolic balance laws.

- Dr. Sam Krupa (MPI Leipzig): A posteriori error estimates for discontinuous solutions to hyperbolic conservation laws.
- Prof. Dr. Siegfried Müller (RWTH Aachen): Model adaptive schemes for hyperbolic problems.
- Prof. Dr. Martin Frank (KIT), Dr. Graham Kaland: relaxation in moment methods for kinetic equations.
- Dr. Neeraj Sarna (MPI Magdeburg): Reduced models for hyperbolic equations.

Jens Lang

- Prof. Dr. Weiner (Universität Halle-Wittenberg): IMEX-Peer methods.
- Prof. Dr. David Silvester (University of Manchester): Uncertainty quantification.
- Prof. Dr. Robert Scheichl (Universität Heidelberg): Uncertainty quantification.
- Prof. Dr. Martin Gugat (Universität Erlangen-Nürnberg): Probabilistic constrained optimization on flow networks.
- Dr. Rainald Ehrig (ZIB): Kardos programming.
- Dr. Annemarie Lang (Charite Berlin): Modeling of osteoarthritis.
- Prof. Dr. Bernhard A. Schmitt (Universität Marburg): Discrete adjoint implicit Peer methods.
- Prof. Dr. Michael Hinze (Universität Koblenz-Landau): Model order reduction for flow problems.
- Prof. Dr. Weizhang Huang (University of Kansas), Lennard Kamenski (WIAS Berlin): Anisotropic mesh methods.

Mirjam Walloth

- Prof. Dr. Thomas Wick (Universität Hannover), Prof. Dr. Winnifried Wollner (TU Darmstadt), Katrin Mang (Universität Hannover): Adaptive numerical simulation of quasi-static fracture phase-field models.
- Prof. Dr. Andreas Veeser (University of Milan, Italy): A posterior error estimators for contact and obstacle problems.
- Dr. Marita Thomas (WIAS Berlin): Convergence of adaptive solution of phase-field models.

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)

3.2 Publications in Journals and Proceedings

3.2.1 Journals

[1] A. Bauer, S. Wegt, M. Bopp, S. Jakirlic, C. Tropea, A. Krafft, N. Shokina, J. Hennig, G. Teschner, and H. Egger. Comparison of wall shear stress estimates obtained by laser Doppler velocimetry, magnetic resonance imaging and numerical simulations. *Experiments in Fluids*, 60:112, 2019.

[2] A. Böttcher and H. Egger. Structure preserving discretization of Allen-Cahn type problems modeling the motion of phase boundaries. *Vietnam J. Math.*, 48:847–863, 2020.

[3] N. Chatterjee and U. S. Fjordholm. Convergence of second-order, entropy stable methods for multi-dimensional conservation laws. *ESAIM Math. Model. Numer. Anal.*, 54(4):1415–1428, 2020.

[4] J. Dölz. A higher order perturbation approach for electromagnetic scattering problems on random domains. *SIAM/ASA Journal on Uncertainty Quantification*, 8:748–774, 2020.

[5] J. Dölz, H. Harbrecht, S. Kurz, M. D. Multerer, S. Schöps, and F. Wolf. Bembel: The fast isogeometric boundary element c++ library for Laplace, Helmholtz, and electric wave equation. *SoftwareX*, 11:100476, 2020.

[6] H. Egger. Structure preserving approximation of dissipative evolution problems. *Numer. Math.*, 143:85–106, 2019.

[7] H. Egger, O. Habrich, and V. Shashkov. On the Energy stable Galerkin approximation of Hamiltonian and gradient systems. *Comput. Meth. Appl. Math.*, 2020. in press.

[8] H. Egger and N. Philippi. On the transport limit of singularly perturbed convection-diffusion problems on networks. *Math. Meth. Appl. Sci.*, 44:5005–5020, 2020.

[9] H. Egger and B. Radu. A mass-lumped mixed finite element method for acoustic wave propagation. *Numer. Math.*, 145:239–269, 2020.

[10] H. Egger and B. Radu. A second order finite element method with mass lumping for Maxwell's equations on tetrahedra. *SIAM J. Numer. Analysis*, 2020. accepted.

[11] H. Egger and B. Radu. A second order multipoint flux mixed finite element method on hybrid meshes. *SIAM J. Numer. Anal.*, 58:1822–1844, 2020.

[12] H. Egger and M. Sabouri. On the structure preserving high-order approximation of quasistatic poroelasticity. arXiv:1912.13086, 2019. Accepted.

[13] H. Egger and M. Schlottbom. A perfectly matched layer approach for radiative transfer in highly scattering regimes. *SIAM. J. Numer. Anal.*, 57:2166–2188, 2019.

[14] H. Egger, K. Schmidt, and V. Shashkov. Multistep and Runge-Kutta convolution quadrature methods for coupled dynamical systems. *Comput. Appl. Math.*, 2019.

[15] H. Egger and L. Schöbel-Kröhn. Chemotaxis on networks: analysis and numerical approximation. *ESAIM: M2AN*, 54:1339–1372, 2020.

[16] H. Egger and G. Teschner. On the stable estimation of flow geometry and wall shear stress from magnetic resonance images. *Inverse Problem*, 35:095001, 2019.

[17] C. Erath, G. Gantner, and D. Praetorius. Optimal convergence behavior of adaptive FEM driven by simple $(h - h/2)$-type error estimators. *Comput. Math. Appl.*, 79(3):623–642, 2020.

[18] C. Erath and D. Praetorius. Adaptive vertex-centered finite volume methods for general second-order linear elliptic partial differential equations. *IMA J. Numer. Anal.*, 39(2):983–1008, 2019.

[19] C. Erath and D. Praetorius. Optimal adaptivity for the SUPG finite element method. *Comput. Methods Appl. Mech. Engrg.*, 353:308–327, 2019.

[20] C. Erath and R. Schorr. Stable non-symmetric coupling of the finite volume method and the boundary element method for convection-dominated parabolic-elliptic interface problems. *Comput. Methods Appl. Math.*, 20(2):251–272, 2020.

[21] J. Giesselmann and P. G. LeFloch. Formulation and convergence of the finite volume method for conservation laws on spacetimes with boundary. *Numer. Math.*, 144(4):751–785, 2020.

[22] J. Giesselmann, F. Meyer, and C. Rohde. A posteriori error analysis and adaptive non-intrusive numerical schemes for systems of random conservation laws. *BIT*, 60(3):619–649, 2020.

[23] C. Gräßle, M. Hinze, J. Lang, and S. Ullmann. POD model order reduction with space-adapted snapshots for incompressible flows. *Advances in Computational Mathematics*, 45:2401–2428, 2019.

[24] W. Huang, L. Kamenski, and J. Lang. Conditioning of implicit Runge-Kutta integration for finite element approximation of linear diffusion equations on anisotropic meshes. *J. Comput. Appl. Math.*, 2019. Available online 1 October 2019, 112497.

[25] J. Lang, R. Scheichl, and D. Silvester. A fully adaptive multilevel stochastic collocation strategy for solving elliptic pdes with random data. *Journal of Computational Physics*, 419:109692, 2020.

[26] K. Mang, M. Walloth, T. Wick, and W. Wollner. Mesh adaptivity for quasi-static phase-field fractures based on a residual-type a posteriori error estimator. *GAMM-Mitteilungen*, 43(1), 2020.

[27] F. Meyer, C. Rohde, and J. Giesselmann. *a posteriori* error analysis for random scalar conservation laws using the stochastic Galerkin method. *IMA J. Numer. Anal.*, 40(2):1094–1121, 2020.

[28] P. Mindt, J. Lang, and P. Domschke. Entropy-preserving coupling of hierarchical gas models. *SIAM Journal on Mathematical Analysis*, 51:4754–4775, 2019.

[29] C. Müller, S. Ullmann, and J. Lang. A Bramble-Pasciak conjugate gradient method for discrete Stokes equations with random viscosity. *SIAM/ASA J. Uncertainty Quantification*, 7(3):787–805, 2019.

[30] N. Sarna, J. Giesselmann, and M. Torrilhon. Convergence analysis of Grad's Hermite expansion for linear kinetic equations. *SIAM J. Numer. Anal.*, 58(2):1164–1194, 2020.

[31] M. Schneider, J. Lang, and R. Weiner. Super-convergent implicit-explicit peer methods with variable step sizes. *J. Comput. Appl. Math.*, 2019. Available online 26 September 2019, 112501.

[32] L. Schöbel-Kröhn. *Analysis and numerical approximation of nonlinear evolution equations on network structures*. PhD thesis, 2020.

[33] J. Schröder, T. Wick, S. Reese, P. Wriggers, R. Müller, S. Kollmannsberger, M. Kästner, A. Schwarz, M. Igelbüscher, N. Viebahn, H. R. Bayat, S. Wulfinghoff, K. Mang, E. Rand, T. Bog, D. d'Nagella, M. Elhaddad, P. Hennig, A. Düster, W. Garhuom, S. Hubrich, M. Walloth, W. Wollner, C. Kuhn, and T. Heister. A selection of benchmark problems in solid mechanics and applied mathematics. *Archives of Computational Methods in Engineering*, 28:713–751, 2020.

[34] N. Shokina, A. Bauer, G. Teschner, W. B. Buchenberg, C. Tropea, H. Egger, J. Hennig, and A. J. Krafft. MR-based wall shear stress measurements in fully developed turbulent flow using the Clauser plot method. *J. Magn. Res.*, 305:16–21, 2019.

[35] N. Shokina, G. Teschner, A. Bauer, C. Tropea, H. Egger, J. Hennig, and A. Krafft. Parametric sequential method for mri-based wall shear stress quantification. *IEEE Transactions on Medical Imaging*, 2020.

[36] N. Shokina, G. Teschner, A. Bauer, C. Tropea, H. Egger, J. Hennig, and A. J. Krafft. Quantification of wall shear stress in large blood vessels using magnetic resonance imaging. *J. Comput. Techn.*, 24:4–27, 2019.

[37] Z. Sun, M. Braack, and J. Lang. An adaptive moving finite element method for steady low Mach number compressible combustion problems. *International Journal for Numerical Methods in Fluids*, 92:1081–1095, 2020.

[38] M. Walloth. A reliable, efficient and localized error estimator for a discontinuous galerkin method for the Signorini problem. *Applied Numerical Mathematics*, 135:276–296, 2019.

[39] M. Walloth. Residual-type a posteriori error estimator for a quasi-static Signorini contact problem. *IMA Journal of Numerical Analysis*, 40(3):1937–1971, 2019.

[40] M.-C. Weber, L. Fischer, A. Damerau, I. Ponomarev, M. Pfeiffenberger, T. Gaber, S. Götschel, J. Lang, S. Röblitz, F. Buttgereit, R. Ehrig, and A. Lang. Macroscale mesenchymal condensation to study cytokine-driven cellular and matrix-related changes during cartilage degradation. *Biofabrication*, 12:045016, 2020.

[41] Y. Yang, P. Kühn, M. Yi, H. Egger, and B.-X. Xu. Non-isothermal phase-field modeling of heat-melt-microstructure-coupled processes during powder bed fusion. *JOM*, 72:1719–1733, 2020.

3.2.2 Proceedings and Chapters in Collections

[1] J. Dölz, S. Kurz, S. Schöps, and F. Wolf. Recent advances of isogeometric boundary element methods for electromagnetic scattering problems. *Oberwolfach Reports*, 17, 2020.

[2] H. Egger, J. Dölz, and V. Shashkov. A convolution quadrature method for Maxwell's equations in dispersive media. In *Proceedings SCEE 2020*. Springer, 2020.

[3] H. Egger, M. Harutyunyan, M. Merkel, and S. Schöps. On the stability of harmonic mortar methods with application to electric machines. In *Proceedings SCEE 2020*. Springer, 2020. in press.

[4] H. Egger and T. Kugler. Uniform exponential stability of Galerkin approximations for damped wave systems. In *Advanced Finite Element Methods with Applications, Selected papers from the 30th Chemnitz Finite Element Symposium*. Springer, 2019.

[5] H. Egger, T. Kugler, and B.-L. Sailer. Stability preserving approximations of a semilinear hyperbolic gas transport model. Springer, 2019. in press.

[6] H. Egger, T. Kugler, and V. Shashkov. An inexact Petrov-Galerkin approximation for gas transport in pipeline networks. In *Proceedings of ICOSAHOM 2018*. Springer.

[7] H. Egger and N. Philippi. A hybrid discontinuous galerkin method for transport equations on networks. In *International Conference on Finite Volumes for Complex Applications*, pages 487–495. Springer, 2020.

[8] H. Egger and B. Radu. Comparison of the hybrid and multipoint-flux method. *PAMM*, 19(1):e201900280, 2019.

[9] H. Egger and B. Radu. A mass-lumped mixed finite element method for Maxwell's equations. In *Proceedings of SCEE 2018*. Springer, 2020. in press.

[10] H. Egger and V. Shashkov. On energy preserving high-order discretizations for nonlinear acoustics. In *Proceedings ENUMATH 2019*. Springer, 2019. in press.

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

[12] B. Geißler, A. Martin, A. Morsi, M. Walther, O. Kolb, J. Lang, and L. Wagner. Optimization. In A. Pirsing and A. Morsi, editors, *Decision Support Systems for Water Supply Systems, Smart Water System to Improve the Operation of Water Supply Systems by Using Applied Mathematics*, volume 2 of *EMS Series in Industrial and Applied Mathematics*, pages 73–104, doi:10.4171/207, 2020. European Mathematical Society.

[13] J. Giesselmann and H. Joshi. Model adaptation of balance laws based on a posteriori error estimates and surrogate fluxes. In *Finite volumes for complex applications IX – methods, theoretical aspects, examples. FVCA 9, Bergen, Norway, June 15–19, 2020. In 2 volumes. Volume I and II*, pages 375–383. Cham: Springer, 2020.

[14] J. Giesselmann and H. Joshi. Model adaptation of chemically reacting flows based on a posteriori error estimates. In *Hyperbolic problems: theory, numerics, applications. Proceedings of the 17th international conference, HYP2018, Pennsylvania State Univer-*

sity, University Park, PA, USA, June 25–29, 2018, pages 442–448. Springfield, MO: American Institute of Mathematical Sciences (AIMS), 2020.

[15] J. Giesselmann, F. Meyer, and C. Rohde. An a posteriori error analysis based on non-intrusive spectral projections for systems of random conservation laws. In *Hyperbolic problems: theory, numerics, applications. Proceedings of the 17th international conference, HYP2018, Pennsylvania State University, University Park, PA, USA, June 25–29, 2018*, pages 449–456. Springfield, MO: American Institute of Mathematical Sciences (AIMS), 2020.

[16] J. Giesselmann and D. Zacharenakis. A posteriori analysis for the Navier-Stokes-Korteweg model. In *Hyperbolic problems: theory, numerics, applications. Proceedings of the 17th international conference, HYP2018, Pennsylvania State University, University Park, PA, USA, June 25–29, 2018*, pages 682–690. Springfield, MO: American Institute of Mathematical Sciences (AIMS), 2020.

[17] C. Gräßle, M. Hinze, J. Lang, S. Ullmann, and J. Lang. Model order reduction for space-adaptive simulations of Navier-Stokes. volume 19 of *Proceedings of Applied Mathematrics and Mechanics*, doi:10.1002/pamm.201900435, 2019. Wiley-VCH Verlag GmbH & Co. KGaA Weinheim.

[18] J. Guillot, G. Koenig, H. Minbashian, E. Frenod, H. Fluorescent, and J. Brajard. Partial differential equations for oceanic artificial intelligence. In *CEMRACS 2019 Proceedings (Geophysical Fluids, Gravity Flows), Marseille*, 2019.

[19] K. Mang, M. Walloth, T. Wick, and W. Wollner. Adaptive numerical simulation of a phase-field fracture model in mixed form tested on an l-shaped specimen with high poisson ratios. *Numerical Mathematics and Advanced Applications - ENUMATH 2019*, 2020.

[20] H. Minbashian and J. Giesselmann. Deep learning for hyperbolic conservation laws with non-convex flux. In *Proceedings in Applied Mathematics & Mechanics*, pages 1–6. Wiley-VCH GmbH, 2020.

[21] M. Schneider and J. Lang. Well-Balanced and Asymptotic Preserving IMEX-Peer Methods. Numerical Mathematics and Advanced Applications ENUMATH 2019, doi:10.1007/978-3-030-55874-1, 2021. Springer International Publishing.

[22] A. Voss-Böhme and A. Gerisch. Multi-scale analysis of contact-dependent interaction in tissue aggregation and invasion. In O. Wolkenhauer, editor, *Systems Medicine*, pages 156–168. Academic Press, Oxford, 2021, published online August 2020.

3.3 Preprints

[1] S. Basava, K. Mang, M. Walloth, T. Wick, and W. Wollner. Adaptive and pressure-robust discretization of incompressible pressure-driven phase-field fracture. arXiv:2006.16566, Fachbereich Mathematik, TU Darmstadt, 2020.

[2] A. Brunk, B. Dünweg, H. Egger, O. Habrich, M. Lukacova-Medvidova, and D. Spiller. Analysis of a viscoelastic phase separation model. arXiv:2012.04234, 2020.

[3] A. Dedner, J. Giesselmann, T. Pryer, and J. K. Ryan. Residual estimates for post-processors in elliptic problems. arXiv:1906.04658, 2019.

[4] J. Dölz, H. Egger, and M. Schlottbom. A model reduction approach for inverse problems with operator valued data. arXiv:2004.11827, 2020.

[5] J. Dölz, H. Egger, and V. Shashkov. A convolution quadrature method for maxwell's equations in dispersive media. arXiv:2004.00359, 2020.

[6] J. Dölz, H. Harbrecht, C. Jerez-Hanckes, and M. Multerer. Isogeometric multilevel quadrature for forward and inverse random acoustic scattering. arXiv:2010.14613, 2020.

[7] P. Domschke, O. Kolb, and J. Lang. Fast and reliable transient simulation and continuous optimization of large-scale gas networks. arXiv:2012.02737, 2020.

[8] H. Egger and J. Giesselmann. Stability and asymptotic analysis for instationary gas transport via relative energy estimates. arXiv:2012.14135, 2020.

[9] H. Egger and B. Radu. A second order finite element method with mass lumping for wave equations in H(div). arXiv:1912.07057, 2019.

[10] H. Egger and B. Radu. A second order finite element method with mass lumping for Maxwell's equations on tetrahedra. arXiv:2002.05575, 2020.

[11] H. Egger and M. Sabouri. On the structure preserving high-order approximation of quasistatic poroelasticity. arXiv:1912.13086, 2019.

[12] H. Egger and V. Shashkov. On energy preserving high-order discretizations for nonlinear acoustics. arXiv:1912.07037, 2019.

[13] M. Elasmi, C. Erath, and S. Kurz. Non-symmetric isogeometric fem-bem couplings. arXiv:2007.09057, 2020.

[14] D. Frenzel and J. Lang. A third-order weighted essentially non-oscillatory scheme in optimal control problems governed by nonlinear hyperbolic conservation laws. arXiv:2009.12392, 2020.

[15] J. Giesselmann and E. Mäder-Baumdicker. A posteriori error estimates for wave maps into spheres. arXiv:2010.07552, 2020.

[16] J. Giesselmann, F. Meyer, and C. Rohde. Error control for statistical solutions. arXiv:1912.04323, 2019.

[17] M. Gugat and J. Giesselmann. Boundary feedback stabilization of a semilinear model for the flow in star-shaped gas networks. submitted to ESAIM: Control, Optimisation and Calculus of Variations, 2020.

[18] J. Lang. Rosenbrock-Wanner methods: Construction and mission. arXiv:2002.12028, 2020.

[19] J. Lang, P. Domschke, and E. Strauch. Adaptive single- and multilevel stochastic collocation methods for uncertain gas transport in large-scale networks. arXiv:2012.03565, 2020.

[20] J. Lang and B. A. Schmitt. Discrete adjoint implicit peer methods in optimal control. arXiv:2002.12081, 2020.

[21] M. Ljulj, K. Schmidt, A. Semin, and J. Tambača. Homogenization of the time-dependent heat equation on planar one-dimensional periodic structures. arXiv:1912.12989, 2019.

[22] Y. Mao, A. Gerisch, J. Lang, M. Böhm, and F. Müller-Plathe. Uncertainty quantification guided parameter selection in a fully coupled molecular dynamics-finite element model of the mechanical behaviour of polymers. submitted to Journal of Chemical Theory and Computation, 2020.

[23] N. Sarna, J. Giesselmann, and P. Benner. Data-driven snapshot calibration via monotonic feature matching. arXiv:2009.08414, 2020.

[24] K. Schmidt and A. Semin. Surface homogenization of an array of Helmholtz resonators for a viscoacoustic model using two-scale convergence. arXiv:2003.11965, 2020.

[25] M. Schuster, E. Strauch, M. Gugat, and J. Lang. Probabilistic constrained optimization on flow networks. arXiv:2009.00352, 2020.

[26] N. Shokina, G. Teschner, A. Bauer, C. Tropea, H. Egger, J. Hennig, and A. J. Krafft. Parametric sequential method for MRI-based wall shear stress quantification. arXiv:2004.11827, 2020.

[27] P. Steinbach, D. O. Schulte, B. Welsch, I. Sass, and J. Lang. Quantification of bore path uncertainty in borehole heat exchanger arrays. arXiv:2103.00271, 2021.

[28] S. Ullmann, C. Müller, and J. Lang. Stochastic Galerkin reduced basis methods for parametrized linear elliptic partial differential equations. arXiv:1812.08519, 2020.

3.4 Reviewing and Refereeing

Jürgen Dölz: Applied Mathematical Modelling, MathSciNet, Numerische Mathematik, SIAM Journal on Matrix Analysis and Applications

Pia Domschke: Mathematical Methods of Operations Research

Herbert Egger: Mathematical Reviews, ERC, DFG; Applied Mathematics and Computation, Applied Numerical Mathematics, BIT Numerical Mathematics, Computers and Mathematics with Applications, ESAIM: Mathematical Modelling and Numerical Analysis, European Transactions on Numerical Analysis, Inverse Problems, Journal of Computational Physics, Mathematical Methods in the Applied Sciences, Mathematics and Computers in Simulation, Numerical Functional Analysis and Optimization, Numerische Mathematik, SIAM Journal on Control and Optimization, SIAM Journal on Numerical Analysis, SIAM Journal on Scientific Computing, SMAI Journal of Computational Mathematics

Christoph Erath: Mathematical Reviews, Zentralblatt; Applied Numerical Mathematics, Computers and Mathematics with Applications, Science China Mathematics

Alf Gerisch: Journal of Computational and Applied Mathematics, Journal of Mathematical Biology, Royal Society Open Science, Philosophical Transactions B, Journal of Theoretical Biology, The Fund for Scientific Research (FNRS, Belgium), Institute Research Fellowships Program (IIT Roorkee, India), LE STUDIUM – Loire Valley Institute for Advanced Studies (France)

Jan Giesselmann: Mathematical Reviews; Applied Numerical Mathematics, Networks Heterogeneous Media, Computational Methods in Applied Mathematics, Discrete & Continuous Dynamical Systems-B, Journal on Scientific Computing, Journal of Computational and Applied Mathematics, ESAIM: Mathematical Modelling and Numerical Analysis, Mathematics of Computation, Mathematical Methods in Applied Sciences, SIAM Journal on Applied Mathematics, SIAM Journal on Mathematical Analysis, SIAM Journal on Numerical Analysis, SIAM Journal on Scientific Computing

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: Applied Numerical Mathematics, Journal of Computational and Applied Mathematics, ESAIM: Mathematical Modelling and Numerical Analysis, Nonlinearity

Mirjam Walloth: ESAIM: Mathematical Modelling and Numerical Analysis, International Journal of Applied and Computational Engineering, IMA Journal of Numerical Analysis

3.5 Software

BEMBEL: *Boundary Element Method Based Engineering Library*
BEMBEL is an open source library for isogeometric boundary element methods for Laplace, Helmholtz and Maxwell problems. Available on Github and on `www.bembel.eu`

Contributor at TU Darmstadt: J. Dölz, H. Harbrecht, S. Kurz, M. Multerer, S. Schöps, and F. Wolf

ANACONDA: *Solving Hyperbolic Partial Differential Algebraic Equations on Networks*
ANACONDA is a software package to solve hyperbolic partial differential algebraicequations 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, Elisa Strauch, and formerly Oliver Kolb

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 uncertainty quantification and optimisation.

Contributor at TU Darmstadt: Jens Lang, Alf Gerisch, Philipp Steinbach

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://dowiki.mathematik.tu-darmstadt.de/numa/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. A first version has been distributed in 1994. Different versions exist now 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 8 academic (free) licenses were given. There were 4 commercial requests, but due to misconceptions concerning the royalty fee from the partners side 3 of these were not satisfied, whereas one given. 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. Many visits were very minimalistic, may be due to problems with long range connections, but during 2019 there were 18868 visits, larger ones from 49 countries, viewing 135482 pages and in 2020 9071 such visits from 12 countries viewing 112667 pages. Any application comes with prede-

fined 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 only were done. For more information, see numawww.mathematik.tu-darmstadt.de

Contributor at TU Darmstadt: Peter Spellucci

4 Theses

4.1 PhD Dissertations

2019

Kugler, Thomas, *Galerkin methods for simulation of wave propagation on a network of pipes* (Herbert Egger)

Schorr, Robert, *Numerical Methods for Parabolic-Elliptic Interface Problems* (Christoph Erath)

2020

Frenzel, David, *Weighted Essentially Non-Oscillatory Schemes in Optimal Control Problems Governed by Nonlinear Hyperbolic Conservation Laws* (Jens Lang)

Schöbel-Kröhn, Lucas, *Analysis and Numerical Approximation of Nonlinear Evolution Equations on Network Structures* (Herbert Egger)

4.2 Master Theses

2019

Accorsini, Lisamarie, *Masslumping Verfahren höherer Ordnung für die effiziente Berechnung der linearen Wellengleichung mittels FEM* (Herbert Egger)

Kosara, Thomas, *Modellierung und Simulation akustischer Wellenausbreitung unter Beachtung nichtlinearer Effekte* (Herbert Egger)

Philippi, Nora Marie, *Analysis and Numerical Approximation of Transport Processes on Networks* (Herbert Egger)

Strelow, Erik Laurin, *Relaxierung von diskreten Steuervariablen mittels äußerer Konvexifizierung* (Jens Lang)

2020

Kunkel, Teresa, *Estimation of interface motion by velocity identification in a level-set method* (Herbert Egger)

4.3 Bachelor Theses

2019

Ihrig, Anna-Lisa, *Numerische Zeitintegration für Neuronale Netzwerke* (Jens Lang)

Wilka, Hendrik, *Superconvergent Explicit Peer Methods with Step Size Control: Theory and Applications* (Jens Lang)

2020

Anthes, Christopher, *Eingebettete explizite Runge-Kutta-Verfahren höherer Ordnung* (Jens Lang)

Antunes Vieira, Marilia, *Exponentielle Runge-Kutta-Verfahren* (Jens Lang)

Englert, Johannes Andreas, *Analysis and Discretization of an elastic model on graphs* (PD Kersten Schmidt)

Fries, Marco Dorian, *Linearly Implicit Two-Step Peer Methods: Theory and Application* (Jens Lang)

Keil, Niels Heinrich, *Finite Volumen Verfahren für Euler Gleichungen zur Wettervorhersage auf Arakawa C-Gittern* (Jens Lang)

Kühnel, Bianca Margit, *Sensorplatzierung und 2-Zusammenhang* (Martin Kiehl)

Martin, Tatjana, *Implizit-Explizite Runge-Kutta Methoden mit optimierten Speicher* (Jens Lang)

Pfaff, Sven, *Numerische Simulation von Mehrkörpersystemen* (Herbert Egger)

Urban, Mira, *Modellierung und Numerische Simulation von Nervenzellen mittels Neuronenmodelle* (Jens Lang)

Windt, Anna, *Relaxation Runge-Kutta Methods: Theory and Application* (Jens Lang)

Özalp, Elise, *Sympletic Runge-Kutta Methods for Hamiltonian Systems* (Alf Gerisch)

5 Presentations

5.1 Talks and Visits

5.1.1 Invited Talks and Addresses

Jürgen Dölz

15/03/2019 *On the Intersection of Non-local Operators and Uncertainty Quantification*
Seminar on Numerical Analysis, TU Delft (The Netherlands)

03/07/2019 *On the Intersection of Non-local Operators and Uncertainty Quantification*
Seminar on Numerical Analysis, Universität Bonn

05/10/2019 *Electromagnetic Scattering on Random Domains*
Seminar on Mathematical Theory of Uncertainty Quantification, University of Twente, Enschede (The Netherlands)

Pia Domschke

19/03/2019 *Error-controlled adaptive simulation of gas transmission networks*
Women in Optimization 2019, Bonn

Herbert Egger

08/01/2019 *Systematic approximation of evolution problems with dissipation, Hamiltonian, or gradient structure*
Kolloquium AG Modellierung-Numerik-Differentialgleichungen, TU Berlin

15/05/2019 *Structure preserving approximation of nonlinear evolution problems*
Mathematics Colloquium, Universität Duisburg/Essen

09/09/2019 *Systematic discretization of some nonlinear evolution problems*
Conference on Reliable Methods of Mathematical Modeling, TU Wien

19/09/2019 *Structure preserving approximation of quasistatic poroelasticty*
Modelling 2019, Olomouc

02/10/2019 *Energy stable approximation of nonlinear wave propagation problems*
ENUMATH Conference, Egmond an Zee

22/06/2020 *On model order reduction for inverse problems in tomographic imaging applications*
SSD Seminar, RWTH Aachen

15/09/2020 *Structure preserving discretization of dissipative Hamiltonian dynamics*
DMV Annual Meeting, TU Chemnitz

28/10/2020 *Stability and asymptotic analysis for instationary gas transport via relative energy estimates*
Thematic Einstein Semester on Energy-based mathematical methods for reactive multiphase flows, Kickoff Conference, Berlin

07/12/2020 *On model order reduction for inverse problems with operator valued data*
Worshop on Computational Inverse Problems for Partial Differential Equations, Oberwolfach

Christoph Erath

12/03/2019 *Numerische Mathematik in der Sekundarstufe*
PH Vorarlberg, Austria

Alf Gerisch

08/05/2019 *What is ... Mathematical modeling of cancer invasion in tissue?*
What is? seminar, TU Darmstadt

06/03/2020 *Modelling and Simulation of Collective Cell Migration: Cross-diffusion and Attracting/Repelling Nonlocal Interactions*
Frankfurt Institute for Advanced Studies (FIAS), Frankfurt (Main)

Jan Giesselmann

09/01/2019 *A posteriori error estimators for systems of hyperbolic conservation laws*
Oberseminar KIT

21/05/2019 *Relative Entropies for Hyperbolic Problems on Networks*
Workshop on Nonlinear Hyperbolic Problems: modeling, analysis, and numerics, Oberwolfach

19/06/2019 *Model-adaptive discontinuous Galerkin schemes for compressible fluid flows*
MAFELAP 2019, Brunel University London, UK

04/07/2019 *A Posteriori Error Estimates of Numerical Methods for Random Conservation Laws*
Innovative Training Network Workshop on Shocks and Interfaces, Oxford

19/07/2019 *Relative entropy based model-adaptive numerical schemes in fluid mechanics*
ICIAM 2019, Valencia

19/07/2019 *Aposteriori estimates for random systems of hyperbolic conservation laws*
ICIAM 2019, Valencia

09/09/2019 *A Posteriori Error Estimates of Numerical Methods for Random Hyperbolic Conservation Laws*
14th Hirschegg Workshop on Conservation Laws, Hirschegg (Kleinwalstertal)

27/09/2019 *Relative entropy for the Euler-Korteweg system with non-monotone pressure*
SMF Week - Inhomogeneous Flows: Asymptotic Models and Interfaces Evolution, Luminy

15/11/2019 *A posteriori error analysis for nonlinear systems of hyperbolic conservation laws*
CSC Seminar, Max Planck Institut für Dynamik komplexer Technischer Systeme, Magdeburg

09/01/2020 *Relative Entropy for Gas Flows on Networks*
Seminar of Graduate School Energy, Entropy, and Dissipative Dynamics, RWTH Aachen

Martin Kiehl

23/02/2019 *Gier – Nicht immer ein Weg zum Erfolg*
Mathematikolympiade Hessen, Darmstadt

16/03/2019 *Mathematische Modellierung mit Funktionen*
Tag der Mathematik, Bensheim

25/09/2019 *Mit Mathematik Probleme spielerisch lösen*
Schülernachmittag, TU Darmstadt

22/02/2020 *Spieltheorie – Was ist der beste Zug*
Mathematikolympiade Hessen, Darmstadt

Jens Lang

26/04/2019 *Adaptive Moving Meshes in Large Eddy Simulation for Turbulent Flows*
Towards Computable Flows Workshop honoring the 68th birthday of Gert Lube, Göttingen

27/05/2019 *An Adaptive Multilevel Stochastic Collocation Method for Elliptic PDEs with Uncertain Data*
ADMOS, Alicante

23/07/2019 *Super-Convergent IMEX-Peer Methods with Variable Time Steps*
SCICADE, Innsbruck

Nora Philippi

23/11/2020 *On the transport limit of singularly perturbed convection-diffusion problems on networks*
Mini-workshop on Robots Learning, Optimization and Control, FAU

Elisa Strauch

09/05/2019 *Stochastic Collocation Method for Partial Differential Equations with Random Input Data*
CAA Seminar, Universität Erlangen-Nürnberg

23/11/2020 *Probabilistic Constraints in Optimization Problems on Flow Networks*
Mini-workshop on Robots Learning, Optimization and Control, Universität Erlangen-Nürnberg

Mirjam Walloth

19/02/2019 *A posteriori estimator for the adaptive solution of a quasi-static fracture phase-field model*
90th Annual Meeting of the International Association of Applied Mathematics and Mechanics (GAMM), Wien

14/05/2019 *Reliable, efficient and robust a posteriori estimators for the variational inequality in fracture phase-field models*
WIAS Berlin

20/06/2019 *Residual-type a posteriori estimators for the singularly perturbed variational inequality in quasi-static fracture phase-field models*
The Mathematics of Finite Elements and Applications (MAFELAP) 2019, Brunel University London, UK

28/08/2019 *A residual-type a posteriori estimator for the adaptive discretization in space and time of a viscoelastic contact problem*
8th GACM Colloquium on Computational Mechanics (GACM), Kassel

30/09/2019 *Adaptive discretization methods for the numerical simulation of static and time-dependent contact problems*
European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019), Egmond aan Zee

16/01/2020 *Residual-type a posteriori estimator for a quasi-static contact problem*
Fachbereich Mathematik und Informatik, Universität Münster

03/02/2020 *Residual-type a posteriori estimators for the adaptive solution of quasi-static fracture phase-field models*
Fakultät Mathematik, KIT

5.1.2 Contributed Talks

Neelabja Chatterjee

29/10/2019 *Convergence analysis of a numerical scheme for a general class of Mean field Equation*
Seminar der AG Numerik, TU Darmstadt

23/11/2020 *Convergence of second-order, entropy stable scheme in multi-dimension*
Seminar der AG Numerik, TU Darmstadt

Jürgen Dölz

22/01/2019 *A higher order perturbation approach for electromagnetic scattering problems on random domains*
WONAPDE 2019, Concepcion (Chile)

20/02/2019 *A higher order perturbation approach for electromagnetic scattering problems on random domains*
90th GAMM Annual Meeting (GAMM 2019), Vienna, Austria

27/02/2019 *On the best approximation of the hierarchical matrix product*
SIAM CSE 2019, Spokane (Washington, USA)

13/06/2019 *H-matrix accelerated second moment analysis for potentials with rough correlation*
PASC 2019, Zürich

06/02/2020 *Recent advances of isogeometric boundary element methods for electromagnetic scattering problems*
Mini-workshop on Boundary Element Methods, Oberwolfach

Herbert Egger

31/05/2019 *Variationally consistent modeling and simulation of laser-based additive manufactering*
SPP 2256 Information Event, DFG Bonn

27/06/2019 *Some notes on high-order methods*
Workshop on High-order and spectral methods, TU Darmstadt

10/07/2019 *Nonlocal diffusion, poroelastodynamics, and network vibrations*
3rd Darmstadt/Graz Workshop, TU Darmstadt

19/11/2019 *Spinodal decomposition of polymer-solvent systems*
TRR 146 Retreat, Nierstein

24/02/2020 *Energy-based modeling and numerical approximation of coupled dynamical systems*
4th Darmstadt/Graz Workshop, TU Graz

03/06/2020 *On the inf-sup stability of harmoncic coupling for the simulation of electric machines*
AG Seminar Numerik, TU Darmstadt

30/09/2020 *On relative energy estimates for macroscopic models describing phase separating systems*
CECAM Conference on Multiscale Simulation Methods in Soft Matter Systems III, Nierstein

19/10/2020 *Quantitative variational phase-field modeling and simulation of PBF additive manufacturing*
SPP 2256 Kickoff Meeting

Christoph Erath

12/09/2019 *On the nonsymmetric coupling method for parabolic-elliptic interface problems*
Reliable Methods of Mathematical Modeling, TU Wien, Austria

16/09/2019 *Efficient solving of a time-dependent interface problem*
OeMG-Conference (Austrian Mathematical Society), Dornbirn, Austria

04/10/2019 *Parabolic-elliptic interface problem on an unbounded domain: full discretization with the method of lines*
Fast BEM 2019, Hirschegg (Kleinwalsertal)

Hrishikesh Joshi

19/06/2019 *Model adaptation for chemically reacting flows: an a posteriori estimator based approach*
Numerical Methods for Hyperbolic Problems (NumHyp 2019), Malaga, Spain

09/09/2019 *Model adaptation for hyperbolic balance laws*
14th Hirschegg Workshop on Conservation Laws, Hirschegg (Kleinwalsertal)

15/06/2020 *Model adaptation of balance laws based on a posteriori error estimates and surrogate fluxes*
Finite Volumes for Complex Applications (FVCA9), Bergen, Norway (virtual)

Hadi Minbashian

02/08/2019 *A dual-weighted residual error estimate for hyperbolic problems*
CEMRACS 2019, Marseille

Christopher Müller

09/07/2019 *A stochastic Galerkin reduced basis method with adaptive snapshots*
Seminar der AG Numerik, TU Darmstadt

11/09/2019 *A stochastic Galerkin reduced basis (SGRB) method for convection-diffusion-reaction equations based on adaptive snapshots*
Workshop on Frontiers of Uncertainty Quantification in Fluid Dynamics (FRONTUQ 2019), Pisa, Italy

30/09/2019 *A stochastic Galerkin reduced basis (SGRB) method for parametrized elliptic PDEs based on adaptive snapshots*
European Numerical Mathematics and Advanced Applications Conference (ENUMATH 2019), Egmond aan Zee, The Netherlands

Nora Philippi

06/05/2020 *On the transport limit of singularly perturbed convection-diffusion problems on networks*
Seminar der AG Numerik, TU Darmstadt

18/06/2020 *A hybrid discontinuous Galerkin method for transport equations on networks*
Finite Volumes for Complex Applications IX (FVCA9), Bergen, Norway (virtual)

Bogdan Radu

21/02/2019 *A second order multipoint flux mixed finite element method on hybrid meshes*
90th GAMM Annual Meeting (GAMM 2019), Vienna, Austria

01/07/2019 *A second order multipoint flux mixed finite element method on hybrid meshes*
12th Workshop on Analysis and Advanced Numerical Methods for Partial Differential Equations, Strobl, Austria

27/07/2019 *High-order mass lumping for wave propagation*
Workshop on higher order methods, Darmstadt, Germany

12/09/2019 *A Mixed FEM with mass lumping for acoustic wave propagation*
GAMM Workshop Numerische Analysis 2019, 11.-12. September 2019, Uni Essen

04/10/2019 *A second order multipoint flux mixed finite element method on hybrid meshes*
European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019), Egmond aan Zee, The Netherlands

05/08/2020 *What is poroelasticity?*
"What is" presentation, Darmstadt, Germany

Mania Sabouri

27/06/2019 *Introduction to spectral element methods*
Workshop on High-order and Spectral Methods, TU Darmstadt

27/06/2019 *Mortar spectral element method for the p-Laplacian equation*
Workshop on High-order and Spectral Methods, TU Darmstadt

Kersten Schmidt

27/06/2019 *High-order FEM and generalized FEM for resolving singular solutions*
Workshop on High-order and Spectral Methods, Darmstadt

27/08/2019 *Asymptotic analysis of the visco-acoustic equations for absorbing walls of arrays of Helmholtz resonators*
14th International Conference on Mathematical and Numerical Aspects of Wave Propagation, Vienna, Austria

17/09/2019 *Asymptotic analysis of the visco-acoustic equations for absorbing perforated walls*
Singular Days 2019, Kassel

Moritz Schneider

15/07/2019 *Superconvergent IMEX Peer methods with variable step sizes*
International Congress on Industrial and Applied Mathematics (ICIAM 2019), Valencia, Spain

04/10/2019 *Superconvergent IMEX Peer methods with variable step sizes*
European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019), Egmond aan Zee, The Netherlands

08/07/2020 *Superconvergent IMEX Peer methods with variable step sizes*
SIAM Annual Meeting (AN20), Toronto, Canada (virtual)

Vsevolod Shashkov

22/02/2019 *Convolution quadrature methods for coupled nonlinear-linear dynamical systems*
90th GAMM Anual Meeting (GAMM 2019), Vienna, Austria

20/05/2020 *On convolution quadrature for Maxwell's equations in dispersive media*
Seminar der AG Numerik, TU Darmstadt

Philipp Steinbach

06/05/2020 *Uncertainty Quantification of Borehole Thermal Energy Storage Facilities*
EGU General Assembly 2020, online

24/06/2020 *Uncertainty Quantification of Borehole Thermal Energy Storage Facilities*
Seminar der AG Numerik, TU Darmstadt

Elisa Strauch

15/07/2019 *Stochastic Collocation Method for Hyperbolic PDEs with Random Initial Data*
The XV International Conference on Stochastic Programming (ICSP XV), Trondheim, Norway

Gabriel Teschner

02/10/2019 *A framework for estimation of flow geometry and wall shear stress from MRV*
Chemnitz Symposium on Inverse Problems 2019, Frankfurt

12/11/2019 *A framework for estimation of flow geometry and wall shear stress from MRV*
Seminar der AG Numerik, TU Darmstadt

Mirjam Walloth

22/01/2019 *A posteriori estimator for the singularly perturbed variational inequality for a fracture phase-field model*
Seminar der AG Numerik, TU Darmstadt

02/07/2019 *A posteriori estimators for the adaptive solution of quasi-static fracture phase-field models*
Modern Finite Element Technologies Mathematical and Mechanical Aspects (MFET 2019), Bad Honnef

Dimitrios Zacharenakis

13/09/2019 *Asymptotic preserving schemes for gas flows on large networks*
14th Hirschegg Workshop on Conservation Laws, Hirschegg (Kleinwalsertal)

04/10/2019 *Asymptotic analysis on large-scale gas networks*
European Conference on Numerical Mathematics and Advanced Applications (ENUMATH 2019), Egmond aan Zee, The Netherlands

5.1.3 Visits

Jan Giesselmann, King Abdullah Universiy of Science and Technology, Thuwal, Saudi-Arabia, April 2019

Jan Giesselmann, Foundation for Research and Technology - Hellas, Crete, Greece, March 2020

5.2 Organization and Program Commitees of Conferences and Workshops

Pia Domschke

– Minisymposium: Numerical methods to advance mathematical biology research (jointly with Alf Gerisch (TU Darmstadt) and Chandrasekhar Venkataraman (Sussex, UK)) at the European Conferences on Numerical Mathematics and Advanced Applications (ENUMATH2019), 30.09.19–04.10.19, Egmond aan Zee, The Netherlands

Herbert Egger

- Minisymposium: Recent developments in the numerical approximation of transport equations, Mafelap 2019, 18.06.19–21.06.19, Brunel University London, UK
- Workshop on High-order and Spectral Methods, 27.06.19, TU Darmstadt (jointly with Mania Sabouri)
- Section on Numerical analysis, GAMM Conference 2020, 16.03.20–20.03.20, Kassel

Christoph Erath

- Strategietagung TU Darmstadt und TU Graz, 10.07.19–11.07.19, TU Darmstadt

Alf Gerisch

- Minisymposium: Numerical methods to advance mathematical biology research (jointly with Pia Domschke (TU Darmstadt) and Chandrasekhar Venkataraman (Sussex, UK)) at the European Conferences on Numerical Mathematics and Advanced Applications (ENUMATH2019), 30.09.19–04.10.19, Egmond aan Zee, The Netherlands

Mania Sabouri

- Workshop on High-order and Spectral Methods, 27.06.19, TU Darmstadt (jointly with Herbert Egger)

6 Workshops and Visitors at the Department

6.1 Guest Talks at the Department

14/01/2019 Dr. Mané Harytyunyan (TU Kaiserslautern), *Modellierung, Analyse und Diskretisierung von magnetorestriktiven Materialien* (Herbert Egger)

05/02/2019 Prof. Dr. Jennifer K. Ryan (Universität Düsseldorf and University of East Anglia, UK), *Constructing Accurate Post-Processing Convolution Kernels* (Jan Giesselmann)

20/02/2019 Marcel Klinge (Universität Halle-Wittenberg), *A comparison of one-step and two-step AMF methods* (Jens Lang)

04/06/2019 Kishore Nori (RWTH Aachen), *Viscous extension of Moment models for Shallow flows: Theory and Numeric* (Jan Giesselmann)

11/06/2019 Dr. Neeraj Sarna (MPI Dynamik komplexer technischer Systeme, Magdeburg), *Entropy stable schemes for linear kinetic equations* (Jan Giesselmann)

12/06/2019 Dr. Reinhald Ehrig (Zuse Institute Berlin), *Model development and FE calculations for the characterization of human osteoarthritis* (Jens Lang)

27/06/2019 Ass. Prof. Dr. Frankziska Weber (Carnegie Mellon University, USA), *Numerical approximation of statistical solutions for systems of hyperbolic conservation laws* (Jan Giesselmann)

22/10/2019 Rahel Brügger (Universität Basel), *On the Solution of a Time-dependent Inverse Shape Identification Problem of Heat Equation* (Herbert Egger)

05/11/2019 Dipl. Math. Daniel Sebastian (TU Wien), *How functional error estimates could unite adaptivity and error control for boundary element methods* (Christoph Erath)

21/11/2019 Dr. Philipp Öffner (Universität Zürich), *About the stability of numerical schemes for hyperbolic conservation laws* (Jan Giesselmann)

03/12/2019 Camile Kunz (FIAS Frankfurt), *An overview of numerical approaches for a coupled chemotaxis-reaction-diffusion system* (Alf Gerisch)

10/12/2019 Dr. Alexander Konschin (Universität Bremen), *Streuung an lokal gestörten periodischen Medien und die Bloch-Floquet-Transformation* (Herbert Egger)

30/01/2020 Dr. Julian Köllermeier (KU Leuven, Belgium), *Moment Models for Kinetic Equations — On Efficient Numerical Methods* (Jan Giesselmann)

04/02/2020 Dr. Maria Lymbery (Universität Duisburg-Essen), *On the numerical solution of the fully dynamic MPET system* (Herbert Egger)

06/02/2020 Prof. Dr. Markus Bause (Helmut-Schmidt-Universität Hamburg), *On Generalized Space-Time Finite Element Methods for Flow and Waves* (Herbert Egger)

13/05/2020 Dr. Matthias Schlottbom (University of Twente, The Netherlands), *A model reduction approach for inverse problems with operator valued data* (Herbert Egger)

27/05/2020 Melvin Liebsch (TU Darmstadt and CERN), *Bayesian Inference in Magnetic Measurement of Accelerator Magnets* (Herbert Egger)

10/06/2020 Laura D'Angelo (TU Darmstadt), *Quasi-3D Quench Simulation of Superconducting Magnets* (Herbert Egger)

17/06/2020 Iryna Kultchytsa (TU Darmstadt), *Parallel-in-time calculation of the periodic steady-state solution with application in electrical engineering* (Herbert Egger)

17/07/2020 Richard Löscher (TU Graz), *A space-time finite element method for the wave equation using a modified Hilbert transformation* (Herbert Egger)

16/10/2020 Dr. Kathrin Smetana (University of Twente, The Netherlands), *Stable Petrov-Galerkin methods for (kinetic) transport equations* (Herbert Egger)

07/12/2020 Jun.-Prof. Dr. Sandra May (TU Dortmund), *Time-dependent conservation laws on cut cell meshes and the small cell problem* (Herbert Egger)

16/12/2020 Ass. Prof. Dr. Elena Rossi (University Modena and Reggio Emilia, Italy), *Traffic flows at road junctions: a macroscopic multilane approach* (Jan Giesselmann)

23/12/2020 Prof. Dr. Martin Gugat (Universität Erlangen-Nürnberg), *On problems of dynamic optimal nodal control for gas networks* (Jan Giesselmann)

6.2 Visitors at the Department

Prof. Dr. Olaf Steinbach (TU Graz, Austria), March 2019.

Dr. Sam G. Krupa (Max Planck Institute Leipzig), July - August 2020.

Prof. Dr. Josip Tambača (University of Zagreb, Croatia), February – March 2020.

Matko Ljulj (University of Zagreb, Croatia), February – March 2020.

6.3 Workshops and Conferences at the Department

- Mathematische Modellierungswoche, Fuldatal, 06.10.19–11.10.19 (organized by Martin Kiehl, Jan Giesselmann 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 Termo-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 Universität Halle-Wittenberg every three years

7.2 Awards and Offers

Awards

Jens Lang: Berlin Research Award for Alternatives to Animal Experiments, December 12, 2019

Offers of Appointments

Jan Giesselmann: Professorship (W3) for Applied Mathematics, Universität Paderborn

Jan Giesselmann: Professorship (W3) for Numerical Mathematics, Ruhr–Universität Bochum

7.3 Secondary Schools and Public Relations

The department of mathematics is involved in various activities for schools, secondary school students, and public relations. In addition to providing printed information material, the department of mathematics presents itself to the public on its web pages. These were fundamentally revised in 2020 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, 10 scientists (F. Aurzada, P. Domschke, R. Haller-Dintelmann, A. Knof, B. Kümmerer, M. Otto, A.-M. von Pippich, U. Reif, A. Schwartz, B. Seyfferth) have offered lectures

covering a wide range of topics. In 2019, lectures within the frame of Math on Demand have taken place in the context of school visits at our department (see list below). In 2020, there have been no lectures due to the Covid-19 pandemic. Further information is available on our homepage:
https://www.mathematik.tu-darmstadt.de/studium/orientierungsangebote/studieninteressierte_1/math_on_demand/index.de.jsp

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, as well as scientific talks from the fields of Analysis, Numerical Analysis and Optimisation in 2019 and from the fields of Algebra, Geometry and Numerical Analysis in 2020.
- Presentation of the department and its study programmes at the university information day, TUDay, every May: with talks by the student advisor, sample lectures, tutorial classes, and meetings with students of the department; about 80 participants over the course of the day (two lectures from the field of Logic in 2019 and two lectures from the fields of Algebra and Analysis in 2020). Due to the Covid-19 pandemic, the TUDay in 2020 took place virtually.
- Participation in the university fair "vocatium", a fair for school students who are interested in a university study programme (28.05.19 in Offenbach, Dr. Seeberg; 2020 (online))
- Participation in two university fairs abroad in 2019 in Russia and Poland to recruite international students (October and November 2019, Nathalie Becker).
- Participation in a virtual university fair for international prospective students in Ukraine and Belarus (27.11.20, Nathalie Becker).
- Due to the Covid-19 pandemic, student advisory for prospective students mostly was held online via Zoom by Dr. Seeberg in 2020.
- Annual organisation of an afternoon with several talks about mathematics for secondary school students, “Darmstädter Schülerinnen- und Schülernachmittag zur Mathematik” (organisation: Prof. Kohler; in 2019 with talks from the fields of Algebra, Numerical Analysis and Stochastics). In 2020, the event had to be cancelled due to the Covid-19 pandemic.
- 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 by female mathematicians. About 30 participants in each year (organized by the department’s gender equality officers; lectures from the field of Numerical Analysis in 2019 and from the field of Algebra in 2020).

- 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), by Prof. Kiehl, academic staff and students. In the recent years, the department had the opportunity to host the finals with about 150 participants.
  Mathematical afternoon (lectures were delivered by Prof. Kiehl and Prof. Haller-Dintelmann (2019)) and Prof. Kiehl and Prof. Schwartz (2020).

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

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

- Lecture titled "Kryptographie" in the context of the "Kinder-Uni" by Prof. Bruder and Insa Apel in 2019.

- 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. The ”Knobelstraßen” take place annually shortly before Christmas.

Other activities

- In connection with the "Profilwerkstatt" Darmstadt, production of a short video to promote the Master’s programme Mathematics in 2020. Protagonists were Prof. Schwartz and a student enrolled in this study programme.

- Talk titled "Endlos summieren?" at Berufliche Schule Gelnhausen (25.01.19, Prof. Haller-Dintelmann).

- Talk titled "Wie gewinnt man eine Goldmedaille im Skifliegen?" and "Wie löst man die Wettbewerbsaufgaben?" (16.03.19, Prof. Kiehl).

- Talk titled "Mit welcher Wahrscheinlichkeit stirbt ein Familienname aus?", visit from the Max-Planck-Gymnasium Groß-Umstadt (18.06.19, Prof. Aurzada).

- Visit of the lecture "Lineare Algebra II" in the context of the visit of the Gymnasium Michelstadt (26.06.19, Prof. Pfetsch, Dr. Hojny).

- Talk titled "Mit Mathematik Probleme spielerisch lösen", visit from the Georg-August-Zinn-Schule Reichelsheim/Odenwald (25.09.19, Prof. Kiehl).

- Talk titled "Was Sie schon immer über perfektoide Räume wissen wollten und nie zu fragen wagten" (25.10.19, Prof. Wedhorn).

- Talk titled "Verknotete Mathematik: Why Knot?", visit from the Martin-Niemöller-Schule Wiesbaden (18.02.20, Prof. Kümmerer).

- Talk titled “Das Newton-Verfahren: Wie entsteht eigentlich schöne Mathematik?”, at the "Landes-Olympiade Mathematik" (22.02.20, Prof. Schwartz).
- Annual Graduation Event: celebration with friends and family of the graduated students (organisation: Prof. Aurzada and staff). Talk titled "Die diskrete Mathematik der Demokratie: Oder die Qual mit der Wahl" by Prof. Gritzmann, TU München (24.05.19).

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