# Biennial Report

**Department of Mathematics**
**Research Group Numerical Analysis and Scientific Computing**
2021 and 2022

TECHNISCHE UNIVERSITÄT DARMSTADT

## General Remark

This document contains a subset of the information of the Biannual Report of the Department of Mathematics at TU Darmstadt for 2021 and 2022. 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

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# 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 design of theoretical tools for the purpose of the latter, the derivation of a priori and 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 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, in modeling and simulation of compressible single- and multi-phase flows, in geophysical flow problems with dispersion, as well as non-Newtonian fluid flow.

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, approximation and (quasi-)optimality results, the design and analysis of *a posteriori* error estimates, the uncertainty quantification for problems with variable inputs, and the structure preserving model reduction and approximation 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 *Computational Engineering* and *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.

**Members of the research group**

**Professors**
Herbert Egger, Jan Giesselmann, Martin Kiehl, Jens Lang, Tabea Tscherpel

**Retired professors**
Peter Spellucci

**Postdocs**
Neelabja Chatterjee, Alf Gerisch, Christopher Müller, Kersten Schmidt, Aleksey Sikstel

**Research associates**

Aidan Chaumet, Franziska Eickmann, Oliver André Habrich, Hrishikesh Joshi, Teresa Kunkel, Fabio Leotta, Richard Franz Löscher, Nora Marie Philippi, Bogdan Radu, Moritz Schneider, Vsevolod Shashkov, Philipp Steinbach, Elisa Strauch, Erik Laurin Strelow, Gabriel Teschner, Hendrik Wilka

**Secretaries**

Elke Dehnert, Dagmar Thies

## Projects of the research group

### Project: Neural networks for approximation of nonlinear hyperbolic conservation laws

Recently, neural networks have found success in approximating solutions of PDEs, especially for high-dimensional problems. However, for nonlinear hyperbolic conservation laws, the established approach of *Physics Informed Neural Networks* (PINNs) fails. Nonlinear hyperbolic conservation laws exhibit discontinuous solutions after finite time even for smooth initial data, which leads to the failure of standard PINNs in these situations. The project develops alternative training strategies that can be understood as learning the weak formulation of the PDE instead. Solutions of the weak formulation may be non-unique. We look at entropy inequalities to learn only entropy solutions. So far we have studied problems with periodic boundary conditions. Given Dirichlet boundary data on a bounded domain, for hyperbolic conservation laws it depends on the state of the solution if the boundary data is achieved or not, such that boundary data must be understood in a suitable weak sense. We aim to extend our learning framework to incorporate boundary data weakly.

**Contact:** Aidan Chaumet, Jan Giesselmann

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[1] A. Chaumet and J. Giesselmann. Efficient wPINN-approximations to entropy solutions of hyperbolic conservation laws. arXiv:2211.12393, 2022.

### Project: Projection methods for shallow water models with dispersion

We consider the nonlinear and dispersive Green–Naghdi system of equations which models free surface flows. The dispersive pressure terms lead to a non-hyperbolic structure for which common strategies for instance to impose boundary conditions are not available anymore. This motivates the use of the Green-Naghdi system in projection structure consisting of four equations for the water height, averaged horizontal and vertical velocities and standard deviation of vertical velocity and two constraints. The projection structure allows for a splitting scheme into an advection step and a correction step after introducing a time stepping. The simplest version does not take the pressure into account in the first step. This leads to a shallow water and advection step as a first step and the second step is a correction step that incorporates the constraints by means of introducing the pressure functions. This can even be done for the case of non-homogeneous boundary conditions in an entropy stable manner

[1]. However, to obtain more flexibility on the way of prescribing boundary conditions on the pressure and to ensure that no artificial boundary conditions are imposed, the method needs refinement. For this reason we are investigating an incremental method that includes the pressure terms in the first step as source terms and updates only pressure differences in the correction step. This may also allow for insights on the significance of an inf-sup condition.

**Partner:** Martin Parisot (Inria, University of Bordeaux, France); Sebastian Noelle (RWTH Aachen)

**Contact:** Franziska Eickmann, Tabea Tscherpel

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[1] S. Noelle, M. Parisot, and T. Tscherpel. A class of boundary conditions for time-discrete Green-Naghdi equations with bathymetry. *SIAM J. Numer. Anal.*, 60(5):2681–2712, 2022.


### Project: Uncertainty quantification guided parameter selection in a fully coupled molecular dynamics-finite element model of the mechanical behavior of polymers

The objective of investigating macroscopic polymer properties with a low computing cost and a high resolution has led to the development of efficient hybrid simulation tools. Systems generated from such simulation tools can fail in service if the effect of uncertainty of model inputs on its outputs is not accounted for. This work focuses on quantifying the effect of parametric uncertainty in our coarse-grained molecular dynamics-finite element coupling approach using uncertainty quantification. We consider uniaxial deformation simulations of a polystyrene sample at $T = 100\text{K}$ in our study. Parametric uncertainty is assumed to originate from parameters in the molecular dynamics model with a nonperiodic boundary (the force constant between polymer beads and anchor points, the number of anchor points and the size of the surrounding dissipative particle dynamics domain) and a parameter to blend the energies of particles and continuum (weighting factor). Key issues that arise in uncertainty quantification are discussed on the basis of the quantities of interest including mass density, end-to-end distance and radial distribution function. This work reveals the influence of key input parameters on the properties of polymer structure and facilitates the determination of those parameters in the application of this hybrid molecular dynamics-finite element approach.

**Partner:** Yunfeng Mao (Tongji University, China); Michael C. Böhm (TU Darmstadt); Florian Müller-Plathe (TU Darmstadt)

**Contact:** Jens Lang, Alf Gerisch

#### References


[1] Y. Mao, A. Gerisch, J. Lang, M. C. Böhm, and F. Müller-Plathe. Uncertainty quantification guided parameter selection in a fully coupled molecular dynamics-finite element model of the mechanical behavior of polymers. *J. Chem. Theory Comput.*, 17(6):3760–3771, 2021.


### Project: Mathematical modeling 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, mechanical interactions in tissue development

and the cascade of steps in fracture healing can be modeled as time-dependent PDEs. We consider models that include cross-diffusion processes, study the effect of multiple adhesion terms of different forms and consider mechanochemical models of pattern formation.
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. Mechanochemical models lead to implicit PDEs which require a dedicated numerical treatment. In our approaches, 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 (Politecnico di Torino, Italy); Chiara Villa (Sorbonne University, Paris, France); Mariya Ptashnyk (Heriot-Watt University, Edinburgh, UK); Anja Voß-Böhme (HTW Dresden); Jonathan Sherratt (Heriot-Watt University, Edinburgh, UK)

**Contact:** Alf Gerisch

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[2] C. Villa, A. Gerisch, and M. A. Chaplain. A novel nonlocal partial differential equation model of endothelial progenitor cell cluster form ation during the early stages of vasculogenesis. *J Theor Biol*, 534:110963, 2022.

[3] A. Voss-Böhme and A. Gerisch. Multi-scale analysis of contact-dependent interaction in tissue aggregation and invasion. In O. Wolkenhauer, editor, *Systems Medicine: Integrative, Qualitative and Computational Approaches*, pages 156–168. Academic Press, Oxford, 2021.

**Project: Regularized moment methods for kinetic equations**

Moment equations employing entropy closures are an established method for solving kinetic equations since they lead to equations that share many properties with compressible fluid mechanics equations and possess a natural entropy structure. However, solving these equations numerically is rather delicate since the entropy closure makes it necessary to solve constrained minimization problems for each flux evaluation and numerical errors might make these problems unfeasible. This difficulty can be overcome using regularized minimization problems, as introduced in [2]. We have proven convergence in relative entropy 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

**Contact:** Jan Giesselmann

### References


[1] G. W. Alldredge, M. Frank, and J. Giesselmann. On the convergence of the regularized entropy-based moment method for kinetic equations. *SMAI-JCM*, 9:1–29, 2023.

[2] 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: A posteriori error estimates for Keller-Segel models with linear and non-linear diffusion**

Keller Segel models are a family of models describing the movement of bacteria attracted by a chemical substance that they also create. Many of these models lead to finite time blow-up (mass concentration) for certain initial data which makes the construction and error analysis of numerical schemes challenging. We focus on the derivation of conditional a posteriori error estimates for finite volume and discontinuous Galerkin schemes that provide computable upper bounds for the difference between exact and numerical solutions. The estimates are conditional in the sense that some numerical quantity can be evaluated and if it is below a certain threshold the error bound is valid.

**Partner:** Kiwoong Kwon (Kyungpook National University, Republic of Korea); Niklas Kolbe (RWTH Aachen)

**Contact:** Jan Giesselmann

**Project: A posteriori error estimates for hyperbolic conservation laws based on a-contraction**

The goal of this project is to derive novel a posteriori error estimates for systems of hyperbolic conservation laws in one space dimension. The goal is to obtain error estimators that are of the same order as the error if the solution is smooth and that converge even when the exact solution is discontinuous thereby vastly improving upon the state of the art. In a first step we focus on scalar model problems with convex flux but restrict ourselves to techniques that shall be extensible to systems. We decompose the computational domain into parts where the initial data are increasing and parts where they are decreasing. In the increasing parts we use classical finite volume schemes and reconstructions as in [1] while we use wave-front tracking in the decreasing parts. The a-contraction methodology [2] will allow us to relate residuals and errors in an optimal way.

**Partner:** Sam Krupa (MPI Leipzig)

**Contact:** Jan Giesselmann

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[1] A. Dedner and J. Giesselmann. A posteriori analysis of fully discrete method of lines discontinuous Galerkin schemes for systems of conservation laws. *SIAM J. Numer. Anal.*, 54(6):3523–3549, 2016.

[2] S. G. Krupa. Criteria for the $a$-contraction and stability for the piecewise-smooth solutions to hyperbolic balance laws. *Commun. Math. Sci.*, 18(6):1493–1537, 2020.


**Project: A posteriori error control for statistical solutions of barotropic Navier-Stokes equations**

This project addresses the numerical approximation of statistical solutions of the barotropic Navier-Stokes equations, one of the fundamental equations in fluid mechanics. Statistical solutions are a novel solution concept for compressible Navier-Stokes equations that is motivated by turbulence modeling and is thought to address issues with well-posedness that persist for deterministic solution concepts. Statistical solutions can be understood as time-parametrized probability measures on function spaces induced by a random initial datum. Hence, a statistical solution can be approximated by an empirical measure obtained from samples from the initial distribution that are evolved with a numerical scheme for the deterministic, barotropic Navier-Stokes equations. In the convection-dominated case that we focus on, a typical numerical scheme would be of Runge-Kutta discontinuous Galerkin type. We aim to provide reliable, efficient, and robust a posteriori error estimators for these schemes, i.e., upper error bounds for errors caused by discretization in space-time and stochastic space that are computable from the numerical solution. We will combine the relative entropy stability framework with suitable reconstructions of the numerical solution to establish these error bounds. Furthermore, we plan to employ our a posteriori error estimator to construct adaptive, highly efficient multi-level Monte Carlo schemes for approximating quantities of interest pertinent to statistical solutions.

**Partner:** Sebastian Krumscheid (KIT)

**Contact:** Jan Giesselmann

**Project: Dissipative solutions for the Navier-Stokes-Korteweg system and their numerical treatment**

Many problems in computational fluid dynamics are described by the compressible Euler or Navier-Stokes (NS) equations. Recently, dissipative weak (DW) solutions have been introduced as a generalization to classical solution concepts. In a series of works, DW solutions have been established as a meaningful concept from the analytical and numerical points of view. DW solutions do not have to fulfill the equations weakly but only up to some defect and oscillations measures. They can be identified as limits of consistent and stable approximations and convergence towards DW solutions has been demonstrated for several structure-preserving numerical methods. Further, they are a natural extension of classical solutions since DW solutions coincide with them if either the classical solution exists, referred to as weak-strong uniqueness principle, or if DW solutions enjoy certain smoothness. A further extension to the Navier-Stokes system is the Navier-Stokes-Korteweg (NSK) system which includes capillarity terms in the equations. Our motivation for considering NSK in our project is driven by the recent observations made by Slemrod that the rigorous passage of solutions from the mesoscopic equations (Boltzmann) to macroscopic systems, known as Hilbert sixth's problem, will fail for the classical systems (NS and Euler) because of the appearance of van der Waals–Korteweg capillarity terms in a macroscopic description. Therefore, Korteweg systems are more suitable for describing real fluid motions. In our project, we will extend the framework of DW solutions to NSK equations. We will define DW solutions in such a way that they form a natural extension of classical solutions, i.e. such that they satisfy a weak-strong uniqueness principle, for the local and non-local NSK model. In addition, we plan to prove their global existence by demonstrating convergence of structure-preserving numerical schemes. First, structure-preserving low order schemes will be constructed and analyzed, whereas later we focus as well on the development and convergence properties of higher order finite element schemes.

**Partner:** Philipp Öffner (Universität Mainz)

**Contact:** Jan Giesselmann

**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 Polymerforschung Mainz)

**Support:** DFG TRR 146

**Contact:** Herbert Egger

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[1] A. Brunk, B. Dünweg, H. Egger, O. Habrich, M. Lukacova-Medvidova, and D. Spiller. Analysis of a viscoelastic phase separation model. *J. Phys.: Condens. Matter*, 33:234002, 2021.

[2] H. Egger, O. Habrich, and V. Shashkov. Energy stable Galerkin approximation of Hamiltonian and gradient systems. *Comput. Meth. Appl. Math.*, 21:335–349, 2021.

[3] D. Spiller, A. Brunk, O. Habrich, H. Egger, M. Lukacova-Medvidova, and B. Duenweg. Systematic derivation of hydrodynamic equations for viscoelastic phase separation. *J. Phys.: Condens. Matter*, 33:364001, 2021.


**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 simulations 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: Observer-based data assimilation for barotropic gas transport using distributed measurements**

The goal of data assimilation is to estimate the state of some physical system by combining available measurement data with a physical model of the system. In our case, we consider the flow of gas through gas pipe networks described by the one-dimensional barotropic Euler equations complemented with energy-conserving coupling conditions at the pipe junctions. Then, we set up an observer system that contains additional source terms of Luenberger type depending on distributed measurements of one of the state variables. Using an extension of the relative energy method we show that the state of the observer system converges exponentially in the long time limit towards the original system state, i.e., we reconstruct the complete system state from measurements of only one state variable.

**Partner:** Martin Gugat (Universität Erlangen-Nürnberg)

**Support:** DFG TRR 154

**Contact:** Jan Giesselmann, Teresa Kunkel

**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/low Mach 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/low Mach 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:** 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.

[2] H. Egger, J. Giesselmann, T. Kunkel, and N. Philippi. An asymptotic-preserving discretization scheme for gas transport in pipe networks. *IMA Journal of Numerical Analysis*, 2022.

#### Project: Implicit Peer triplets for ODE constrained optimal control problems

It is well known that in the first-discretize-then-optimize approach in the control of ordinary differential equations the discrete 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 different formulations and 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 published in J. Comput. Appl. Math., 262:73–86, 2014, and discuss the construction of 3-stage methods for the order pair (3,2) in detail. The impact of nodes having equal differences is highlighted. It turns out that the most attractive methods are related to backward differentiation formulas. Three 3-stage methods are constructed, which show the expected orders in numerical tests.

Further, we are concerned with the construction and convergence analysis of novel implicit Peer triplets of two-step nature with four stages for nonlinear ODE constrained optimal control problems. We combine the property of super-convergence of some standard Peer method for inner grid points with carefully designed starting and end methods to achieve order four for the state variables and order three for the adjoint variables in a first-discretize-then-optimize approach together with A-stability. The notion triplets emphasize that these three different Peer methods have to satisfy additional matching conditions. Four such Peer triplets of practical interest are constructed. In addition, as a benchmark method, the well-known backward differentiation formula BDF4, which is only $A(73.35^o)$-stable, is extended to a special Peer triplet to supply an adjoint consistent method of higher order and BDF type with equidistant nodes. Within the class of Peer triplets, we found a diagonally implicit $A(84^o)$-stable method with nodes symmetric in $[0,1]$ to a common center that performs equally well. Numerical tests with four well established optimal control problems confirm the theoretical findings also concerning A-stability.

**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. *J. Comput. Appl. Math.*, 416:114596, 2022.

[2] J. Lang and B. A. Schmitt. Implicit A-stable peer triplets for ODE constrained optimal control problems. *Algorithms*, 15:310, 2022.

#### Project: Gas transport in large-scale 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 semi-convex 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.
We also investigate quantification of uncertainties that arise from intra-day oscillations in the demand for natural gas transported through large-scale networks. The short-term transient dynamics of the gas flow is modelled by a hierarchy of hyperbolic systems of balance laws based on the isentropic Euler equations. We extend a novel adaptive strategy for solving elliptic PDEs with random data, recently proposed and analysed by Lang, Scheichl, and Silvester [J. Comput. Phys., 419:109692, 2020], to uncertain gas transport problems. Sample-dependent adaptive meshes and a model refinement in the physical space is combined with adaptive anisotropic sparse Smolyak grids in the stochastic space. A single-level approach which balances the discretization errors of the physical and stochastic approximations and a multilevel approach which additionally minimizes the computational costs are considered. Two examples taken from a public gas library demonstrate the reliability of the error control of expectations calculated from random quantities of interest, and the further use of stochastic interpolants to, e.g., approximate probability density functions of minimum and maximum pressure values at the exits of the network.
In a further step, we considered both a stationary and a dynamic flow model with uncertain boundary data on networks. We introduce two different ways how to compute the probability for random boundary data to be feasible, discussing their advantages and disadvantages. In this context, feasible means that the flow corresponding to the random boundary data meets some box constraints at the network junctions. The first method is the spheric radial decomposition and the second method is a kernel density estimation. In both settings, we consider certain optimization problems and we compute derivatives of the probabilistic constraint using the kernel density estimator. Moreover, we derive necessary optimality conditions for an approximated problem for the stationary and the dynamic case. Throughout the study, we use numerical examples to illustrate our results by comparing them with a classical Monte Carlo approach to compute the desired probability.

**Partner:** Pia Domschke (Frankfurt School of Finance & Management); Martin Gugat, Michael Schuster (Universität Erlangen-Nürnberg)

**Contact:** Jens Lang, Elisa Strauch

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[2] J. Lang, P. Domschke, and E. Strauch. Adaptive single- and multilevel stochastic collocation methods for uncertain gas transport in large-scale networks. In *Mesh generation and adaptation—cutting-edge techniques*, volume 30 of *SEMA SIMAI Springer Ser.*, pages 113–135. Springer, Cham, 2022.

[3] M. Schuster, E. Strauch, M. Gugat, and J. Lang. Probabilistic constrained optimization on flow networks. *Optim. Eng.*, 23(2):983–1032, 2022.

**Project: Quantification of bore path uncertainty in borehole heat exchanger arrays**

Borehole heat exchanger arrays have become a common implement for the utilization of thermal energy in the soil. Building these facilities is expensive, especially the drilling of boreholes, into which closed-pipe heat exchangers are inserted. Therefore, cost-reducing drilling methods are common practice, which can produce inaccuracies of varying degree. This brings into question how much these inaccuracies could potentially affect the performance of a planned system. In the presented case study, an uncertainty quantification for seasonally operated borehole heat exchanger arrays is performed to analyze the impact of the bore paths' deviations. We introduce an adaptive, anisotropic stochastic collocation method, known as the generalized Smolyak algorithm, which was previously unused in this context and apply it to a numerical model of the borehole heat exchanger array. Our results show that the borehole heat exchanger array performance is surprisingly reliable even with potentially severe implementation errors during their construction. This, coupled with the potential uses of the presented method in similar applications gives planners and investors valuable information regarding the viability of borehole heat exchanger arrays in the face of uncertainty. With this project, we hope to provide a powerful statistical tool to the field of geothermal energy, in which uncertainty quantification methods are still rarely used at this point. The discussed case study represents a jumping-off point for further investigations on the effects of uncertainty on borehole heat exchanger arrays and borehole thermal energy storage systems.

**Partner:** Ingo Sass (Deutsches Geoforschungszentrum Potsdam)

**Contact:** Jens Lang

### References

[1] P. Steinbach, D. O. Schulte, B. Welsch, I. Sass, and J. Lang. Quantification of bore path uncertainty in borehole heat exchanger arrays using adaptive anisotropic stochastic collocation. *Geothermics*, 97(4):102194, 2021.

**Project: A-priori error estimates to smooth solutions of Runge-Kutta discontinuous Galerkin (RKDG) methods for scalar fractional conservation laws**

Fractional conservation laws (FCLs) are generalizations of convection-diffusion equations where the local diffusion may depend on the global dynamics. They appear in many different contexts such as overdriven gas detonation, mathematical finance and flow in porous media. It is well known that solutions to FCLs may develop shocks in finite time if the diffusion fails to counterbalance the convection and thus an entropy formulation is needed to guarantee well-posedness. Accordingly, in the context of numerical methods, low convergence rates have to be expected and are indeed already available in the literature. Contrary to these worst-case estimates, one may be interested in achievable convergence rates when dealing with sufficiently smooth solutions to obtain a more differentiated picture of the numerical performance. This line of reasoning has been customary in the setting of pure conservation laws which often times share similar properties with FCLs. In fact, for conservation laws, optimal error estimates to smooth solutions of higher order RKDG methods are well known. We aim to establish comparable results for a certain class of FCLs in this project.

**Contact:** Jan Giesselmann, Fabio Leotta

**Project: Reduced order models for convection-diffusion-reaction equations with deterministic and 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: Initially, we compute a fixed number of snapshots of the solution on a predefined set of points in the deterministic parameter domain using adaptively constructed stochastic Galerkin finite element subspaces. Then, we 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 setup phase of the reduced order model but also introduces additional error terms. We derive an upper bound for the error of the reduced solution which contains all error sources involved. For every error source, we derive computable upper bounds which are used to steer the construction of the reduced order model.

**Contact:** Christopher Müller, Jens Lang

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**Project: Analysis and numerical approximation of singularly perturbed transport equations on networks**

Transport processes on network structures, described by one-dimensional metric graphs, arise in the modelling of various physical phenomena, e.g., the transport of gas mixtures in gas networks, the contaminant transport in water supply networks or networks of 1D cracks, as well as the heat transport in district heating networks. Related problems also appear in the context of traffic flow. In this project, we are particularly interested in singularly perturbed convection-diffusion processes and their limiting behavior to pure transport. For vanishing diffusion, boundary layers arise at network junctions due to a change in the coupling in the transport limit. Moreover, we investigate the systematic numerical treatment of such problems. A hybrid discontinuous Galerkin method and an adaptive strategy turns out to guarantee stability and uniform error estimates in the asymptotic regime.

**Support:** DFG TRR 154

**Contact:** Herbert Egger, Nora Philippi

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[2] H. Egger and N. Philippi. On the transport limit of singularly perturbed convection-diffusion problems on networks. *Math. Methods Appl. Sci.*, 44(6):5005–5020, 2021.

[3] H. Egger and N. Philippi. An asymptotic preserving hybrid-dG method for convection-diffusion equations on pipe networks. arXiv:2209.04238, 2022.

### Project: Kinetic models for chemotaxis and diffusion limits

The movement of bacteria in presence of a chemical substance is called chemotaxis and can be described by kinetic models. The bacteria react to the chemoattractant and approach more favorable environments. In general, the movement is composed into two phases, a "run" phase of directed moving in straight lines and a "tumble phase" of reorientation influenced by the chemoattractant, which itself depends on the bacteria density. In this project, we consider chemotaxis on networks described by one-dimensional metric graphs. Within edges bacteria can only move in two directions, whereas at network junctions, they can enter each incident edge. In the macroscopic limit, chemotaxis is described by the Keller-Segel model. We are now particularly interested in the existence of solutions, and the convergence of the kinetic model to the limit problem.

**Partner:** Kathrin Hellmuth (Universität Würzburg); Matthias Schlottbom (University of Twente, The Netherlands)

**Contact:** Herbert Egger, Nora Philippi

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[1] R. Borsche, J. Kall, A. Klar, and T. N. H. Pham. Kinetic and related macroscopic models for chemotaxis on networks. *Math. Models Methods Appl. Sci.*, 26(6):1219–1242, 2016.

[2] H. Egger and M. Schlottbom. Diffusion asymptotics for linear transport with low regularity. *Asymptot. Anal.*, 89(3-4):365–377, 2014.

[3] H. Egger and L. Schöbel-Kröhn. Chemotaxis on networks: analysis and numerical approximation. *ESAIM Math. Model. Numer. Anal.*, 54(4):1339–1372, 2020.

### 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), Monique Dauge (University of Rennes 1), Ralf Hiptmair (ETH Zürich)

**Contact:** Kersten Schmidt

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[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 (BAM), Anita Schulz (HTW Berlin)

**Contact:** Kersten Schmidt

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[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] K. Schmidt and A. Thöns-Zueva. Impedance boundary conditions for acoustic time harmonic wave propagation in viscous gases in two dimensions. *Math. Meth. Appl. Sci.*, 45(12):7404–7425, 2022.

[4] 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: Magnetic oriented approach for modelling and simulation of electric circuits**

The modified nodal analysis (MNA) is probably the most widely used formulation for the modeling and simulation of electric circuits. Its conventional form uses electric node potentials and currents across inductors and voltage sources as unknowns, thus taking an electrical viewpoint. In this project, we develop and analyze an alternative magnetic oriented nodal analysis (MONA) approach, which is based on flux linkage potentials and charge differences across capacitors and voltage sources. Despite the different modeling perspective, the approach is applicable to the same general class of circuits and leads to regular systems of differential algebraic equations under the same topological assumptions as required for the MNA. Moreover, while the MNA leads to systems of index $\leq 2$, the index of the MONA systems is $\leq 1$, which facilitates the numerical treatment.

**Partner:** Idoia Cortes Garcia (Eindhoven University of Technology, The Netherlands)

**Support:** DFG TRR 361, DFG SPP 2256, SFB F90-N, DFG GSC 233

**Contact:** Herbert Egger, Vsevolod Shashkov

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[1] V. Shashkov, I. Cortes Garcia, and H. Egger. MONA-A magnetic oriented nodal analysis for electric circuits. *International Journal of Circuit Theory and Applications*, 50(9):2997–3012, 2022.


**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:** Bai-Xiang Xu (TU Darmstadt)

**Support:** DFG GSC 233, DFG SPP 2256

**Contact:** Herbert Egger, Vsevolod Shashkov

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

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

[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.

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### 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:** DFG GSC 233, DFG TRR 146

**Partner:** Jürgen Dölz (Universität Bonn)

**Contact:** Herbert Egger, Vsevolod Shashkov

### References


[1] J. Dölz, H. Egger, and V. Shashkov. A convolution quadrature method for Maxwell's equations in dispersive media.

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

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

**Project: Physics informed neural networks for gas transport problems**

Physics informed neural networks emerged from the machine learning community and offer a new way to approximate solutions of partial differential equations. Since then, numerous extensions have been proposed and applications have been studied. In this project we want to explore potential applications and examine their benefit to solve gas transport problems. These problems include simulation tasks ranging from pipes to pipeline systems as well as optimization tasks that seek energy efficient controls of elements in the pipeline system. Due to the transport nature of the underlying balance laws, these tasks have unique challenges that we want to solve with the physics informed approach.

For example, to avoid similar simulations with slightly varied controls, reduced order methods are used to speed up the optimization process. However, the commonly used reduced basis methods are not well suited to build a reduced model for gas transport. Here, we build reduced models based on physics informed neural networks. We also apply a second strategy to solve the optimization problem by solving adjoint-based optimality conditions at the same time as the simulation conditions. Both approaches can been seen as extensions to the originally described physics informed neural networks and are made possible by the great flexibility of this method.

Physics informed neural networks are not yet universally applicable in all gas transport scenarios. Special challenges arise when simulating the gas flow in real world scenarios, i.e. long pipes and a realistic speed of sound. Here, we try to understand the noticed obstacles and look into possible solutions.

Finally, we are interested in mathematical analysis of the aforementioned methods.

**Partner:** Marc Pfetsch (TU Darmstadt)

**Support:** Graduate School Computational Engineering, TU Darmstadt

**Contact:** Alf Gerisch, Jens Lang, Erik Laurin Strelow

**Project: Local interpolation and projection operators for conforming finite element spaces**

We introduce and investigate projection operators mapping to Lagrange elements for arbitrary polynomial order. More specifically, a Scott–Zhang type interpolation operator is constructed that — additionally to the usual properties — is compatible with dual spaces of Sobolev spaces, in the sense that it is stable in the corresponding negative norms. This allows for optimal rates of convergence in situations of low regularity of weak solutions. For comparison we discuss operators with similar properties such as locality, stability and the projection property. Such operators are useful tools to prove interpolation error estimates for parabolic problems and smoothen rough right-hand sides in a least squares finite element method. For first order spaces those results are contained in [1] and extensions are under investigation.

**Partner:** Lars Diening, Johannes Storn (Universität Bielefeld)

**Contact:** Tabea Tscherpel

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[1] L. Diening, J. Storn, and T. Tscherpel. Interpolation operator on negative Sobolev spaces. arXiv:2112.08515, 2021.

### Project: $L^2$-projection mapping to conforming finite element spaces and grading of adaptively refined meshes

In this project we investigate the $L^2$-projection mapping to conforming finite element spaces on a family of adaptively refined triangulations. While stability results in Sobolev spaces are available for quasi-uniform triangulations, this is not true in general for adaptively refined meshes. Indeed, certain decay properties are strongly linked to the grading of the underlying family of meshes. However, Sobolev stability of the $L^2$-projection is essential for the numerical analysis of parabolic problems. Even in the simple case of the heat equation it is known to be equivalent to quasioptimality for the semi-discrete approximation (Tantardini, Veeser, 2016, SIAM J. Numer. Anal.). In [1] we have extended existing results on the $L^p$- and $W^{1,p}$-stability of the projection mapping to Lagrange finite element spaces under realistic assumptions on the mesh grading. In particular this allows for stability results for arbitrary polynomial degrees. For several 2D adaptive refinement schemes the mesh grading has been examined in the literature. For the 3D case the mesh refinements are much more challenging to investigate and to date there are no grading results available. This is subject of ongoing research.

**Partner:** Lars Diening, Johannes Storn (Universität Bielefeld)

**Contact:** Tabea Tscherpel

#### References

[1] L. Diening, J. Storn, and T. Tscherpel. On the Sobolev and $L^p$-stability of the $L^2$-projection. *SIAM J. Numer. Anal.*, 59(5):2571–2607, 2021.

### Project: Dimensions of divergence-free finite element spaces

Mixed finite element spaces can be used to approximate incompressible fluid equations such as the Stokes equations. In this setup to ensure stability a discrete inf-sup condition on the velocity and the pressure space is needed. For optimal error estimates on the velocity, mixed finite element spaces for which the discretely divergence-free velocity functions are also exactly divergence-free are well-suitable.

For piecewise polynomial functions on general triangulations as velocity space (Scott–Vogelius element) and the pressure space chosen as the divergence thereof, the inf-sup condition is available only for sufficiently high polynomial degree; in 3D up to now it is only on special triangulations. These assumptions can be relaxed by considering lower polynomial degree on certain split meshes. A comparison of the computational cost has to take both the local number of degrees of freedom and the effect of the split into account. Employing counting arguments in 3D we compare the Scott–Vogelius element with several split methods in terms of computational cost. This also yields insights into discrete de Rham complexes.

**Partner:** L. Ridgway Scott (University of Chicago, United States; Emeritus)

**Contact:** Tabea Tscherpel

#### References

[1] L. R. Scott and T. Tscherpel. Dimensions of exactly divergence-free finite element spaces in 3D. arXiv:2301.00185, 2023.

**Project: Numerical analysis of fluid equations with non-standard boundary conditions**

For non-Newtonian fluids complex boundary behaviour such as stick-slip or even dynamic boundary conditions are highly relevant to describe the fluid motion correctly. In the context of finite element approximations imposing non-homogeneous boundary conditions in a strong manner can lead to solutions of the homogeneous problem; this phenomenon is known as Babuska paradox. To avoid this one may impose boundary conditions weakly, e.g. by the so-called Nietsche method. The object of this project is to show convergence and error estimates for non-standard boundary conditions in fluid equations, starting with the steady case on polygonal domains and later extending this to the unsteady case. This involves the analysis of certain discrete operators that may prove useful in more general situations.

**Partner:** Alexei Gazca Orozco (Universität Freiburg); Erika Maringova (Institute of Science and Technology Austria)

**Contact:** Tabea Tscherpel

**Project: Well-balanced approximation of the Green–Naghdi equations**

The Green–Naghdi equations are a reduced model between the full free surface incompressible Euler equations and the shallow water equations. As such they are not hyperbolic but include extra terms responsible for dispersion. Numerical schemes that preserve stationary solutions are referred to as well-balanced. Already for the shallow water equations in the presence of a non-flat bottom such schemes have been developed and require a careful treatment of the bottom function. For the Green-Naghdi equations the situation is even more delicate, because there are more stationary solutions and more terms to be taken into account. We aim for an improved understanding of the stationary solutions of the Green–Naghdi equations and a well-balanced approximation.

**Partner:** Emmanuel Audusse (University Paris 13, France); Martin Parisot (Inria, University of Bordeaux, France)

**Contact:** Tabea Tscherpel

**Project: Adaptive stochastic collocation for problems with non-smooth dependencies in the random space**

In many applications we assume some uncertainties in the corresponding models, which we typically approximate with finite dimensional random spaces. It is common to investigate functionals, which map from these spaces to quantities of interest (QoI). Stochastic collocation methods allow us to gather information on stochastic quantities of these functionals, e.g. expected values. In this project we consider problems where these functionals have non-smooth regions. As a first step we investigate algorithms on sparse grids which allow us to identify regions where discontinuities in the first derivative occur. Additionally we work on sparse grid approximations, which operate differently based on the identified smoothness. We want to achieve that our method uses efficient high order approximations in smooth areas. As an application we consider gas networks: Using our method we want to calculate probabilities, in which the network operates below certain thresholds.

**Contact:** Jens Lang, Hendrik Wilka

**Support:** DFG TRR 154

# 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 also 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 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 is now in its third funding period.

The energy transition ("Energiewende") in Germany and its success are currently – more than ever – 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. Originally, natural gas was planned to bridge the transition in the next decades, since it was readily accessible, tradable, and storable. However, the pressure to accelerate the transition is increasing. Moreover, hydrogen as an alternative energy carrier is gaining importance and can be transported through pipelines. Although its physical behavior can be treated using similar mathematical equations as for natural gas, there are several issues that require attention, especially if hydrogen is mixed with natural gas.
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 Professors Disser, 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.

Seven professors of the Department of Mathematics are Principal Investigators within the Graduate School Computational Engineering (Aurzada, Bothe, Disser, Giesselmann, Lang, Pfetsch, Ulbrich) 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. Dr.-Ing. Marschall is Research Group Leader with scientific focus on Two-Phase and Interfacial Flows. Together they supervise more than 11 interdisciplinary PhD projects within the Graduate School in close cooperation with a co-supervisor from Engineering or Computer Science. Former members of the Graduate School who contributed during 2021-2022 are Profs. Egger, Schwartz and Wollner.

## 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.

# 3 Scientific and Industrial Cooperations

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

**Herbert Egger**

- Prof. Dr. Matthias Schlottbom (University of Twente, The Netherlands), Prof. Dr. Jürgen Dölz (Universität Bonn): Model reduction for inverse problems.
- Dr. Aaron Brunk, Prof. Dr. Maria Lukacova (Universität Mainz): Spinodal decomposition of polymer solvent systems.
- Dr. Mania Sabouri (Universität Kassel): High-order methods for poroelasticity.
- Prof. Dr. Jürgen Dölz (Universität Bonn): Convolution quadrature methods.
- Ass.-Prof. Dr. Idoia Cortes Garcia (TU Eindhoven, The Netherlands): Simulation of electric circuits.
- Melina Merkel (TU Darmstadt), Prof. Dr. Sebastian Schöps (TU Darmstadt): Electric machine simulation.
- Prof. Dr. Bai-Xian Xu (TU Darmstadt): Analysis and simulation of additive manufacturing processes.
- Prof. C. Tropea (TU Darmstadt), Prof. J. Hennig, Dr. A. Krafft (UK Freiburg): MRI-based Wall Shear Stress Quantification.

**Alf Gerisch**

- Prof. Dr. Mark A. J. Chaplain (University of St. Andrews, UK), Prof. Dr. Kevin J. Painter (Polytechnic University of Turin, Italy), Dr. Chiara Villa (Sorbonne University, Paris, France), Dr. Mariya Ptashnyk (Heriot-Watt University, Edinburgh, UK), Prof. Dr. Anja Voß-Böhme (HTW Dresden): Mechano-biological and non-local models of tissue development.
- 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.
- Prof. Dr. Ram Jiwari (IIT Roorkee, India): Radial basis function differential quadrature methods for time-dependent PDEs.

**Jan Giesselmann**

- SFB Transregio 154: Mathematische Modellierung, Simulation und Optimierung am Beispiel von Gasnetzwerken, Speaker: Prof. Dr. Alexander Martin (Universität Erlangen-Nürnberg).
- Prof. Dr. Martin Gugat (Universität Erlangen-Nürnberg): Boundary observers for hyperbolic balance laws.
- Prof. Dr. Christiane Helzel (Universität Düsseldorf): A posteriori error estimator for kinetic equations describing rod like particles.

- Prof. Dr. Sebastian Krumscheid (KIT, Karlsruhe): A posteriori error control for statistical solutions of barotropic Navier-Stokes equations.
- Dr. Sam G. Krupa (MPI Leipzig): A posteriori error estimates for discontinuous solutions to hyperbolic conservation laws.
- Prof. Dr. Sandra May (University Uppsala, Finland): A priori error estimates for finite volume schemes on cut-cell meshes.
- Prof. Dr. Min-Gi Lee (Kyungpook National University, Korea), Kiwoong Kwon (Kyungpook National University, Korea), Dr. Niklas Kolbe (RWTH Aachen): A posteriori error estimates for Keller-Segel models with linear and non-linear diffusion.
- Group of Prof. Dr. Maria Lukacova (Universität Mainz): Robust a posteriori error estimates for Allen-Cahn equations with non-constant mobility.
- Dr. Philipp Öffner (Universität Mainz): Dissipative solutions for the Navier-Stokes-Korteweg system and their numerical treatment.
- Dr. Aleksey Sikstel (Universität Köln): A posteriori error estimates for discontinuous solutions to hyperbolic conservation laws.

**Jens Lang**

- Dr. Pia Domschke (Frankfurt School of Finance & Management): Gas transport in networks.
- Prof. Dr. Martin Gugat (Universität Erlangen-Nürnberg): Probabilistic constrained optimization on flow networks.
- Prof. Dr. Ingo Sass (Deutsches Geoforschungszentrum Potsdam): Borehole heat exchanger.
- Prof. Dr. Bernhard A. Schmitt (Universität Marburg): Discrete adjoint implicit Peer methods.
- Prof. Dr. Rüdiger Weiner (Universität Halle-Wittenberg): IMEX-Peer methods.
- Prof. Dr. Weizhang Huang (University of Kansas, USA), Lennard Kamenski (WIAS Berlin): Anisotropic mesh methods.

**Tabea Tscherpel**

- Prof. Dr. Lars Diening, Dr. Johannes Storn (Universität Bielefeld): Grading of adaptively generated triangulations and projection operators onto conforming finite element spaces.
- Prof. Dr. L. Ridgway Scott (University of Chicago, Emeritus, USA): Divergence-free finite element spaces.
- Dr. Alexei Gazca Orozco (Universität Freiburg), Dr. Erika Maringova (Institute of Science and Technology Austria): Numerical analysis for fluid models with complex boundary conditions.

- Dr. Martin Parisot (Inria, University of Bordeaux, France), Prof. Dr. Emmanuel Audusse (University Paris 13, France), Prof. Dr. Sebastian Noelle (RWTH Aachen): Numerical approximation of the Green–Naghdi equations.

# 4 Publications

## 4.1 Co-Editors of Publications

### 4.1.1 Editors of Journals

**Alf Gerisch**

– *PLOS ONE* (Academic Editor)

**Jan Giesselmann**

– *Applied Numerical Mathematics* (Editor)

**Jens Lang**

– *Applied Numerical Mathematics* (Editor)

## 4.2 Publications in Journals and Proceedings

### 4.2.1 Journals


[1] M. Arnold, H. Podhaisky, R. Weiner, E. Celledoni, J. Frank, and J. Lang. Numerical solution of differential and differential-algebraic equations. Selected papers from NUMDIFF-15 [Preface]. *J. Comput. Appl. Math.*, 387:112611, 2021.

[2] A. Brunk, B. Dünweg, H. Egger, O. Habrich, M. Lukacova-Medvidova, and D. Spiller. Analysis of a viscoelastic phase separation model. *J. Phys.: Condens. Matter*, 33:234002, 2021.

[3] A. Dedner, J. Giesselmann, T. Pryer, and J. K. Ryan. On the convergence of the regularized entropy-based moment method for kinetic equations. *J. Sci. Comput.*, 88, no. 2:Paper No. 34, 28, 2021.

[4] L. Diening, J. Storn, and T. Tscherpel. Interpolation operator on negative Sobolev spaces. accepted at Math. Comp., 30.12.22.

[5] J. Dölz, H. Egger, and M. Schlottbom. A model reduction approach for inverse problems with operator valued data. *Numer. Math.*, 148:889–917, 2021.

[6] J. Dölz, H. Egger, and V. Shashkov. A fast and oblivious matrix compression algorithm for Volterra integral operators. *Advances in Computational Mathematics*, 47(6):81, 2021.

[7] P. Domschke, O. Kolb, and J. Lang. Fast and reliable transient simulation and continuous optimization of large-scale gas networks. *Math. Methods Oper. Res.*, 95(3):475–501, 2022.

[8] H. Egger, J. Giesselmann, T. Kunkel, and N. Philippi. An asymptotic-preserving discretization scheme for gas transport in pipe networks. *IMA J. Numer. Anal.*, 2022.

[9] H. Egger, O. Habrich, and V. Shashkov. Energy stable Galerkin approximation of Hamiltonian and gradient systems. *Comput. Meth. Appl. Math.*, 21:335–349, 2021.

[10] H. Egger and N. Philippi. On the transport limit of singularly perturbed convection-diffusion problems on networks. *Math. Methods Appl. Sci.*, 44(6):5005–5020, 2021.

[11] H. Egger and B. Radu. A second order finite element method with mass lumping for Maxwell's equations on tetrahedra. *SIAM J. Numer. Anal.*, 59:864–885, 2021.

[12] H. Egger and M. Sabouri. On the structure preserving high-order approximation of quasistatic poroelasticity. *Math. Comp. Sim.*, 189:237–252, 2021.

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## 4.3 Preprints

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## 4.4 Reviewing and Refereeing

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

**Alf Gerisch:** Journal of Biomechanics, Journal of Computational and Applied Mathematics, IMA Journal of Applied Mathematics, Journal of Theoretical Biology, Mathematical Biosciences and Engineering, The Fund for Scientific Research (FNRS, Belgium)

**Jan Giesselmann:** Zentralblatt; Mathematics of Computation, Journal of Scientific Computing, Differential Integral Equations, Discrete Continuous Dynamical Systems-S, Mathematical Methods in the Applied Sciences, Applied Numerical Mathematics, SIAM/ASA Journal on Uncertainty Quantification, Journal of Applied Mathematics and Computing, SIAM Journal on Mathematical Analysis, SIAM Journal on Control and Optimization, IMA Journal of Numerical Analysis, Nonlinear Analysis Real World Applications, Communications in Optimization Theory, Science Advances, ZAMP

**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, BIT

**Kersten Schmidt:** European Journal of Applied Mathematics, Journal of Computational and Applied Mathematics, SIAM Journal for Applied Mathematics

**Tabea Tscherpel:** IMA Journal of Numerical Analysis, Numerische Mathematik

## 4.5 Software

**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, and formerly Sebastian Ullmann (now at Dassault Systèmes) and Bettina Schieche (now at Münchener Hyp)

**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, optimisation and phase-field simulation.

Contributor at TU Darmstadt: Jens Lang, Alf Gerisch

**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 hexahedredal meshes with locally varying and anisotropic polynomial orders for Poisson and Helmholtz problems, problems in electromagnetics, quantum physics, viscous acoustics (based on Navier-Stokes equations), elasticity and coupling of those models. The matrices can be assembled and linear systems can be solved in parallel where we also give access to external direct solvers. There 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 version January 2015*

donlp2 is a software for the solution of general nonlinear programming problems. Different versions exist concerning the programming language (strict f77, f90, C99), the user interface and some options (for example elimination of redundant linear equality constraints and an interface known as "reverse communication"). donlp2 is free for research, whereas commercial use requires licensing by TU Darmstadt.

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. 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. It is accessible from anywhere in the world and indeed users from about 80 countries are visiting it. Any application comes with predefined test cases which can be used without programming knowledge at all. Presently only the English version receives further development, but the German version will be maintained. This English version has been extended by new iterated quadrature formulas and an improved download of results. For more information, see `numawww.mathematik.tu-darmstadt.de`

Contributor at TU Darmstadt: Peter Spellucci

# 5 Theses

## 5.1 PhD Dissertations

**2021**

Schneider, Moritz, *Super-convergent Implicit-Explicit Peer Methods* (Jens Lang)

Steinbach, Philipp, *Modeling, Simulation and Quantification of Drilling-Related Geometric Uncertainty for Borehole Heat Exchanger Arrays* (Jens Lang)

**2022**

Joshi, Hrishikesh, *Mesh and model adaptation for hyperbolic balance laws* (Jan Giesselmann)

Radu, Bogdan, *Finite Element Mass Lumping for H(div) and H(curl)* (Herbert Egger)

Strauch, Elisa, *Adaptive Multi-Level Monte Carlo and Stochastic Collocation Methods for Hyperbolic Partial Differential Equations with Random Data on Networks* (Jens Lang)

Teschner, Gabriel, *Data Driven Estimation of Wall Shear Stress from Magnetic Resonance Imaging* (Herbert Egger)

## 5.2 Master Theses

**2021**

Borkowski, Markus, *The Hodge-Laplace Equation on the Sphere* (Stefan Kurz, Herbert Egger)

Özalp, Elise, *Physics Informed Deep Learning for Partial Differential Equations* (Jens Lang)

Wilka, Hendrik, *Numerische Realisierung der Karhunen-Loève-Entwicklung in 3D mit H-Matrizen* (Jens Lang)

**2022**

Pfaff, Sven, *Oberflächenhomogenisierung und Analysis einer Finite-Elemente-Methode* (Kersten Schmidt)

## 5.3 Bachelor Theses

**2021**

Asmußen, Martin Jürgen, *Explizite Extrapolationsverfahren für Gewöhnliche Differentialgleichungen: Theorie und Anwendung* (Jens Lang)

Kopp, Erik Georg, *Parameteroptimierung chemischer Reaktionssysteme unter Beschränkungen* (Martin Kiehl)

Ludwig, Olivia Marie, *Essential modeling aspects and parameters for the long term prognosis of epidemical diseases like COVID19* (Martin Kiehl)

Seibel, Timon Philipp, *Fast Iterative Solution Methods for the Radiative Transfer Equation* (Herbert Egger)

**2022**

Binder, Patrick, *Approximationseigenschaften von Splines* (Jens Lang)

Chaumet, Aidan Raoul, *Relative Energy Stability Estimates for the Euler-Poisson System* (Jan Giesselmann)

Companys Franzke, Margarida Elisabeth, *Random batch Methoden für wechselwirkende Teilchen* (Jan Giesselmann)

Gabor, Vanessa Martha, *Stochastische Modellierung und Numerische Simulation der COVID-19 Pandemie* (Jens Lang)

Hoffmann, Marc, *Convergence of Moment Approximations of Linear Kinetic Equations describing semiconductors* (Jan Giesselmann)

Vasconcelos Afonso, Tiago, *Vergleich verschiedener Zielfunktionale bei der Lösung pant. Dgln mittels neuronalen Netzen* (Jan Giesselmann)

# 6 Presentations

## 6.1 Talks and Visits

### 6.1.1 Invited Talks and Addresses

**Neelabja Chatterjee**

27/03/2021 *Convergence Analysis of a numerical scheme for a general class of mean field equations*
Recent Advances in Applied Mathematics: Theory and Computations, Calcutta, India

**Herbert Egger**

14/07/2021 *An arbitrary order variational discretization for Maxwell´s equations in nonlinear media*
ICOSAHOM 2021, Vienna

27/09/2021 *MONA: A magnetic oriented nodal analysis*
DMV-ÖMG Annual Conference 2021 (online)

**Alf Gerisch**

30/09/2021 *Mechanical models of pattern formation in biological tissues: the role of the stress-strain constitutive model*
CMO/BIRS Workshop Modeling and Computational Approaches to Individual and Collective Cell Movement in Complex Environments (online)

19/09/2022 *On the simulation of models of cell migration involving myopic diffusion and cell-cell adhesion*
Minisymposium Mathematics for cell migration under the influence of the microenvironment: from single cells to populations, European Conference on Mathematical and Theoretical Biology (ECMTB 2022), Heidelberg

**Jan Giesselmann**

02/03/2021 *$L^2$ theory with shifts for a posteriori error analysis of finite volume schemes for hyperbolic conservation laws*
Workshop on Hyperbolic Balance Laws: modeling, analysis, numerics, Oberwolfach

14/02/2022 *A Posteriori Error Control of Numerical Schemes for Random Conservation Laws*
Conference on Mathematics of Wave Phenomena 2022, Karlsruhe

07/03/2022 *A Posteriori Error Estimates for 1D Systems of Hyperbolic Conservation Laws*
Perspectives on Multiphase Fluid Dynamics, Continuum Mechanics and Hyperbolic Balance Laws, CIRM, Luminy, France

14/03/2022 *On the Convergence of the Regularized Entropy-Based Moment Method for Kinetic Equations*
SIAM Conference on Analysis of Partial Differential Equations, Minisymposium Data-Driven Closures for Kinetic and Fluid Models, Berlin

19/05/2022 *Structure preserving finite element schemes for Euler Equations on Networks*
Meeting of WG 5 of COST Action Mat-Dyn-Net, Namur, Belgium

**Teresa Kunkel**

30/09/2021 *A uniformly convergent mixed finite element method for isothermal gas transport in pipe networks*
DMV-ÖMG Annual Conference 2021 (online)

23/11/2022 *What is ... ? Euler equations and their solution concepts*
What is ... ? Seminar, TU Darmstadt

**Jens Lang**

12/01/2021 *A Fully Adaptive Multilevel Stochastic Collocation Strategy for Solving Elliptic PDEs with Random Data*
WCCM 2021 (online)

14/07/2022 *Mathematical Solutions for Individualized Medical Treatment*
School of Medicine, Departments of Orthopaedic Surgery & Bioengineering, University of Pennsylvania, USA

26/07/2022 *Adaptive Stochastic Collocation Methods for Uncertain Unsteady Gas Transport in Networks*
WCCM 2022 (online)

28/07/2022 *Implicit A-Stable Peer Triplets for ODE Constrained Optimal Control Problems*
SCICADE 2022, Reykjavik, Iceland

**Christopher Müller**

03/02/2021 *What is ... ? A goal-oriented formulation?*
What is ... ? Seminar, TU Darmstadt

**Tabea Tscherpel**

03/12/2022 *Sobolev stability of the $L^2$-projection mapping to finite element spaces*
Recent trends in mathematical modelling, Kácov, Czech Republic

### 6.1.2 Contributed Talks

**Aidan Chaumet**

24/05/2022 *Relative Energy Stability Estimates for the Euler-Poisson System*
Seminar der AG Numerik, TU Darmstadt

**Herbert Egger**

13/04/2021 *Hansjörg-Wacker Memorial Prize Laudatio*
ECMI Conference, Wuppertal

**Franziska Eickmann**

24/11/2022 *Mathematical modeling and numerical simulation of bedload sediment transport in shallow flows*
Seminar der AG Numerik, TU Darmstadt

**Jan Giesselmann**

24/06/2022 *Weak-strong stability for wave-maps*
Conference on Hyperbolic Problems, Malaga, Spain

24/08/2022 *Euler equations on networks: Parabolic limit and asymptotic preserving numerics*
BENASQUE IX Partial differential equations, optimal design and numerics, Benasque, Spain

26/08/2022 *Observer based data assimiliation for transient models of gas transport*
BENASQUE IX Partial differential equations, optimal design and numerics, Benasque, Spain

**Teresa Kunkel**

13/09/2021 *Robust error analysis of a mixed finite element method for friction dominated, low Mach gas transport*
15th Hirschegg Workshop on Conservation Laws, Hirschegg

22/06/2022 *Observer-based data assimilation for isothermal gas transport using distributed measurements*
Conference on Hyperbolic Problems, Malaga, Spain

11/07/2022 *Observer-based data assimilation for isothermal gas transport using distributed measurements*
Equadiff 15, Brno, Czech Republic

**Nora Philippi**

03/03/2021 *Relative energy estimates, asymptotic stability and structure preserving discretization for isentropic flow in gas networks*
Trends in Mathematical Modelling, Simulation and Optimisation: Theory and Applications (online)

29/09/2021 *Singular perturbation of transport problems on pipe networks*
DMV-ÖMG Annual Conference 2021 (online)

29/10/2021 *Relative energy estimates, asymptotic stability and structure preserving discretization for isentropic flow in gas networks*
Research seminar, HU Berlin

20/06/2022 *An asymptotic preserving discretization scheme for gas transport in pipe networks*
Conference on Hyperbolic Problems, Malaga, Spain

14/07/2022 *A structure and asymptotic preserving discretization scheme for gas transport in pipe networks*
Equadiff 15, Brno, Czech Republic

17/08/2022 *An asymptotic preserving hybrid discontinuous Galerkin method for singularly perturbed convection-diffusion problems on networks*
GAMM Annual meeting, Aachen

**Kersten Schmidt**

13/11/2021 *Acoustic impedance conditions and the Helmholtz equation*
SAM Alumni Reunion & Science Slam, ETH Zürich

28/07/2022 *Adapted contour integration for nonlinear eigenvalue problems in wave-guide coupled resonators*
15th International Conference on Mathematical and Numerical Aspects of Wave Propagation, Paris, France

18/08/2022 *Adapted contour integration for nonlinear eigenvalue problems in wave-guide coupled resonators*
93rd Annual Meeting of the International Association of Applied Mathematics and Mechanics, Aachen

**Vsevolod Shashkov**

10/07/2022 *MONA - A magnetic oriented nodal analysis for electric circuits*
SCEE 2022, Amsterdam, Netherlands

15/05/2022 *MONA - A magnetic oriented nodal analysis for electric circuits*
JKU Linz

**Aleksey Sikstel**

25/05/2022 *A local a-posteriori error estimator for systems of hyperbolic conservation laws*
SHARK-FV Conference, Minho, Portugal

23/06/2022 *A local a-posteriori error estimator for systems of hyperbolic conservation laws*
Conference on Hyperbolic Problems, Malaga, Spain

**Elisa Strauch**

19/04/2021 *Stochastic Collocation Method for Hyperbolic PDEs with Random Data*
CE Research Colloquium, TU Darmstadt

**Erik Laurin Strelow**

01/02/2021 *Physics informed neural networks for gas networks*
CE Research Colloquium, TU Darmstadt

### 6.1.3 Visits

Jan Giesselmann, TU Berlin, September 2021

Jan Giesselmann, Institute for Advanced Study, Princeton, USA, February 2022

Teresa Kunkel, Universität Erlangen-Nürnberg, November 2021 and October 2022

Jens Lang, University of Pennsylvania, School of Medicine, USA, July 2022

## 6.2 Organization and Program Commitees of Conferences and Workshops

**Jan Giesselmann**

- Member of Organizing Committee Meeting of Working Group 5 of COST Action Mat-Dyn-Net, Namur, Belgium, May 18–20 2022

**Jens Lang**

- International Conference: Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-16) (jointly with Martin Arnold (Halle), Elena Celledoni (Trondheim), Jason Frank (Utrecht), Maren Hantke (Halle), Raphael Kruse (Halle), and Helmut Podhaisky (Halle)), Sep 6–10, 2021, Martin Luther University of Halle-Wittenberg, Halle/Saale

- Minisymposium: Certification of Computer Simulations and Model Adaptation (jointly with Ludovic Chamoin (Paris-Saclay), Serge Prudhomme (Montreal) and Juan José Rodenas (Valencia)) at 14th World Congress on Computational Mechanics (WCCM), Jan 11–15, 2021, Online

- Minisymposium: Certification of Computer Simulations and Model Adaptation (jointly with Ludovic Chamoin (Paris-Saclay), Serge Prudhomme (Montreal), Juan José Rodenas (Valencia), and Fredrick Larsson (Göteborg)) at 15th World Congress on Computational Mechanics (WCCM), Jul 31 – Aug 5, 2022, Online

- Workshop: Adaptive Moving and Anisotropic Meshes for the Numerical Approximation of PDEs (jointly with Chris Budd (Bath), Weizhang Huang (Kansas), and Simona Perotto (Milano)), May 9–13, 2022, ICMS Edinburgh

# 7 Workshops and Visitors at the Department

## 7.1 Guest Talks at the Department

18/01/2021 Dr. Milana Pavic-Colic (University of Novi Sad), *Cauchy Problem and moment equations for the Boltzmann model describing polyatomic gas* (Jan Giesselmann)

25/01/2021 Prof. Dr. Ansgar Jüngel (TU Vienna), *Structure-preserving finite-volume schemes for cross-diffusion systems* (Herbert Egger)

01/02/2021 Prof. Dr. Hana Mizerova (Comenius University in Bratislava and Czech Academy of Sciences), *Convergent finite volume scheme for compressible Euler equation* (Jan Giesselmann)

08/02/2021 Dr. Aleksey Sikstel (Universität Erlangen-Nürnberg), *Analysis and Numerical Methods for Coupled Hyperbolic Conservation Laws* (Jan Giesselmann)

21/04/2021 Dr. Stephan Gerster (RWTH Aachen), *Stochastic Galerkin Formulations for Hyperbolic Conservation Laws* (Jan Giesselmann)

05/05/2021 PD Dr. Stefan Takacs (JKU Linz), *Condition number bounds for IETI-DP methods that are explicit in h and p* (Herbert Egger)

02/06/2021 Dr. Clemens Hofreither (RICAM Linz), *Rational approximation in the context of fractional diffusion* (Herbert Egger)

09/06/2021 Prof. Dr. Tobias Breiten (TU Berlin), *Feedback control of nonlinear infinite-dimensional and port-Hamiltonian systems* (Jan Giesselmann)

16/06/2021 Dr. Clemens Pechstein (Dassault Systèmes Austria GmbH), *A unified convergence theory for Robin-Schwarz methods – continuous and discrete, including crosspoints* (Herbert Egger)

30/06/2021 Aaron Brunk (JGU Mainz), *Wellposedness and numerical analysis for a viscoelastic phase separation model via energy and relative energy methods* (Herbert Egger)

07/07/2021 PD Dr. Peter Mewis (TU Darmstadt), *Strömungssimulation in Fließgewässer* (Jan Giesselmann)

26/10/2021 Richard Löscher (TU Graz), *A General Approach to Mass Lumping Using Hilbert Complexes* (Herbert Egger)

09/11/2021 Dr. Piotr Minakowksi (OvGU Magdeburg), *Error Estimates for Neural Network Solutions of Partial Differential Equations* (Jan Giesselmann)

16/11/2021 Nicola De Nitti (Universität Erlangen-Nürnberg), *Control of advection-diffussion equations on networks and singular limits* (Herbert Egger)

06/12/2021 Ass. Prof. Carolina Urzua-Torres (TU Delft), *A New Approach to Space-Time Boundary Integral Equations for the Wave Equation* (Herbert Egger)

10/05/2022 Dr. Stephan Gerster (University of Como), *Feedback control for hyperbolic balance laws* (Jan Giesselmann)

17/05/2022 Nadine Stahl (Universität Trier), *Efficient State Estimation using Reduced Order Models for Pipeline Networks* (Jan Giesselmann)

14/06/2022 Dr. Jim Magiera (Universität Stuttgart), *Components of a Molecular-Continuum Interface Solver for Liquid-Vapor Flow: Moving Mesh, Molecular Dynamics and Machine Learning* (Jan Giesselmann)

19/06/2022 Dr. Marlies Pirner (Universität Würzburg), *Hypocoercivity for a nonlinear generation-recombination model* (Jan Giesselmann)

11/07/2022 Dr. Yuhuan Yuan (Universität Mainz), *Convergence and error estimates of the Godunov Method for Multidimensional Compressible Euler Equations* (Jan Giesselmann)

25/10/2022 Lucas Maier (Universität Stuttgart), *Numerical Simulation of Multi-phase Flow in Porous Media with a Phase-field Model* (Jens Lang)

01/12/2022 Dr. Niklas Kolbe (RWTH Aachen), *New numerical and data-based approaches for networked scalar conservation laws* (Jan Giesselmann)

08/12/2022 Prof. Dr. Sebastian Krumscheid (KIT), *Multilevel Monte Carlo methods for forward Uncertainty Quantification* (Jan Giesselmann)

15/12/2022 Dr. Jörn Wichmann (Universität Bielefeld), *An averaged space-time discretization of the stochastic p-Laplace system* (Tabea Tscherpel)

## 7.2 Visitors at the Department

Kiwoong Kwon (Kyungpook National University, Korea), September to October 2022.

Prof. Dr. Sandra May (Uppsala University, Schweden), September 2022.

Dr. Jörn Wichmann (Universität Bielefeld), December 2022.

## 7.3 Workshops and Conferences at the Department

– Mathematische Modellierungswoche, October 17–22, 2021, Fuldatal (organized by Martin Kiehl, Jan Giesselmann (TU Darmstadt) and Tobias Braumann (Zentrum für Mathematik, Bensheim))

– Mathematische Modellierungswoche, October 23–28, 2022, Fuldatal (organized by Martin Kiehl, Jan Giesselmann (TU Darmstadt) and Tobias Braumann (Zentrum für Mathematik, Bensheim))

# 8 Other scientific and organisational activities

## 8.1 Memberships in Scientific Boards and Committees

**Martin Kiehl**

– Vorsitzender des Aufsichtsrats, Zentrum für Mathematik, Bensheim

**Jens Lang**

– Member of Board of Deans of the Graduate School Computational Engineering, TU Darmstadt, since 2008

– Member of Scientific Committee of the Conference on the Numerical Solution of Differential and Differential-Algebraic Equations to be held at the Martin-Luther University Halle-Wittenberg every three years

## 8.2 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.

The following is a list of further public relations activities.

**Activities for secondary school students and prospective students**

- Since 2020, th job and study information fair HoBIT, (Hochschul- und Berufsinformationstage) has been taking place in a new form. In January, members of the university inform about the different offers during podcast-like online discussions. Mathematics is represented by professors and students. In May, a significantly smaller fair takes place. The Department of Mathematics uses exhibits to convey the fascination of mathematics and provides information about studying in talks with about 100 pupils.

- Participation in the university fair "vocatium", a fair for school students who are interested in a university study programme (Offenbach and Mannheim)

- Several visits from schools, especially Leistungskurse (advanced courses in mathematics). The typical program consists of a mathematical lecture, information about the study and a meeting with students. Tours, for example of the ULB (Library) or the high-performance computer, are also organized on request.

- Due to the Covid-19 pandemic, student advisory for prospective students mostly was held online via Zoom by Dr. Seeberg in 2021.

- Activities for secondary school students and prospective students
  Tutoring courses in the scope of the Hessian programme "Löwenstark " for students of year 6 to 8. Topics covered are fractions, terms and variables, and geometry.

- Lecture titled "Mathematisches Problemlösen" in the context of the youth camp "Albert-Schweitzer-Uni" for 8-15-year-olds in Lindenfels by Jan Herzog in 2021.

- Annual organisation of the mathematical problem solving event "Knobelstraßen" for high school and university student by the working group on subject didactics in 2021 (online) and 2022 (in person). They take place annually shortly before Christmas. School groups that are unable to attend receive materials upon request.

- Annual Graduation Event: celebration with friends and family of the graduated students (organisation: Prof. Große-Brauckmann and staff) June 2022.

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