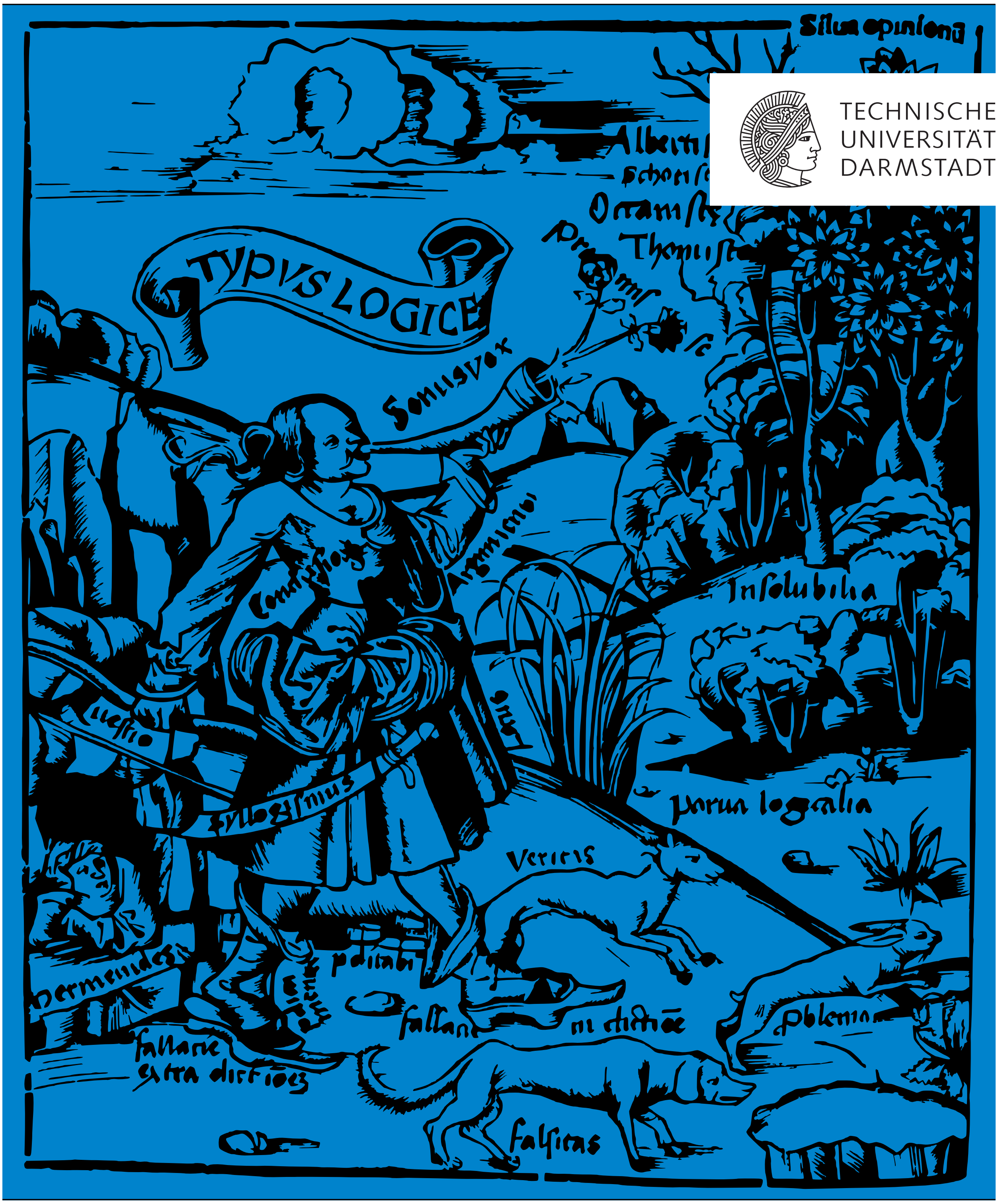
Biannual Report

Department of Mathematics
Research Group Numerical Analysis and Scientific Computing
2015 and 2016



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General Remark

This document contains a subset of the information of the Biannual Report of the Department of Mathematics at TU Darmstadt for 2015 and 2016. It has simply been obtained by extracting all the information provided by our Research Group Numerical Analysis and Scientific Computing from the complete report. All empty chapters have been removed. This is only meant to be supplementary, because it is hard to filter out information from the complete document.

Research Group Numerical Analysis and Scientific Computing

April 2018

Contents

1 Research Group Numerical Analysis and Scientific Computing

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

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

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

The research group *Numerical Analysis and Scientific Computing* has been and is engaged among others in various coordinated research activities, e.g., in the Graduate Schools (Excellence Initiative) GSC 233 Computational Engineering and GSC 1070 Energy Science and Engineering, the Transregional Collaborative Research Centers (Transregio/SFB) TRR 154 Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks and TRR 146 Multiscale Simulation Methods for Soft Matter Systems, the International Research Training Group IGK 1529 Mathematical Fluid Dynamics, the German Research Foundation (DFG) Priority Programs SPP 1253 Optimisation with Partial Differential Equations, SPP 1276 Multiple Scales in Fluid Mechanics and Meteorology (MetStröm), and SPP 1420 Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials, and the Funding Program “Future-oriented Technologies and Concepts for an Energy-efficient and Resource-saving Water Management - ERWAS” of the Federal Ministry of Education and Research (BMBF) (`http://www.bmbf.nawam-erwas.de/en`). In addition, the group has various industry partners, including cooperations with Robert Bosch GmbH Stuttgart, BASF Ludwigshafen, and Infineon München.

Members of the research group

Professors

Herbert Egger, Christoph Erath, Martin Kiehl, Jens Lang

Retired professors

Peter Spellucci

Postdocs

Pia Domschke, Sofia Eriksson, Alf Gerisch, Michelle Lass, Raimondo Penta, Jan-Frederik Pietschmann, Sebastian Ullmann, Mirjam Walloth

Research Associates

Anke Böttcher, David Frenzel, Thomas Kugler, Axel Ariaan Lukassen, Pascal Mindt, Christopher Müller, Bogdan Radu, Alexander Rath, Moritz Schneider, Lucas Schöbel-Kröhn, Robert Schorr, Dirk Schröder, Tobias Seitz, Christopher Spannring, Zhen Sun, Gabriel Teschner, Sara Tiburtius, Lisa Wagner

Secretaries

Elke Dehnert, Sigrid Hartmann

Project: Numerical approximation of phase field models in elastic bodies

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

Contact: A. Böttcher, H. Egger

References

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

[2] R. Müller, A. Böttcher, B. Xu, J. Aurich, and D. Gross. Driving forces on interfaces in elastic-plastic two phase materials. *ZAMM. Angew. Math. Mech.*, 90:812–820, 2010.

Project: Mixed finite element methods for the acoustic wave equation

The study of wave propagation is an important topic in the field of engineering and it finds application in various fields such as in antenna design, radar detection, noise cancellation, fiber optics, signal filtering, seismic prospection and many others. Therefore, the efficient and accurate simulation of wave phenomena is of big relevance from a practical point of view. Successful numerical methods have to take into account various problem specific aspects: discrete problems are typically of large scale and efficient time stepping schemes are required; computational domains have to be truncated and artificial boundaries have to be introduced; a systematic derivative and adjoint calculus are required in order to tackle optimization, control, and inverse problems; the approximation of solutions at high wave number requires very fine grids; special treatment of material interfaces may be needed. Our goal is to model the APE (acoustic perturbed equation) and to analyze its discrete system in the context of mixed finite element methods. Further, we will then extend the obtained results to the elastodynamics and Maxwell's equations.

Support: Graduate School Computational Engineering, DFG

Contact: H. Egger, B. Radu

References

[1] H. Egger and B. Radu. Super-convergence and post-processing for mixed finite element approximations of the wave equation. *arXiv:1608.03818*, 2016.

Project: Tikhonov stability in Hilbert scales under Hölder stability

We consider the stable solution of nonlinear ill-posed problems by Tikhonov regularization in Hilbert scales. Order-optimal convergence rates are established for a priori and a posteriori parameter choice strategies under a conditional stability assumption for the inverse problem. The role of a hidden source condition is investigated and the relation to previous results for regularization in Hilbert scales is elaborated. The applicability of the results is discussed for some model problems, and the theoretical results are illustrated by numerical tests.

Partner: B. Hofmann (TU Chemnitz)

Contact: H. Egger

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

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

Partner: K. Fellner, T. Q. Tang (TU Graz); J.-F. Pietschmann (WWU Münster)

Contact: H. Egger

References

[1] H. Egger, K. Fellner, J.-F. Pietschmann, and B. Q. Tang. A finite element method for volume-surface reaction-diffusion systems. *arXiv:1511.00846*, 2015.

Project: Boundary treatment and accelerated reconstruction in Fluorescence optical tomography

Flourescence optical tomography is a non-invasive imaging modality that allows one to obtain space- and time-resolved information about biological processes in-vitro and in-vivo. Two of the main challenges in the practical use of this method are: (i) the automatic detection and handling of unknown geometry, and (ii) the computational handling and inversion of huge data sets. The goal of this project is to enhance existing computational methods in order to address these challenges.

Partner: M. Schlottbom (UT Twente)

Contact: H. Egger

References

[1] H. Egger and M. Schlottbom. A class of Galerkin schemes for time-dependent radiative transfer. *SIAM Journal on Numerical Analysis*, 54:3577–3599, 2015.

[2] H. Egger and M. Schlottbom. Numerical methods for parameter identification in stationary radiative transfer. *Computational Optimization and Applications*, 62:67–83, 2015.

Project: Asymptotic preserving schemes for compressible flow on networks

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

Partner: M. Lukačova (JGU Mainz)

Contact: H. Egger

References

[1] H. Egger. A mixed variational discretization for non-isothermal compressible flow in pipelines. *arXiv:1611.03368*, 2016.

[2] H. Egger. A robust conservative mixed finite element method for compressible flow on pipe networks. *arXiv:1609.04988*, 2016.

[3] H. Egger and T. Kugler. Damped wave systems on networks: Exponential stability and uniform approximations. *arXiv:1605.03066*, 2016.

Project: Spinodal decomposition of polymer-solvent systems

Mathematical models for the dynamics of polymer systems on the mesoscopic scale are based on a bead-spring description of polymer chains and the Navier-Stokes solver for the surrounding solvent. Despite their structural simplicity, a simulation of these models on relevant scales is still computationally infeasible. Theoretical models are better suited for numerical simulations on macroscopic scales but they often yield unrealistic results due to insufficient information about the underlying constitutive equations. This project intends to close the gap between the mesoscopic and the macroscopic world for a particular model system with highly complex non-equilibrium dynamics, namely a phase-separating polymer solution. A particular focus lies on the development of new concepts of multiscale methods and coarse-graining. The main goal of the project is to develop efficient and robust parameter identification strategies that allow us to estimate the required constitutive laws in the macroscopic model via calibration to simulation results for the underlying mesoscale models obtained by a coupled Lattice-Boltzmann–Molecular-Dynamics algorithm.

Partner: B. Dünweg (MPIP Mainz); M. Lukačova (JGU Mainz)

Contact: H. Egger

References

[1] H. Egger, T. Kugler, and N. Strogies. Parameter identification in a semilinear hyperbolic system. *arXiv:1606.03580*, 2016.

[2] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of chemotaxis models with volume-filling. *SIAM J. Appl. Math.*, 75(2):275–288, 2015.

Project: Identification of nonlinear diffusion laws in quasi-linear parabolic and elliptic equations

We consider the inverse problem of identifying a nonlinear diffusion coefficient in second order quasi-linear parabolic and elliptic equations with principal part in divergence form, given knowledge of a partial Dirichlet-to-Neumann map. The proofs are based on a localization procedure at the boundary. Since this is mostly independent of the particular structure of the problem, our approach is able to handle arbitrary unknown lower order terms, as long as they fulfill mild regularity conditions, mixed boundary conditions and even systems of equations.

Partner: M. Schlottbom (UT Twente); J.-F. Pietschmann (WWU Münster)

Contact: H. Egger

References

[1] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of chemotaxis models with volume-filling. *SIAM J. Appl. Math.*, 75(2):275–288, 2015.

[2] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of nonlinear heat conduction laws. *J. Inverse Ill-Posed Probl.*, 23(5):429–437, 2015.

Project: Convergence of some adaptive FVM

We consider the vertex-centered finite volume method with first-order conforming ansatz functions. The adaptive mesh refinement is driven by the local contributions of the weighted-residual error estimator. We prove that the adaptive algorithm leads to linear convergence with generically optimal algebraic rates for the error estimator and the sum of energy error plus data oscillations. While similar results have been derived for finite element and boundary element methods, the present work appears to be the first for adaptive finite volume methods, where the lack of the classical Galerkin orthogonality leads to new challenges.

Partner: D. Praetorius (TU Wien)

Contact: C. Erath

References

[1] C. Erath and D. Praetorius. Convergence of some adaptive finite volume methods. *SIAM J. Numer. Anal.*, 54:2228–2255, 2016.

Project: A non-symmetric coupling of the finite volume method and the boundary element method

As model problem we consider the prototype for flow and transport of a concentration in porous media in an interior domain and couple it with a diffusion process in the corresponding unbounded exterior domain. To solve the problem, we develop a new non-symmetric coupling between the vertex-centered finite volume and boundary element method. This discretization naturally provides conservation of local fluxes and, with an upwind option, also stability in the convection dominated case. We aim to provide a first rigorous analysis of the system for different model parameters, stability, convergence, and a priori estimates. This includes the use of an implicit stabilization, known from the finite element and boundary element method coupling. Some numerical experiments conclude the work and confirm the theoretical results.

Partner: G. Of (TU Graz); F.-J. Sayas (University of Delaware, USA)

Contact: C. Erath

References

[1] C. Erath, G. Of, and F.-J. Sayas. A non symmetric coupling of the finite volume method and the boundary element method. *Numer. Math.*, pages 1–28, published online, 2016.

Project: A nonconforming a posteriori estimator for the coupling of cell-centered finite volume and boundary element methods

The coupling of the cell-centered finite volume and the boundary element method is an interesting approach to solving elliptic problems on an unbounded domain, where local flux conservation is important. Based on the piecewise constant interior finite volume solution, we define a Morley-type interpolant built on a non-conforming finite element. Together with the Cauchy data of the exterior boundary element solution, this allows us to define a residual-based a posteriori error estimator. With respect to an energy norm, we prove reliability and efficiency of this estimator and use its local contributions to steer an adaptive mesh-refining algorithm. In two examples we illustrate the effectiveness of the new adaptive coupling method and compare it with the coupling approach with a conforming Morley interpolant.

Contact: C. Erath

References

[1] C. Erath. A nonconforming a posteriori estimator for the coupling of cell-centered finite volume and boundary element methods. *Numer. Math.*, 131:425–451, 2015.

Project: Semi-Lagrangian schemes for transport in a (climate) dynamical core

In today's atmospheric numerical modeling, scalable and highly accurate numerical schemes are of particular interest. To address these issues, Galerkin schemes, such as the spectral element method, have received more attention in the last decade. They also provide other state-of-the-art capabilities such as improved conservation. However, the tracer transport of hundreds of tracers, e.g., in the chemistry version of the Community Atmosphere Model, is still a performance bottleneck. Therefore, we consider two conservative semi-Lagrangian schemes. Both are designed to be multi-tracer efficient, third order accurate, and allow significantly longer time steps than explicit Eulerian formulations. We address the difficulties arising on the cubed-sphere projection and on parallel computers, and show the high scalability of our approach. Additionally, we use the two schemes for the transport of passive tracers in a dynamical core and compare our results with a current spectral element tracer transport advection used by the High-Order Method Modeling Environment.

Partner: M. A. Taylor (Sandia National Laboratories, USA); R. D. Nair (NCAR, USA)

Contact: C. Erath

References

[1] C. Erath, M. A. Taylor, and R. D. Nair. Two conservative multi-tracer efficient semi-lagrangian schemes for multiple processor systems integrated in a spectral element (climate) dynamical core. *Commun. Appl. and Ind. Math.*, 7:71–95, 2016.

Project: Optimal adaptivity for the SUPG FEM

For convection dominated problems, the streamline upwind Petrov-Galerkin method (SUPG) (also named streamline diffusion finite element method (SDFEM)) promotes a non-oscillatory finite element solution. Based on robust a posteriori error estimators, we propose an adaptive mesh-refining algorithm for SUPG and prove that the generated SUPG solutions converge with asymptotically optimal rates towards the exact solution.

Partner: S. A. Funken (Universität Ulm); D. Praetorius (TU Wien)

Contact: C. Erath

Project: Time-dependent cell-centered FVM-BEM coupling

An interesting approach to deal with problems on unbounded domains is to couple the finite volume method with the boundary element method. Previously, novel work has been done for problems of diffusion convection reaction type in an interior domain coupled to a diffusion process in an unbounded exterior problem [1, 2]. In this project, we extend the cell-centered FVM-BEM coupling methodology [2] to problems of other types involving time, e.g., parabolic-elliptic interface problems.

Contact: C. Erath, S. Eriksson

References

[1] C. Erath. Coupling of the finite volume element method and the boundary element method: an a priori convergence result. *SIAM Journal on Numerical Analysis*, 50:574–594, 2012.

[2] C. Erath. A new conservative numerical scheme for flow problems on unstructured grids and unbounded domains. *J. Comput. Phys.*, 245:476–492, 2013.

Project: Higher order integration methods for the optimal control of hyperbolic equations

Many problems in natural science can be modeled with hyperbolic differential equations such as traffic modeling and fluid mechanics. The main difficulty of these equations is that solutions may become discontinuous even if the initial data and boundary conditions are smooth. In many applications we are interested in optimizing a given objective through optimal control. The main issue is that the control-to-state mapping is not differentiable with respect to common variational concepts. However, it can be shown that the control-to-state mapping is shift-differentiable. This concept implies the Fréchet-differentiability of objective functionals and yields adjoint-based formulas for their derivative. We investigate the numerical treatment of the adjoint equation and the computation of the optimal control.

Partner: S. Ulbrich (TU Darmstadt)

Support: Graduate School Computational Engineering, DFG

Contact: D. Frenzel, J. Lang

Project: Multiscale structure-functional modeling of musculoskeletal mineralized tissues

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

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

Partner: K. Raum (Charité-Universitätsmedizin Berlin); Q. Grimal (Biomedical Imaging Lab, UPMC Paris, France)

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

Contact: A. Gerisch, R. Penta, S. Tiburtius

References

[1] M. Granke, Q. Grimal, W. J. Parnell, K. Raum, A. Gerisch, F. Peyrin, A. Saïed, and P. Laugier. To what extent can cortical bone millimeter-scale elasticity be predicted by a two-phase composite model with variable porosity? *Acta Biomaterialia*, 12:207–215, 2015.

[2] R. Penta and A. Gerisch. The asymptotic homogenization elasticity tensor properties for composites with material discontinuities. *Continuum Mechanics and Thermodynamics*, 29:187–206, 2016.

[3] R. Penta and A. Gerisch. Investigation of the potential of asymptotic homogenization for elastic composites via a three-dimensional computational study. *Computing and Visualization in Science*, 17:185–201, 2016.

[4] R. Penta, K. Raum, Q. Grimal, S. Schrof, and A. Gerisch. Can a continuous mineral foam explain the stiffening of aged bone tissue? A micromechanical approach to mineral fusion in musculoskeletal tissues. *Bioinspiration & Biomimetics*, 11:035004, 2016.

Project: Numerical methods for time-dependent PDE problems from mathematical biology

Biological processes like the invasion of tissue by cancer cells, the adhesion-driven reorganization of tissue, and the cascade of steps in fracture healing can be modeled as time-dependent PDEs. For the reliable, efficient and accurate simulation of these models, dedicated numerical schemes are required. We focus on general methods for taxis-diffusion-reaction systems and on particular schemes for the evaluation of the spatially nonlocal terms in models of cellular adhesion. In our approach, we follow the method of lines with finite volumes in space and linearly-implicit methods in time.

Partner: M. A. J. Chaplain (University of St. Andrews, UK); K. J. Painter (Heriot-Watt University, Edinburgh, UK); D. Trucu (University of Dundee, UK); L. Geris (University of Liège, Belgium)

Contact: A. Gerisch, P. Domschke

References

[1] P. Domschke, D. Trucu, A. Gerisch, and M. Chaplain. Structured models of cell migration incorporating molecular binding processes. arXiv:1607.05353, July 2016.

[2] K. J. Painter, J. M. Bloomfield, J. A. Sherratt, and A. Gerisch. A nonlocal model for contact attraction and repulsion in heterogeneous populations. *Bulletin of Mathematical Biology*, 77:1132–1165, 2015.

[3] D. Trucu, P. Domschke, A. Gerisch, and M. A. Chaplain. Multiscale computational modelling and analysis of cancer invasion. In L. Preziosi, M. A. Chaplain, and A. Pugliese, editors, *Mathematical Models and Methods for Living Systems: Levico Terme, Italy 2014*, pages 275–321. Springer International Publishing, 2016.

Project: Defect corrected averaging for highly oscillatory problems

The accurate solution of partial differential equations with highly oscillatory source terms over long time scales constitutes a challenging problem. There exists a variety of methods dealing with problems that include processes, equations or variables on fine and coarse scales. Multiscale methods have in common that they neither fully resolve the fine scale, nor completely ignore it. On the one hand, these methods strive, without significantly sacrificing accuracy or essential properties of the system, to be much more efficient than methods that fully resolve the fine scale. On the other hand, these methods should be considerably more accurate than methods that completely ignore the fine scale. Within this project, we develop a defect corrected averaging procedure, which is based on a modified coarse scale problem that approximates the solution of the fine scale problem in stroboscopic points. Nevertheless, our approximation process is clearly different from the stroboscopic averaging method. We give an error estimate for the solution of the modified problem. The computational efficiency of the approximation is further improved by the application of preconditioning techniques. Tests on numerical examples show the efficiency and reliability of our approach.

Partner: J. Wensch (TU Dresden)

Contact: A. Gerisch

References

[1] J. Wensch, A. Gerisch, and A. Naumann. Defect corrected averaging for highly oscillatory problems. *Applied Mathematics and Computation*, 261:90–103, 2015.

Project: Hierarchical Galerkin methods for hyperbolic problems with parabolic asymptotic

This project is part of the Transregional Collaborative Research Centre TRR 154 *Mathematical modeling, simulation and optimization of gas networks*, and deals with the construction and analysis of numerical methods for singularly perturbed hyperbolic problems with parabolic limit. The main goal is to devise efficient asymptotic preserving numerical schemes together with reliable a posteriori error estimators. Of particular interest are the isothermal one-dimensional Euler equations with friction, which are used to model gas flow in pipes and networks. Basic physical principles, like the conservation of mass, the balance of momentum, and the boundedness of solutions should be preserved on the discrete level on single pipes and across junctions.

Support: Project C04 within DFG TRR 154

Contact: H. Egger, T. Kugler, J. Lang

References

[1] H. Egger and T. Kugler. Damped wave systems on networks: Exponential stability and uniform approximations. *arXiv:1605.03066*, 2016.

[2] H. Egger, T. Kugler, and N. Strogies. Parameter identification in a semilinear hyperbolic system. *arXiv:1606.03580*, 2016.

Project: Anisotropic meshes and explicit Runge-Kutta methods

We study the stability of explicit Runge-Kutta integration schemes for the linear finite element approximation of linear parabolic equations. The derived bound on the largest permissible time step is tight for any mesh and any diffusion matrix within a factor of $2(d+1)$, where d is the spatial dimension. Both full mass matrix and mass lumping are considered. The bound reveals that the stability condition is affected by two factors. The first one depends on the number of mesh elements and corresponds to the classic bound for the Laplace operator on a uniform mesh. The other factor reflects the effects of the interplay of the mesh geometry and the diffusion matrix.

Partner: W. Huang (University of Kansas, USA); L. Kamenski (WIAS Berlin)

Contact: J. Lang

References

[1] W. Huang, L. Kamenski, and J. Lang. Stability of explicit one-step methods for P1-finite element approximation of linear diffusion equations on anisotropic meshes. *SIAM J. Numer. Anal.*, 54:1612–1634, 2016.

Project: On asymptotic global error estimation and control of finite difference solutions for semilinear parabolic equations

In this project, we extend the global error estimation and control addressed in Lang and Verwer [SIAM J. Sci. Comput. 29, 2007] for initial value problems to finite difference solutions of semilinear parabolic partial differential equations. The approach presented there is combined with an estimation of the PDE spatial truncation error by Richardson extrapolation to estimate the overall error in the computed solution. Approximations of the error transport equations for spatial and temporal global errors are derived using asymptotic estimates that neglect higher order error terms for sufficiently small step sizes in space and time. Asymptotic control in a discrete L^2-norm is achieved through tolerance proportionality and uniform or adaptive mesh refinement.

Partner: K. Debrabant (Southern University of Denmark)

Contact: J. Lang

References

[1] K. Debrabant and J. Lang. On asymptotic global error estimation and control of finite difference solutions for semilinear parabolic equations. *Computer Methods in Applied Mechanics and Engineering*, 288:110–126, 2015.

Project: Robustness of a new molecular dynamics-finite element coupling approach for soft matter systems analyzed by uncertainty quantification

Key parameters of a recently developed coarse-grained molecular dynamics-finite element coupling approach have been analyzed in the framework of uncertainty quantification (UQ). We have employed a polystyrene sample for the case study. The new hybrid approach contains several parameters that cannot be determined on the basis of simple physical arguments. Among others, this includes the so-called anchor points as information transmitters between the particle-based molecular dynamics (MD) domain and the surrounding finite element continuum, the force constant between polymer beads and anchor points, the number of anchor points, and the relative sizes of the MD core domain and the surrounding dissipative particle dynamics domain. Polymer properties such as density, radius of gyration, end-to-end distance, and radial distribution functions are calculated as a function of the above model parameters. The influence of these input parameters on the resulting polymer properties is studied by UQ. Our analysis shows that the hybrid method is highly robust. The variation of polymer properties of interest as a function of the input parameters is weak.

Partner: Shengyuan Liu, Mohammed Rahimi, Michael C. Böhm, Florian Müller-Plathe (Theoretical Chemistry, TU Darmstadt)

Contact: J. Lang, A. Gerisch

References

[1] S. Liu, A. Gerisch, M. Rahimi, J. Lang, M. C. Böhm, and F. Müller-Plathe. Robustness of a new molecular dynamics-finite element coupling approach for soft matter systems analyzed by uncertainty quantification. *The Journal of Chemical Physics*, 142:104105, 2015.

Project: Adjoint-based error control for the simulation and optimization of gas and water supply networks

In this work, the simulation and optimization of transport processes through gas and water supply networks is considered. Those networks mainly consist of pipes as well as other components like valves, tanks and compressor/pumping stations. These components are modeled via algebraic equations or ODEs while the flow of gas/water through pipelines is described by a hierarchy of models starting from a hyperbolic system of PDEs down to algebraic equations. We present a consistent modeling of the network and derive adjoint equations for the whole system including initial, coupling and boundary conditions. These equations are suitable to compute gradients for optimization tasks but can also be used to estimate the accuracy of models and the discretization with respect to a given cost functional. With these error estimators we present an algorithm that automatically steers the discretization and the models used to maintain a given accuracy. We show numerical experiments for the simulation algorithm as well as the applicability in an optimization framework.

Partner: Oliver Kolb (Universität Mannheim)

Contact: J. Lang, P. Domschke

References

[1] P. Domschke, O. Kolb, and J. Lang. Adjoint-based error control for the simulation and optimization of gas and water supply networks. *Applied Mathematics and Computation*, 259:1003–1018, 2015.

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

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

Contact: J. Lang, A. Gerisch

References

[1] D. Schröder, A. Gerisch, and J. Lang. Space-time adaptive linearly implicit peer methods for parabolic problems. *J. Comp. Appl. Math.*, 316:330–344, 2016.

Project: PDAS strategy for the KS system of chemotaxis

This project focuses on a numerical scheme applied to the Keller-Segel (KS) system of chemotaxis. The KS chemotaxis system describes the space and time evolution of a population of cells governed by the effects of diffusion and a directed motion in response to chemical gradients. The model problem is composed of a set of coupled nonlinear parabolic partial differential equations, which can be reformulated as a parabolic obstacle problem provided that the conservation of positivity is satisfied. The discrete problem resulting from the finite element discretization is solved by using the primal dual active set (PDAS) strategy. The performance and efficiency of the algorithm are studied and interpreted as a semismooth Newton method.

Contact: H. Egger, M. Lass

Project: A numerical approach to obstacle problems with convection diffusion operators

Numerical solutions of obstacle problems with convection diffusion operators are considered. Different multigrid strategies are applied to the algebraic problems arising from the finite element or finite difference approximations of the given problem. The goal is to obtain optimal computational complexity similar to the multigrid convergence property of PDE-based problems. Experimental results are presented to show the numerical performance and efficiency of the proposed method.

Partner: A. Borzì (Universität Würzburg); E.-J. Park (Yonsei University, South Korea)

Contact: M. Lass

Project: Multigrid methods for the optimal control of elliptic variational inequalities

This research project aims to contribute to the development and advancement of finding faster and more efficient numerical techniques for optimal control problems governed by elliptic variational inequalities (VIs). The prototypical problem is the optimal control of a VI of obstacle type. Different nonlinear multigrid techniques are evaluated and utilized to directly solve an appropriate optimality system of the optimal control problem without regularization. The numerical performance and efficiency of the proposed multigrid algorithms are studied and interpreted in comparison with other existing numerical methods, which typically employ an additional regularization loop for solving this type of problems. The motivation for such extensions is to be able to provide optimality solutions with optimal computational complexity and robustness with respect to optimization parameters. The main challenge here is to show the textbook multigrid convergence behaviour similar to the PDE-based problems in order to obtain optimal computational complexity.

Partner: R. Herzog (TU Chemnitz)

Support: Alexander von Humboldt-Stiftung (Georg Forster-Forschungsstipendium)

Contact: M. Lass

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

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

Contact: A. Lukassen, M. Kiehl

Project: Adaptive dynamical multiscale methods

The flow of gas through pipelines is of great interest in the engineering community. There are many challenges to running a gas transmission network. Various contracts have to be fulfilled, e.g., gas fed in by multiple suppliers has to be routed through the network while consumers' demands have to be met. The aim of operating a gas transmission network is to minimize the running costs. Those costs are mainly the running costs of compressor stations and contractual penalties. This leads to an optimal control problem on a network. Similar optimal control problems also occur for example in water supply networks. While monitoring systems are already quite advanced, efficient simulation and optimization tools are only available to some extent. Of course, before considering optimization tasks, reliable simulation algorithms are essential. Since the application of coarse discretizations or simplified models is often adequate in many parts of the considered networks to resolve the dynamics in the daily operation of gas and water supply networks, information about the quality of the computed solutions is very important. Within this project, we develop an algorithm to adaptively control model and discretization errors in simulations for gas and water supply networks with respect to a given quantity of interest using adjoint techniques.

Partner: O. Kolb (Universität Mannheim)

Support: Project B01 within DFG TRR 154

Contact: P. Mindt, P. Domschke, J. Lang

Project: Stochastic Galerkin methods for incompressible flows

Input data for mathematical models are most of the time not known exactly due to measurement errors or a lack of knowledge in general. The stochastic Galerkin method is one particular approach from the field of Uncertainty Quantification, where this influence on the solution of a partial differential equation is investigated. For a class of established representations of the stochastic input, the methodology exhibits exponential convergence rates but at the same time suffers from the curse of dimensionality. In order to solve the associated large coupled systems of equations efficiently, sophisticated iterative methods and preconditioners are required. The goal of this project is to apply and extend existing methods specifically tailored to flow problems with random data.

Support: Graduate School Computational Engineering, DFG

Contact: C. Müller, S. Ullmann, J. Lang

Project: IMEX-Peer methods with optimized stability regions

The spatial discretization of certain time-dependent partial differential equations (e.g. advection-diffusion-reaction systems) yields large systems of ordinary differential equations in time. Their right-hand sides admit a splitting into a stiff and non-stiff part or, to be more precise, a part that has to be solved using an implicit time integrator and a part to which we can apply an explicit method. However, in order to guarantee consistency for both parts, the implicit and explicit integrators must fit together. A natural way to construct such methods is to start with an appropriate implicit scheme and extrapolate it in a suitable manner. Promising candidates are singly-implicit Peer methods. In Peer methods, all internal stages in a time step have the same order. The choice of the implicit method as well as the extrapolation provide us with some degrees of freedom that we use to optimize the full implicit-explicit (IMEX) Peer scheme with respect to its stability region and convergence properties. Another advantage of Peer methods is that we can adapt the step-size during the solution process. The goal in further research is to construct IMEX-Peer methods with large stability regions that include an adaptive step-size control.

Partner: W. Hundsdorfer (CWI Amsterdam, The Netherlands)

Contact: M. Schneider, J. Lang

References

[1] J. Lang and W. Hundsdorfer. Extrapolation-based implicit-explicit peer methods with optimised stability regions. *arXiv:1610.00518*, 2016.

Project: Finite element methods for chemotaxis models on networks

Chemotaxis describes the movement of cells and organisms caused by their reaction to chemical gradients. Since the first mathematical investigation of chemotactic phenomena by Keller and Segel, a variety of PDE models has been developed in order to reproduce the main features of population dynamics governed by chemotaxis. This project is concerned with some of these models in a network setting. Existence and uniqueness of global solutions has been considered for the classical Keller-Segel model on a network. A further goal of this project is the determination of appropriate finite element methods for the classical model as well as for some modifications, including hyperbolic models.

Contact: H. Egger, L. Schöbel-Kröhn

Project: Numerical methods for a parabolic-elliptic interface problem

In this project, we want to find and analyze a suitable discretization method for a coupled system of partial differential equations consisting of the model problem for transport in porous media, that is a (possibly convection dominated) parabolic time-dependent diffusion-convection-reaction equation on a bounded domain and a diffusion process on the complement of the domain, modeled by the Laplace equation, which are coupled at the boundary. To approximate such problem the coupling of a method for the interior problem and the boundary element method (BEM) is of particular interest. In this project we want to consider finite element based or vertex-centered finite volume based methods to approximate the interior problem. Because of the possible convection domination in the interior, we have to use stabilized versions: for FEM we apply the streamline upwind Petrov Galerkin (SUPG) method, and for FVM a classical upwind strategy. There are several methods to couple an interior method with BEM, depending on the formulation of the exterior problem and the transmission conditions between the interior and the exterior problem, one such method is the non-symmetric coupling, which has not been analyzed for the time-dependent case and thus is the main focus of this research project.

Contact: R. Schorr, C. Erath

Support: Graduate School Computational Engineering, DFG

Project: A posteriori error estimates for non-symmetric coupling of finite volume and boundary element method

In this project we considered an interface problem often arising in transport problems: a coupled system of partial differential equations with one (elliptic) transport equation on a bounded domain and one equation (in this case the Laplace problem) on the complement, an unbounded domain. Based on the non-symmetric coupling of the finite volume method and boundary element method we introduced a semi-robust residual error estimator and investigated reliability and efficiency. The upper bound turned out to be robust against variation of the model data, the lower bound, however, additionally depends on the Péclet number and is therefore only semi-robust. Still, the results can be used to steer an adaptive refinement algorithm to (heuristically) improve the rate of convergence.

Contact: C. Erath, R. Schorr

Support: Graduate School Computational Engineering, DFG

References

[1] C. Erath and R. Schorr. An adaptive non-symmetric finite volume and boundary element coupling method for a fluid mechanics interface problem. *In press, SIAM J. Sci. Comput.*, 2016.

Project: Inverse problems for incompressible flow

Flow measurements provide an important source of information for the development, calibration, and discrimination of models for fluid flow. While traditional experimental techniques were able to provide only partial information about the flow field, novel measurement modalities such as particle tracking, tomographic particle imaging, or magnetic resonance velocimetry deliver spatially resolved three-dimensional velocity measurements. Like in many other measurement techniques, the measured flow fields are perturbed by a rather large amount of measurement noise which inhibits a use of the results for further investigations. In this project, we utilize specific flow models and methods from inverse problems and optimal control to reconstruct a physically consistent improved flow field that allows for further post-processing [1]. An important point, especially for in vivo applications, is the geometry determination of the actual flow regime. By using suitable a priori information we aim to use the MRV data directly to reconstruct a smooth representation of the flow geometry. To achieve this goal we combine ideas from variational image segmentation/registration, moving mesh techniques and linear elasticity.

Partner: C. Tropea (TU Darmstadt)

Support: DFG IRTG 1529 and Graduate School Computational Engineering, DFG

Contact: T. Seitz, H. Egger

References

[1] H. Egger, T. Seitz, and C. Tropea. Enhancement of flow measurements using fluid-dynamic constraints. *arXiv:1512.08620*, 2015.

Project: Reduced basis method for partial differential equations with random input data

The incorporation of stochastic quantities in numerics increases the complexity in theory and computation. Stochastic methods like stochastic collocation or Monte Carlo require many computationally expensive solutions of the underlying partial differential equation. The reduced basis method approximates the solution on a low-dimensional subspace in order to speed up the calculation and therefore makes stochastic methods feasible. The core of the project is the a posteriori error estimation of the reduced model influenced by random data for time dependent problems.

Support: Graduate School Computational Engineering, DFG

Contact: C. Spannring, S. Ullmann, J. Lang

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

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

Contact: Z. Sun, J. Lang

Project: Wall shear stress measurements using magnetic resonance imaging

The flow of blood in human vessels is of great interest in medicine. A very important physical quantity is the wall-shear stress (WSS) as is its relative contribution along the wall. Unfortunately, the resolution of magnetic resonance imaging (MRI) is too coarse to determine the behavior of the flow in boundary layers. The aim of this project is to use both the MRI measurements and a fluid dynamical model to provide accurate values of the WSS. From a mathematical point of view there arise a couple of problems like computing an appropriate guess on the geometry of the vessels, finding a proper model containing boundary conditions and minimizing the computational effort in the resulting optimization problem. The cardiology group of the Klinik für Radiologie (Universitätsklinikum Freiburg) will provide the MRI data, the SLA Institut (TU Darmstadt) will assess the accuracy of the developed algorithms by comparing the results with laser Doppler velocimetry (LDA) and CFD simulations for some selected test cases.

Partner: A. Bauer, C. Tropea (TU Darmstadt); A. Krafft, W. Buchenberg, J. Hennig (Universitätsklinikum Freiburg)

Support: DFG

Contact: G. Teschner, T. Seitz, H. Egger

References

[1] H. Egger, T. Seitz, and C. Tropea. Enhancement of flow measurements using fluid-dynamic constraints. arXiv:1512.08620, 2015.

Project: POD-Galerkin reduced order modeling with space-adapted snapshots for uncertainty quantification

We investigate reduced order modeling as a means to accelerate statistical estimation for problems governed by PDEs with random data. A set of representative snapshots of the PDE solution are required to build a POD-Galerkin reduced order model. Implementation and analysis usually rely on the property that all snapshots are elements of one and the same discretized space. Regarding accuracy and efficiency, however, it is attractive to compute the snapshots with space-adaptive numerical methods. In this case, each snapshot may belong to a different discretized space, so that conventional methods cannot be applied. This project investigates theoretical and practical consequence that arise from the fact that the snapshot computations are generalized from a fixed discretization space to adapted discretization spaces.

Support: Graduate School Computational Engineering, DFG

Contact: S. Ullmann, J. Lang

References

[1] S. Ullmann, M. Rotkvic, and J. Lang. POD-Galerkin reduced-order modeling with adaptive finite element snapshots. *Journal of Computational Physics*, 325:244–258, 2016.

Project: EWAVE

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

Partner: A. Martin (FAU Erlangen-Nürnberg); G. Leugering (FAU Erlangen-Nürnberg); G. Steinebach (Hochschule Bonn-Rhein-Sieg); O. Kolb (Universität Mannheim); M. Plath (RWW Rheinisch-Westfälische Wasserwerkgesellschaft mbH); O. Kremsier (GreyLogix Aqua); A. Pirsing (Siemens AG, Siemens Industry Automation); R. Rosen (Siemens AG, Siemens Corporate Technology)

Contact: L. Wagner, J. Lang

References

[1] L. Wagner, J. Lang, and O. Kolb. Second order implicit schemes for scalar conservation laws. In *Lecture Notes in Computational Science and Engineering*, volume 112, pages 33–41, 2016.

Project: Adaptive finite element discretization methods for the numerical simulation of static and dynamic contact problems

Due to the non-smooth and nonlinear character of contact problems, the adaptive numerical simulation based on a posteriori estimators is, on the one hand, in great demand but on the other hand, it is a very challenging task.

One of the most common a posteriori error estimators is the standard residual estimator which is directly derived from the equivalence of the norm of the error and the dual norm of the residual. For contact problems this relation is disturbed due to nonlinearity. Thus, additional effort is required to derive an a posteriori error estimator for contact problems. This project deals with the construction and the analysis of efficient and reliable residual-type a posteriori error estimators for the numerical simulation of contact problems. We consider static and dynamic contact problems and a discretization by means of continous finite elements.

Partner: A. Veeser (UNIMI, Italy); R. Krause (USI, Italy)

Contact: M. Walloth

References

[1] R. Krause, A. Veeser, and M. Walloth. An efficient and reliable residual-type a posteriori error estimator for the Signorini problem. *Numerische Mathematik*, 130:151–197, 2015.

[2] M. Walloth and R. Krause. Adaptive numerical simulation of dynamic contact problems. In A. Abdulle, S. Deparis, D. Kressner, F. Nobile, and M. Picasso, editors, *Numerical Mathematics and Advanced Applications 2013*, pages 273–282, Berlin, Heidelberg, 2015. Springer.

Project: Residual-type estimators for a discontinuous Galerkin method for the Signorini problem

This project deals with the construction and the analysis of residual-type a posteriori error estimators for the discontinuous finite element solution of contact problems. In order to obtain an efficient, reliable and localized estimator, the local properties of the discontinuous solution are exploited appropriately. To illustrate the performance of the estimator, the theoretical results are accompanied by numerical studies.

Contact: M. Walloth

References

[1] R. Krause, A. Veeser, and M. Walloth. An efficient and reliable residual-type a posteriori error estimator for the signorini problem. *Numerische Mathematik*, 130:151–197, 2015.

[2] M. Walloth. A reliable, efficient and localized error estimator for a discontinuous galerkin method for the Signorini problem. *Preprint 2713, Fachbereich Mathematik, TU Darmstadt*, 2016.

2 Collaborative Research Projects and Cooperations

The research group 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 154

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

The aim of the TRR 154 is to offer answers to these challenges by using methods of mathematical modelling, simulation, and optimization and, in turn, to provide solutions of increased quality. Novel mathematical findings are required in different areas such as mathematical modelling, numerical analysis, and simulation as well as integer, continuous, and stochastic optimization 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. Furthermore, efficient hierarchical numerical approximation techniques for the resulting algebraically coupled PDEs need to be developed and a sophisticated error control, taking the interaction with the mixed-integer optimization algorithms into account, is required.

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

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

2.2 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 studing engineering applications and to engineering 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, Egger, Lang, Pfetsch, Ulbrich, Wollner) with expertise in Probability Theory and Stochastic Analysis, Mathematical Modeling and Analysis, Numerical Analysis and Scientific Computing, Numerics of Partial Differential Equations, Discrete Optimization, and Nonlinear Optimization and Optimal Control. Four more members of the department are Research Group Leaders (Disser, Erath, Schwartz, Ullmann) with scientific focus on Online Optimization, Numerical Analysis, Discrete-Nonlinear Optimization, and Uncertainty Quantification. Together they supervise more than 10 interdisciplinary PhD projects within the Graduate School in close cooperation with a co-supervisor from Engineering or Computer Science.

2.3 Graduate School of Energy Science and Engineering

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

The optimal strategy to meet this challenge is, on the one hand, to improve conventional energy technologies and render them progressively more efficient to meet the ever more stringent demands on pollutant emissions and, on the other hand, to simultaneously develop innovative, advanced renewable energy technologies which must be brought to a

competitive technological readiness level and provide safe, reliable and cost-effective solutions.
Two professors of the Department of Mathematics are Principal Investigators within the Graduate School Energy Science and Engineering (Lang, Ulbrich) with expertise in Numerical Analysis, Nonlinear Optimization and Optimal Control.

2.4 International Research Training Group IRTG 1529

The International Research Training Group "Mathematical Fluid Dynamics" (IRTG 1529) is funded by the German Research Foundation (DFG) and the Japan Society for the Promotion of Science (JSPS). It is associated with TU Darmstadt and with two universities located in Tokyo, Waseda University and University of Tokyo.
The research of the program focuses on analytical, numerical and stochastic aspects as well as on modeling, optimization and aerodynamics of fluid dynamics. It distinguishes itself through joint teaching and supervision. The core program consists of interdisciplinary lectures and seminars and includes research and study periods in Tokyo. Presently, there are 12 PhD students and 2 Postdocs on the Darmstadt side and a similar amount on the Japanese side.
The principal investigators in Darmstadt are Volker Betz, Dieter Bothe, Herbert Egger, Reinhard Farwig, Matthias Hieber, Ulrich Kohlenbach, Maria Lukáčová, Cameron Tropea, Stefan Ulbrich and Martin Ziegler. The participating colleagues in Tokyo are Tadahisa Funaki, Yoshikazu Giga, Yosuke Hasegawa, Akitoshi Kawamura, Hideo Kozono, Hirofumi Notsu, Yoshihiro Shibata, Masahiro Yamamoto, Masao Yamazaki and Keita Yokoyama.
IRTG 1529 is organizing seminars, short courses, workshops and conferences on a regular basis in Darmstadt and Tokyo. The list of speakers in 2015 and 2016 includes leading experts of the field, e.g., R. Danchin, G.P. Galdi, Th. Gallay, Y. Giga, J. Goldstein, M. Gubinelli, G. Karch, H. Knüpfer, H. Koch, Th. Nguyen, T. Ogawa, J. Prüss, O. Sawada, G. Seregin, G. Simonett, S. Shimizu, V. Solonnikov, R. Takada, M. Tucsnak and H. Weber.
Highlights of the program were altogether 8 conferences or bigger workshops in 2015 and 2016, e.g., the "International Workshops on Mathematical Fluid Dynamics" at Waseda University, Tokyo, in March 2015 and November 2016 and in Darmstadt in April 2015 and November 2016.
The workshop on "Young Researchers in Fluid Dynamics" in June 2015 attracted many PhD students and informed them about various activities of the IRTG.
In addition, a joint workshop between SPP 1506, Transport Processes at Fluidic Interfaces, and the IRTG took place in October 2015 in Darmstadt.

2.5 Scientific and Industrial Cooperations

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

Pia Domschke

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

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

Herbert Egger

– Prof. Dr. Volker Mehrmann (TU Berlin), Arbi M. Badlyan (TU Berlin), Prof. Dr. Christopher Beattie (Virginia Tech, USA): Systematic discretization of differential equations with port-Hamiltonian structure.

– Prof. Dr. Bernd Hofmann (TU Chemnitz): Tikhonov regularization under stability assumptions.

– Dr. Matthias Schlottbom (UT Twente, The Netherlands): Advanced numerical methods for fluorescence optical tomography.

– Prof. Dr. Maria Lukačova (JGU Mainz): Asymptotic-preserving methods.

– Dr. Michaela Kesina, Prof. Dr. Peter Egger (ETH Zürich): Gibbs sampling methods for econometric models with panel data.

– Prof. Dr. Cameron Tropea (TU Darmstadt), Prof. Dr. Jürgen Hennig (Uniklinik Freiburg): Estimation of Wall-Shear Stress from Magnetic Resonance Velocimetry Data (DFG).

– SFB Transregio 154: Mathematische Modellierung, Simulation und Optimierung am Beispiel von Gasnetzwerken, Speaker: Prof. Dr. Alexander Martin (FAU Erlangen).

Christoph Erath

– Prof. Dr. Dirk Praetorius (TU Wien): Adaptive vertex-centered FVM with convergence rates.

– Dr. Günther Of (TU Graz), Francisco-Javier Sayas (University of Delaware, USA): Nonsymmetric FVM-BEM coupling.

– Prof. Dr. Stefan A. Funken (Universität Ulm), Prof. Dr. Dirk Praetorius (TU Wien): Optimal adaptivity for SUPG FEM.

– Dr. Mark A. Taylor (Sandia National Laboratories, USA), Dr. Ramachandran D. Nair (National Center for Atmospheric Research, USA): Multi-tracer efficient transport for CAM.

Alf Gerisch

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

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

- Prof. Dr. Jens Lang (TU Darmstadt), Dirk Schröder (TU Darmstadt), Prof. Dr. Rüdiger Weiner (Universität Halle-Wittenberg), Dr. Helmut Podhaisky (Universität Halle-Wittenberg): Peer methods and their application in the Finite Element system KARDOS.
- Prof. Dr. Jens Lang (TU Darmstadt), Prof. Dr. Florian Müller-Plathe (TU Darmstadt), Prof. Dr. Michael Böhm (TU Darmstadt): Uncertainty quantification in multiscale models of soft matter systems.

Jens Lang

- Prof. Dr. Willem Hundsdorfer (CWI Amsterdam, The Netherlands): IMEX-Peer methods.
- Prof. Dr. Weizhang Huang (University of Kansas, USA), Lennard Kamenski (WIAS Berlin): Anisotropic mesh methods.
- Jun.-Prof. Dr. Oliver Kolb (Universität Mannheim): Simulation and optimization of gas and water networks.
- Prof. Dr. Kristian Debrabant (University of Southern Denmark): Global error estimation and control for semilinear parabolic equations.
- Bodo Erdmann (ZIB): Kardos programming.

Mirjam Walloth

- Prof. Dr. Rolf Krause (University of Lugano): Adaptive finite element discretization methods for the numerical simulation of static and dynamic contact problems.
- Prof. Dr. Andreas Veeser (University of Milan): Adaptive finite element discretization methods for the numerical simulation of static and dynamic contact problems.

3 Publications

3.1 Co-Editors of Publications

3.1.1 Editors of Journals

Alf Gerisch

- *In Silico Cell and Tissue Science* (Associate Editor)

Jens Lang

- *Applied Numerical Mathematics* (Editor)

3.2 Publications in Journals and Proceedings

3.2.1 Journals

[1] A. Borzì, E.-J. Park, and M. V. Lass. Multigrid optimization methods for the optimal control of convection-diffusion problems with bilinear control. *Journal of Optimization Theory and Applications*, 168(2):510–533, 2016.

[2] K. Debrabant and J. Lang. On asymptotic global error estimation and control of finite difference solutions for semilinear parabolic equations. *Computer Methods in Applied Mechanics and Engineering*, 288:110–126, 2015.

[3] P. Domschke, O. Kolb, and J. Lang. Adjoint-based error control for the simulation and optimization of gas and water supply networks. *Applied Mathematics and Computation*, 259:1003–1018, 2015.

[4] H. Egger, F. Kretzschmar, S. M. Schnepp, I. Tsukerman, and T. Weiland. Transparent boundary conditions for a discontinuous Galerkin Trefftz method. *Appl. Math. Comput.*, 267:42–55, 2015.

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[6] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of chemotaxis models with volume-filling. *SIAM J. Appl. Math.*, 75(2):275–288, 2015.

[7] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of nonlinear heat conduction laws. *J. Inverse Ill-Posed Probl.*, 23(5):429–437, 2015.

[8] H. Egger and M. Schlottbom. Numerical methods for parameter identification in stationary radiative transfer. *Comput. Optim. Appl.*, 62(1):67–83, 2015.

[9] H. Egger and M. Schlottbom. A class of Galerkin Schemes for time-dependent radiative transfer. *SIAM J. Numer. Anal.*, 54(6):3577–3599, 2016.

[10] C. Erath. A nonconforming a posteriori estimator for the coupling of cell-centered finite volume and boundary element methods. *Numer. Math.*, 131:425–451, 2015.

[11] C. Erath, G. Of, and F.-J. Sayas. A non symmetric coupling of the finite volume method and the boundary element method. *Numer. Math.*, pages 1–28, published online, 2016.

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3.2.2 Proceedings and Chapters in Collections

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3.3 Preprints

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3.4 Reviewing and Refereeing

Herbert Egger: Mathematical Reviews; Applicable Analysis, Applied Numerical Mathematics, Computers and Mathematics with Applications, Inverse Problems, Inverse Problems in Imaging, Mathematics of Computation, Mathematical Modeling and Numerical Analysis, Mathematical Models and Methods in Applied Sciences, Numerische Mathematik, SIAM Journal on Numerical Analysis, SIAM Journal on Scientific Computing

Christoph Erath: Mathematical Reviews; SIAM Journal on Numerical Analysis, SIAM Journal on Scientific Computing, Numerische Mathematik, Applied Mathematics and Computation, Journal of Computational and Applied Mathematics, Journal of Scientific Computing, Monthly Weather Review, Geoscientific Model Development Discussion, Finite Volumes for Complex Applications VIII

Alf Gerisch: Applied Mathematics and Computation, Computer Methods in Biomechanics and Biomedical Engineering, SIAM Journal on Scientific Computing, Journal of Computational and Applied Mathematics, Journal of Applied Mathematics and Computing, Journal of Mathematical Biology, Journal of Theoretical Biology, Mathematical Biosciences, Journal of the Royal Society Interface, TU Wien "Innovative Projects/Staff", External reviewer in PhD commitee at MOX Group at TU Milan

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 on Analysis, SIAM Journal Scientific on Computing

Mirjam Walloth: Journal of Computational and Applied Mathematics, SIAM Journal on Numerical Analysis

3.5 Software

HOMME: *Integrating Semi-Lagrangian schemes*

A spectral-element dynamical core based on the High-Order Method Modeling Environment (HOMME) framework is the default dynamical core for the Community Atmosphere Model (CAM, version 5.2 and higher) - CAM-SE. The grid system in HOMME is based on the cubed-sphere geometry resulting from a gnomonic equiangular projection of the sphere. It has been shown that this approach is highly scalable, up to 170 000 cores. Atmospheric models used for practical climate simulation must be capable of handling the transport of hundreds of tracers. For computational efficiency, conservative multi-tracer semi-Lagrangian type transport schemes are appropriate. The integration of two schemes, SPELT and CSLAM, and the coupling to the spectral element dynamical core is part of the software contribution.

Contributor at TU Darmstadt: Christoph Erath

FastCOIN: *Fast adaptive stochastic COllocation INfrastructure*

FastCOIN is a software package that implements an adaptive, anisotropic stochastic collocation approach on sparse grids for the quantification of uncertainty in PDEs or other models with random parameters described by finitely many random variables. This includes, in particular, finite-dimensional parametrizations of correlated random fields. Similar to a Monte Carlo simulation, this approach decouples and, hence, parallelizes the stochastic problem into a set of deterministic problems. FastCOIN is able to resolve a stochastic parameter space of dimensions up to $20-50$.

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

KARDOS: *Solving Time-Dependent Partial Differential Equations*

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

Contributor at TU Darmstadt: Jens Lang, Alf Gerisch, Dirk Schröder

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 interfacing known as “reverse communication”). donlp2 is free for research, whereas commercial use requires licensing by TU Darmstadt. In the period under review the technique of taking numerical gradients has been revised again and several minor flaws were removed. Three commercial licenses have been sold during this period and 38 academic (free) licenses were given. For more information, see `www.mathematik.tu-darmstadt.de/fbereiche/numerik/staff/spellucci/DONLP2/`

Contributor at TU Darmstadt: Peter Spellucci

numawww: *Interactive computing exercises for numerical methods and continuous optimization*

Numawww is a cgi/html-based computing device for general numerical methods and methods of continuous optimization. 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 14 newly implemented methods and many other implementations were completely redesigned. There were about 28500 visits in 2013 and 36000 in 2014 compared to 6000 in 2011 and 12000 in 2012. For more information, see numawww.mathematik.tu-darmstadt.de

Contributor at TU Darmstadt: Peter Spellucci

Triangular Taylor Hood finite elements: *Matlab code for mixed P2/P1 finite elements*
This toolbox solves PDE problems with mixed P2/P1 (Taylor Hood) finite elements. The capabilities of the toolbox are demonstrated with an unsteady thermally driven flow in a tall cavity. Introductory examples of a Poisson problem and a Burgers' problem is also available. For more information, see https://de.mathworks.com/matlabcentral/fileexchange/49169.

Contributor at TU Darmstadt: Sebastian Ullmann

4 Theses

4.1 PhD Dissertations

2015

Tiburtius, Sara, *Homogenization for the multiple scale analysis of musculoskeletal mineralized tissues* (Jens Lang)

2016

Rath, Alexander, *Global Error Estimation for Stiff Differential Equations* (Jens Lang)

Schröder, Dirk, *Peer Methods in Optimal Control* (Jens Lang)

4.2 Diplom Theses

2016

Mercan, Necati, *Eine graphische Oberfläche zur Entwicklung geeigneter Zielfunktionen in der Fahrzeugsimulation* (Martin Kiehl)

4.3 Master Theses

2015

Fricke, Mathis, *Characterization of particle size distributions via angular light scattering* (Herbert Egger)

Heeg, Simon, *Mixed finite element methods for the Darcy flow problem* (Herbert Egger)

Kugler, Thomas, *A Finite Element Method for the Damped Wave Equation* (Herbert Egger)

Leja, Jessica Anna, *Numerische Modellierung von Wandelanleihen und ihre Bedeutung für Immobilienunternehmen* (Jens Lang)

Mindt, Pascal, *Ein implizites Box-Verfahren für Transportgleichungen mit Flussumkehr* (Jens Lang)

Radu, Bogdan, *A mixed finite element method for the acoustic wave equation* (Herbert Egger)

Räsch, Sascha Andreas Boris, *A linear direct/iterative solver on bordered block diagonal matrices for circuit simulations* (Herbert Egger)

Rotkvic, Marko, *Reduzierte Basis-Modelle für Adaptive Finite Elemente Lösungen* (Jens Lang)

2016

Althaus, Lea, *On Acoustic Tomography using Paraxial Approximations* (Herbert Egger)

Berg, Viktoria, *Adaptive Schrittweitenkontrolle für IMEX-PEER-Verfahren* (Jens Lang)

Raab, Pia Josephine, *Residuenbasierte Fehlerschätzer für Hindernisprobleme* (Mirjam Walloth)

Ruppert, Simon Moritz, *Adaptive Finite Element Method for Non-Linear Magnetostatics* (Herbert Egger)

Schneider, Moritz, *Numerical methods for parameter dependent eigenvalue problems* (Herbert Egger)

Schöbel-Kröhn, Lucas Wilfried, *Galerkin Approximation and Asymptotic Stability for the Thermistor Problem* (Herbert Egger)

Schorr, Robert, *Adaptive non-symmetric coupling of Finite Volume Method and Boundary Element Method* (Christoph Erath)

Teschner, Gabriel Christian, *Finite-Elemente-Methoden für die Primitive Equations* (Herbert Egger)

4.4 Bachelor Theses

2015

Büttgenbach, Frank Gert, *Differential-algebraic equations with applications to circuit simulation* (Herbert Egger)

Neudert, Maximilian Gerhard, *Finite Volume Method - an introduction to partial differential equations based on a model problem in two dimensions* (Christoph Erath)

Remmel, Patrick, *Parallel-in-Time methods for the solution of ordinary differential equation systems* (Jens Lang)

Sándor, Balázs, *An improved implementation of A Posteriori Error Estimators in the FEM* (Jens Lang)

2016

Hövelmann, Adrian, *A simulation enviroment for modular constructed electrical circuits useing different ODE and DAE-solver* (Martin Kiehl)

Jansen, Erik, *Step size selection in finite differences with application in the sensitivity analysis for ODEs* (Alf Gerisch)

5 Presentations

5.1 Talks and Visits

5.1.1 Invited Talks and Addresses

Pia Domschke

10/12/2015 *Mathematical modelling of cancer invasion: The role of cell adhesion variability*
Workshop on "New Mathematical and Computational Problems involved in Cell Motility, Morphogenesis and Pattern Formation", Isaac Newton Institute for Mathematical Sciences, Cambridge, UK

14/01/2016 *Structured models of cell migration incorporating molecular binding processes*
Applied Analysis Seminar, Heidelberg

07/07/2016 *Adaptive modelling, simulation and optimization of gas and water supply networks*
IGDK1754 Munich – Graz, München

Herbert Egger

10/03/2015 *Finite element methods for saddlepoint problems with applications to Darcy and Stokes flow I*
Waseda Workhop on Mathematical fluid dynamics, Tokyo, Japan

11/03/2015 *Finite element methods for saddlepoint problems with applications to Darcy and Stokes flow II*
Waseda Workhop on Mathematical fluid dynamics, Tokyo, Japan

12/03/2015 *Finite element methods for saddlepoint problems with applications to Darcy and Stokes flow III*
Waseda Workhop on Mathematical fluid dynamics, Tokyo, Japan

13/03/2015 *Finite element methods for saddlepoint problems with applications to Darcy and Stokes flow IV*
Waseda Workhop on Mathematical fluid dynamics, Tokyo, Japan

20/07/2015 *Modeling and Simulation of Gas Flow in Pipes I*
TRR154 Workshop, FAU Erlangen

21/07/2015 *Modeling and Simulation of Gas Flow in Pipes II*
TRR154 Workshop, FAU Erlangen

22/07/2015 *Modeling and Simulation of Gas Flow in Pipes III*
TRR154 Workshop, FAU Erlangen

23/07/2015 *Modeling and Simulation of Gas Flow in Pipes IV*
TRR154 Workshop, FAU Erlangen

24/07/2015 *Modeling and Simulation of Gas Flow in Pipes V*
TRR154 Workshop, FAU Erlangen

18/01/2016 *Variational Methods for Radiative Transfer*
Karlsruhe PDE Seminar, KIT

14/06/2016 *Parameter identification in a semilinear hyperbolic system*
Seminars "Partielle Differentialgleichungen und Inverse Probleme", TU Chemnitz

26/09/2016 *Variational Methods for Radiative Transfer*
Chemnitz FEM Symposium, TU Chemnitz

29/11/2016 *A variational discretization framework for compressible flow in pipeline networks*
Kolloquium AG Modellierung, Numerik, Differentialgleichungen, TU Berlin

02/12/2016 *Kinetic descriptions for particle systems: modelling and numerical approximation*
TRR 146 Retreat, Mainz

Christoph Erath

14/03/2016 *Adaptive Coupling of Finite Volume and Boundary Elements Methods*
Workshop on boundary elements and adaptivity, Universität Basel (Prof. Dr. Helmut Habrecht)

14/10/2015 *Koppeln auf unstrukturierten Gittern – adaptive FVM-BEM*
Mathematisches Kolloquium (Antrittsvorlesung), TU Darmstadt

10/07/2015 *Adaptive Coupling of Finite Volume and Boundary Element Methods*
Kolloquium, 25. Treffen des Rhein-Main Arbeitskreises, TU Darmstadt

09/06/2015 *Adaptive Coupling of Finite Volume and Boundary Element Methods*
Kollquium, Institut für Numerische Mathematik, TU Graz (Dr. Günther Of, Prof. Dr. Olaf Steinbach)

Alf Gerisch

25/06/2015 *A structured population model for cell migration and cell surface-bound processes*
ICMS Workshop on "Computational and multiscale mathematical modelling of cancer growth and spread", Edinburgh, UK

24/07/2015 *Sensitivity Analysis and Quantification of Uncertainty: Method and application in a model of tumour invasion*
Isaac Newton Institute for Mathematical Sciences, Cambridge, UK

11/12/2015 *Nonlocal models for interaction driven cell movement*
Workshop on "New Mathematical and Computational Problems involved in Cell Motility, Morphogenesis and Pattern Formation", Isaac Newton Institute for Mathematical Sciences, Cambridge, UK

19/10/2016 *What is...? Homogenisierung*
What is...? Seminar, Fachbereich Mathematik, TU Darmstadt

Thomas Kugler

20/01/2016 *What is...? Numerische Methoden für turbulente Strömungen*
What is...? Seminar, Fachbereich Mathematik, TU Darmstadt

Jens Lang

15/03/2015 *IMEX Peer Methods with Optimized Stability*
CWI Amsterdam, The Netherlands

03/07/2015 *Ein Schritt Mehr: Von Rosenbrock zu Peer*
Farewell Colloquium in Honour of Prof. Dr. Bernhard A. Schmitt, Marburg

25/07/2016 *Adaptive Modelling, Simulation and Optimization of Water and Gas Supply Networks*
World Congress of Computation Mechanics 2016, Seoul, South Korea

Pascal Mindt

06/07/2016 *What is...? Ein Finite Volumen Verfahren*
What is...? Seminar, Fachbereich Mathematik, TU Darmstadt

Raimondo Penta

25/11/2015 *Asymptotic homogenization for fluid and drug transport in malignant vessels and the impact of microvascular tortuosity on tumor blood flow*
Seminar of the Applied Mathematics & Mathematical Physics Section, Imperial College London, UK

29/09/2015 *Investigation of multiphase composites via asymptotic homogenization and its application to the bone hierarchical structure*
M3TB2015 – Multiscale Models in Mechano and Tumor Biology: Modeling, Homogenization, and Applications, TU Darmstadt

28/08/2015 *Effective governing equations for poroelastic growing media*
Workshop on Porous Media Modelling in Biological Processes: Perspectives on Analytical and Computational Methods Enabling Data Inversion, University of Dundee, UK

Tobias Seitz

13/02/2016 *Filtering distributed flow measurements using fluid-dynamic constraints*
Workshop on Mathematical Analysis for Nonlinear Phenomena, Kanazawa, Japan

22/06/2016 *What is...? Ein schlecht gestelltes Problem*
What is...? Seminar, Fachbereich Mathematik, TU Darmstadt

Sebastian Ullmann

04/12/2015 *Model order reduction with adaptive finite element POD and application to uncertainty quantification*
Seminar in Numerical Analysis, Universität Basel

02/06/2016 *POD-Galerkin reduced-order modeling with adaptive finite element snapshots*
Numerik Kolloquium, Universität Ulm

5.1.2 Contributed Talks

Anke Böttcher

17/11/2016 *Numerical approximation of Allen-Cahn type equations*
Seminar der AG Numerik, TU Darmstadt

Bogdan Radu

23/06/2016 *Mixed finite element methods for the acoustic wave equation*
Seminar der AG Numerik, TU Darmstadt

07/07/2016 *Mixed finite element methods for the acoustic wave equation*
AANMPDE, Strobl

Pia Domschke

23/02/2015 *Modelling the role of adhesion in the heterogeneous dynamics of cancer invasion*
Research Group Workshop Kleinwalsertal, Hirschegg

21/06/2015 *Structured models of cell migration incorporating membrane reactions (Poster)*
ICMS Workshop on "Computational and multiscale mathematical modelling of cancer growth and spread", Edinburgh, UK

28/09/2015 *Structured models of cell migration incorporating membrane reactions (Poster)*
International Workshop of Multiscale Models in Mechano and Tumor Biology, Darmstadt

08/03/2016 *Adaptive Modelling, Simulation and Optimization of Gas and Water Supply Networks*
GAMM/DMV Conference 2016, Braunschweig

12/07/2016 *Adaptive Modelling, Simulation and Optimization of Gas and Water Supply Networks*
7ECM Berlin 2016

Herbert Egger

29/05/2015 *On numerical methods for parameter identification in radiative transfer*
AIP 2015, Helsinki, Finland

16/03/2016 *On enhancement of flow measurements using fluid-dynamic constraints*
Inverse Problems in the Alps, Obergurgl

06/06/2016 *A fictitious domain levelset method for inclusion detection*
ECCOMAS Congress 2016, Crete, Greece

07/07/2016 *Damped wave systems on networks: Exponential stability and uniform approximations*
AANMPDE 2016, Strobl

02/08/2016 *Damped wave systems on networks: Exponential stability and uniform approximations*
HYP 2016, RWTH Aachen

Christoph Erath

15/06/2016 *Adaptive vertex-centered finite volume methods with convergence rates*
MAFELAP 2016 (eingeladen im Minisymposium), Brunel University London, UK

08/03/2016 *A non symmetric FVM-BEM coupling method*
GAMM 2016, Braunschweig

23/10/2015 *A non symmetric FVM-BEM coupling method*
13. Söllerhaus Workshop on Fast BEM in Industrial Applications, Hirschegg, Österreich

24/02/2015 *Finite Volume Method-Coupling-Boundary Element Method*
Research Group Workshop Kleinwalsertal, Hirschegg

Sofia Eriksson

26/02/2015 *Stable Numerical Methods with Boundary and Interface Treatment for Applications in Aerodynamics*
Research Group Workshop Kleinwalsertal, Hirschegg

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

Alf Gerisch

23/02/2015 *A nonlocal model for contact attraction and repulsion in heterogeneous populations*
Research Group Workshop Kleinwalsertal, Hirschegg

23/02/2016 *Can a Continuous Mineral Foam Explain the Stiffening of Aged Bone Tissue?*
Bio-inspired Materials 2016, Potsdam

12/07/2016 *Cross-diffusion in structured models of cancer invasion*
ECMTB 2016, Nottingham, UK

Thomas Kugler

14/04/2016 *Damped Waves on Networks*
Seminar der AG Numerik, TU Darmstadt

07/07/2016 *Structure Preserving Model Reduction for Damped Wave Propagation on Networks*
AANMPDE, Strobl

06/10/2016 *Structure Preserving Model Order Reduction for Damped Wave Propagation on Networks*
Mathematics of Gas Transport, Berlin

Jens Lang

07/09/2015 *On Global Error Estimation and Control for Stiff Initial Values Problems*
NUMDIFF 2015, Halle

15/09/2015 *Higher Order Time Integrators of PEER Type for Parabolic Problems*
ENUMATH 2015, Ankara, Turkey

Axel Ariaan Lukassen

16/06/2016 *Parameter estimation for chemical systems*
Seminar der AG Numerik, TU Darmstadt

04/10/2016 *Parameter estimation for chemical systems*
Reduced Basis Summer School 2016, Hedersleben

Pascal Mindt

09/06/2016 *Finite Volume Methods on Networks*
Seminar der AG Numerik, TU Darmstadt

Christopher Müller

14/04/2015 *The stochastic Galerkin method*
5th Retreat of the GSC CE, Seeheim-Jugenheim

17/08/2015 *Uncertainty Quantification for PDEs with random data – the stochastic Galerkin method*
CE Research Colloquium, TU Darmstadt

14/11/2016 *Stochastic Galerkin finite element discretization of Stokes flow with random viscosity – iterative solvers and preconditioning*
CE Research Colloquium, TU Darmstadt

24/11/2016 *Stochastic Galerkin finite element discretization of Stokes flow with random viscosity – iterative solvers and preconditioning*
Seminar der AG Numerik, TU Darmstadt

18/12/2016 *Conjugate gradient methods for stochastic Galerkin finite element matrices with saddle point structure*
FOMICS Winter School on Uncertainty Quantification, University of Lugano, Italy

Raimondo Penta

07/04/2016 *The role of microvascular tortuosity in tumor transport phenomena*
BAMC2016, Oxford Mathematical Institute, UK

16/09/2015 *Investigation of multiphase composites via asymptotic homogenization and its application to the bone hierarchical structure*
XXII Italian Congress AIMETA2015, University of Genoa, Italy

17/06/2015 *Multiscale modeling and numerical simulations of multiphase elastic composites with discontinuous material properties*
EMI 2015 International Conference, Engineering Mechanics Institute, Stanford University, USA

15/03/2015 *The role of microvascular tortuosity in tumor transport phenomena*
GAMM 2015 International Conference, Lecce, Italy

Moritz Schneider

27/10/2016 *The Contour Method and its applications*
Seminar der AG Numerik, TU Darmstadt

Lucas Wilfried Schoebel-Kroehn

20/10/2016 *Stability and Galerkin Approximation for the Thermistor Problem with Mixed Boundary Conditions*
Seminar der AG Numerik, TU Darmstadt

Robert Schorr

30/06/2016 *Adaptive non-symmetric coupling of Finite Volume and Boundary Element Method*
Seminar der AG Numerik, TU Darmstadt

04/07/2016 *Adaptive non-symmetric coupling of Finite Volume and Boundary Element Method*
9th Workshop on Analysis and Advanced Numerical Methods for Partial Differential Equations (not only) for Junior Scientists (AANMPDE(JS)-9-16), Strobl

18/07/2016 *Adaptive non-symmetric coupling of Finite Volume and Boundary Element Method*
CE Research Colloquium, TU Darmstadt

Tobias Seitz

02/02/2015 *Inverse problems for incompressible flow*
CE Research Colloquium, TU Darmstadt

26/02/2015 *Inverse problems for incompressible flow*
Research Group Workshop Kleinwalsertal, Hirschegg

12/03/2015 *Inverse problems for incompressible flow*
The 11th Japanese-German International Workshop on Mathematical Fluid Dynamics, Waseda University, Japan

14/04/2015 *Flow reconstruction from MRV measurements*
5th Retreat of the GSC CE, Seeheim-Jugenheim

23/05/2015 *Flow reconstruction from MRV measurements*
Mathematical Theory in Fluid Mechanics, Kácov, Czech Republic

23/10/2015 *Flow enhancement using fluiddynamic constraints*
Waseda University, Japan

17/12/2015 *Filtering distributed flow measurements using fluid-dynamic constraints*
Seminar der AG Numerik, TU Darmstadt

04/03/2016 *Filtering distributed flow measurements using fluid-dynamic constraints*
The 12th Japanese-German International Workshop on Mathematical Fluid Dynamics, Waseda University, Japan

15/03/2016 *Filtering distributed flow measurements using fluid-dynamic constraints*
OCIP 2016, TU München

06/06/2016 *An introduction to Lagrange-Galerkin schemes for fluid mechanics*
CE Research Colloquium, TU Darmstadt

30/10/2016 *Enhancement of flow measurements using fluid-dynamic constraints*
The 13th Japanese-German International Workshop on Mathematical Fluid Dynamics, TU Darmstadt

Christopher Spannring

14/04/2015 *The stochastic Galerkin method*
5th Retreat of the GSC CE, Seeheim-Jugenheim

07/09/2015 *Reduced Basis Method for Parametrized Partial Differential Equations*
CE Research Colloquium, TU Darmstadt

15/09/2016 *Reduced Basis Method for Parabolic Problems with Random Data*
SIMAI 2016, Polytechnic University of Milan, Italy

04/10/2016 *Reduced Basis Method for Parabolic Problems with Random Data*
Reduced Basis Summer School 2016, Hedersleben

17/10/2016 *Reduced Basis Method for Parabolic Problems with Random Data*
CE Research Colloquium, TU Darmstadt

01/12/2016 *Reduced Basis Method for Linear Parabolic Problems with Random Data*
Seminar der AG Numerik, TU Darmstadt

18/12/2016 *Reduced Basis Method for Linear Parabolic Problems with Random Data*
FOMICS Winter School on Uncertainty Quantification, University of Lugano, Italy

Zhen Sun

15/03/2016 *Modelling and Stabilization for Low-Mach-Number Reactive Flow*
Seminar of the Platform - Flexible Energy Converters with Low CO_2 Emissions, Graduate School Energy Science and Engineering, TU Darmstadt

20/10/2016 *Adaptive Finite Element Methods for Low-Mach-Number Reactive Flow*
Seminar of the Platform - Flexible Energy Converters with Low CO_2 Emissions, Graduate School Energy Science and Engineering, TU Darmstadt

Gabriel Teschner

15/12/2016 *Finite Element Methods for the Primitve Equations*
Seminar der AG Numerik, TU Darmstadt

Sara Tiburtius

26/01/2015 *Homogenization for the multiple scale analysis of musculoskeletal mineralized tissues*
Seminar der AG Numerik, TU Darmstadt

Sebastian Ullmann

27/02/2015 *Research in uncertainty quantification*
Research Group Workshop Kleinwalsertal, Hirschegg

16/03/2015 *Uncertainty quantification for thermally driven flow (Poster)*
SIAM CSE, Salt Lake City, USA

13/04/2015 *Reduced-order modeling for UQ*
5th Retreat of the Graduate School CE, Seeheim-Jugenheim

26/05/2015 *Natural convection with random boundary conditions: a comparison of techniques*
UNCECOMP 2015, Crete, Greece

10/09/2015 *Space-adaptive POD for a Burgers problem with stochastic data (Poster)*
GAMM AGUQ Workshop on Uncertainty Quantification, Chemnitz

15/10/2015 *POD-Galerkin for finite elements with dynamic mesh adaptivity*
MoRePaS III, Triest, Italy

12/11/2015 *Adaptive finite element POD for uncertainty quantification*
Workshop Direct and Inverse Problems for PDEs with Random Coefficients, WIAS, Berlin

07/04/2016 *POD-Galerkin modeling with adaptive finite elements for stochastic sampling*
SIAM UQ 2016, Lausanne

17/11/2016 *POD-Galerkin reduced-order modeling with adaptive finite element snapshots*
KoMSO Challenge Workshop, Renningen

Lisa Wagner

14/09/2015 *Higher order time discretization for simulation and optimization of water supply networks*
ENUMATH, Ankara, Turkey

09/06/2016 *Second order implicit schemes for solving balance laws with applications to water supply networks*
Seminar der AG Numerik, TU Darmstadt

17/06/2016 *Second order implicit schemes for solving balance laws with applications to water supply networks*
ECMI, Santiago de Compostela, Spain

Mirjam Walloth

29/05/2015 *Adaptive finite element discretization methods for the numerical simulation of static and dynamic contact.*
IV. ICCCM, Hannover

13/06/2016 *Adaptive finite element discretization methods for the numerical simulation of static and dynamic contact.*
Seminar Lehrstuhl für Festkörpermechanik, Uni Siegen

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

5.1.3 Visits

Herbert Egger, Waseda University, Tokyo, Japan, March 2015

Herbert Egger, FAU Erlangen, July 2015

Herbert Egger, ETH Zürich, March 2016

Herbert Egger, TU Chemnitz, June 2016

Herbert Egger, TU Berlin, December 2016

Christoph Erath, TU Wien, August 2016

Christoph Erath, International Centre for Mathematical Sciences, Edinburgh, UK, March 2015

Alf Gerisch, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, July 2015

Alf Gerisch, Isaac Newton Institute for Mathematical Sciences, Cambridge, UK, November - December 2015

Jens Lang, CWI Amsterdam, The Netherlands, March 2015

Tobias Seitz, Waseda University, Tokyo, Japan, October 2015 – March 2016

Mirjam Walloth, Università della Svizzera italiana, Lugano, Italy, April 2016

Mirjam Walloth, Università degli Studi di Milano, Italy, April 2016

6 Workshops and Visitors at the Department

6.1 Guest Talks at the Department

13/01/2015 Prof. Alexander Lorz (UPMC, France), *On mathematical models of mutation selection* (Jan Pietschmann)

22/02/2015 Prof. Dr. Günther Of (TU Graz), *Coupling of discontinuous Galerkin finite element and boundary element methods* (Herbert Egger)

06/07/2015 Prof. Ilaria Perugia, PhD (Universität Wien), *A Plane Wave Virtual Element Method for the Helmholtz Problem* (Christoph Erath)

14/07/2015 Ricardo Pena Hoepner (Universität Mannheim), *Solutions of the Sinh-Gordon Equation of Spectral Genus Two* (Jens Lang)

17/12/2015 Tobias Seitz (University of Tokyo, Japan), *Filtering distributed flow measurements using fluid dynamic constraints* (Herbert Egger)

02/06/2016 Dr. Adriano De Cezaro (Federal University of Rio Grande, Brasil), *Regularization Approaches for Photo-Acoustic Tomography* (Herbert Egger)

15/06/2016 Prof. Dr. Malte Braack (Universität Kiel), *Outflow boundary conditions for the Navier-Stokes equations* (Jens Lang)

11/07/2016 Prof. Dr. Weizhang Huang (University of Kansas, USA), *A new implementation of the MMPDE moving mesh method and applications* (Jens Lang)

03/11/2016 Prof. Dr. Bülent Karasözen (Middle East Technical University, Turkey), *Energy stable model order reduction for the Allen-Cahn equation* (Jens Lang)

10/11/2016 Prof. Dr. Illia Horenko (USI Lugano), *On a direct data-driven reduction of Bayesian models: where applied mathematics meets data* (Jens Lang)

08/12/2016 Prof. Dr. Karsten Urban (Universität Ulm), *Space-Time-Varitionsformulierung für Reduzierte Basis Methoden (RBMs)* (Jens Lang)

6.2 Visitors at the Department

Jeroen Stolwijk (TU Berlin), January 2015.

Dr. Dumitru Trucu (University of Dundee, UK), August 2015.

Jeroen Stolwijk (TU Berlin), August 2015.

Jeroen Stolwijk (TU Berlin), March 2016.

Oliver Kolb (University of Mannheim), June 2016.

6.3 Workshops and Conferences at the Department

– International Workshop M3TB2015 – Multiscale Models in Mechano and Tumor Biology: Modeling, Homogenization, and Applications, September 28-30, 2015 (organized by Alf Gerisch, Raimondo Penta, Jens Lang)

7 Other scientific and organisational activities

7.1 Memberships in Scientific Boards and Committees

Jens Lang

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

7.2 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 printed information material, the department of mathematics presents itself to the public on its web pages. These are clearly structured and provide quick links for several target groups as well as links leading to specific topics in research and teaching at the department.

Math on demand

In April 2015, the mathematics department of TU Darmstadt launched the program *Math on Demand* for mathematically interested secondary school students and mathematics teachers. The purpose of this program 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 mathematical research. Moreover, we aim to inform the secondary school students about the tremendous opportunities for careers in mathematics and about the mathematics program at TU Darmstadt.

By now eight scientists (F. Aurzada, P. Domschke, B. Kümmerer, M. Otto, A.-M. v. Pippich, U. Reif, A. Schwartz, B. Seyfferth) offer thirteen lectures covering a wide variety of topics. In 2015 and 2016, around 20 lectures or workshops were held for a variety of audiences from the Rhein-Main metropolitan area and its surroundings. Further information is available on the webpage

`http://www.mathematik.tu-darmstadt.de/math-on-demand/`

The following is a list of further public relations activities.

Activities for secondary school students and prospective students

- Presentation of the department with a booth and several talks at the job and study information fair HoBIT, Hochschul- und Berufsinformationstage, three days every January: about 20.000 participants; with a booth staffed by professors, academic staff and students and scientific talks from the fields of Geometry, Logic, and Stochastics in 2015 and from the fields of Algebra, Numerical Analysis and Optimization in 2016.
- Annual participation at the information days for female students, “Schnuppertage für Schülerinnen”, with participation at the central event for female students with interest in STEM/MINT programmes and an on-site presentation of the department including a talk by the student advisor, a sample lecture and talks with female mathematicians, about 30 participants in each year (organization: Dr. Alfes in 2015 and Dr. Wagner in 2016; lectures from the field of Algebra in 2015 and from the field of Numerical Analysis in 2016).
- Support of the annual organization of the Mathematikolympiade Hessen (third level) in cooperation with the Center for Mathematics Bensheim for all grades (about 20 participants per grade each year) (Prof. Kiehl, academic staff and students).
  In the recent years, the department had the opportunity to host the finals. Mathematical afternoon lectures were delivered by Prof. Kiehl and Prof. Aurzada (2015) and Prof. Kiehl and Prof. Scheithauer (2016).
- Organization of the Mathematical Modeling Week for secondary school students in grade 12 in cooperation with Center for Mathematics Bensheim each October (40 participants each year) (Prof. Kiehl).

Contact

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