Biannual Report

Department of Mathematics
Research Group Numerical Analysis and Scientific Computing
2013 and 2014

TECHNISCHE UNIVERSITÄT DARMSTADT

General Remark

This document contains a subset of the information of the Biannual Report of the Department of Mathematics at TU Darmstadt for 2013 and 2014. 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, November 2015

Contents

1 Research Groups

This section gives a brief overview of the research done in the eight research groups.

1.1 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 in fluid dynamics and non-destructive testing, in modeling and simulation of radiative transfer phenomena, in acoustic and optical tomography, in the modeling, simulation, and characterization of ion channels and nanopores, in simulation of transient electromagnetic phenomena, or 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 of novel discretization schemes for wave propagation problems, the design and analysis of a-posteriori error estimates, the construction of asymptotic preserving numerical schemes, and the design of physically consistent discretization schemes.

The research group *Numerical Analysis and Scientific Computing* is engaged among others in the Excellence Cluster EXC 259 Center of Smart Interfaces, the Graduate Schools (Excellence Initiative) GSC 233 Computational Engineering and GSC 1070 Energy Science and Engineering, the Graduate School GSC 1344 Instationary System Modelling for Aircraft Turbines, 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 BASF Ludwigshafen and Infineon München.

Members of the research group

Professors

Herber Egger, Christoph Erath, Martin Kiehl, Jens Lang

Retired professors

Peter Spellucci

Postdocs

Debora Clever, Pia Domschke, Sofia Eriksson, Alf Gerisch, Michelle Lass, Raimondo Penta, Jan-Frederik Pietschmann, Matthias Schlottbom, Mirjam Walloth

Research Associates

Matthias Frankenbach, Karen Kuhn, Axel Ariaan Lukassen, Alexander Rath, Bettina Schieche, Dirk Schröder, Tobias Seitz, Zhen Sun, Sara Tiburtius, Sebastian Ullmann, Lisa Wagner

Secretaries

Elke Dehnert, Sigrid Hartmann, Anke Utecht

Project: Non-Local Effects and Surface-Bound Reactions in Cancer Invasion

The ability to invade tissue and form metastases (secondary tumours) is what makes cancer so dangerous. Key biological processes occurring during invasion are the secretion of matrix degrading enzymes, cell proliferation, the loss of cell-cell adhesion on one hand and enhanced cell-matrix adhesion on the other hand as well as active migration. A better understanding of the effect that biochemical (intracellular) and cellular processes have on tissue scale rearrangement of cells and matrix may help to develop treatment strategies. Hence, the modelling and numerical simulation of cancer cell invasion is of great interest and is the subject of ongoing research. In this project, we focus on two key aspects in the modelling of cancer invasion: cell-cell and cell-matrix adhesion and surface-bound reactions (tissue-level modelling).

Partner: M. A. J. Chaplain (University of Dundee, Scotland); D. Trucu (University of Dundee, Scotland)

Support: DFG Research Fellowship (DO 1825/1-1), Northern Research Partnership PECRE Scheme

Contact: P. Domschke, A. Gerisch

References

[1] P. Domschke, D. Trucu, A. Gerisch, and M. A. J. Chaplain. Mathematical modelling of cancer invasion: Implications of cell adhesion variability for tumour infiltrative growth patterns. *Journal of Theoretical Biology*, 361:41–60, 2014.

[2] P. Domschke, D. Trucu, A. Gerisch, and M. A. J. Chaplain. Structured models of cell migration incorporating membrane reactions. Submitted, 2014.

Project: Adaptive Dynamical Multiscale Methods

The flow of gas through pipelines is of great interest in the engineering community. There are many challenges of 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 extend. 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. Domschke, J. Lang

References

[1] P. Domschke, B. Geißler, O. Kolb, J. Lang, A. Martin, and A. Morsi. Combination of nonlinear and linear optimization of transient gas networks. *INFORMS J. Comput.*, 23(4):605–617, 2011.

[2] P. Domschke, O. Kolb, and J. Lang. Adjoint-based control of model and discretisation errors for gas flow in networks. *Int. J. Math. Model. Numer. Optim.*, 2(2):175–193, 2011.

[3] P. Domschke, O. Kolb, and J. Lang. Adjoint-based error control for the simulation and optimization of gas and water supply networks. Submitted, 2014.

[4] O. Kolb, J. Lang, and P. Bales. An implicit box scheme for subsonic compressible flow with dissipative source term. *Numer. Algorithms*, 53(2):293–307, 2010.

Project: Hierarchical Galerkin methods for hyperbolic problems with parabolic asymptotics

This project is part of the Transregional Collaborative Research Centre TRR 154 *Mathematical modelling, simulation and optimization of gas networks*, and deals with the construction and analysis of numerical methods for singularly perturbed hyperbolic problems with parabolic limit. The main goal is to devise efficient asymptotic preserving numerical schemes 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, J. Lang

References

[1] H. Egger and M. Schlottbom. Diffusion asymptotics for linear transport with low regularity. *Asymptotic Analysis*, 89:365–377, 2014.

[2] O. Kolb, J. Lang, and P. Bales. An implicit box scheme for subsonic compressible flow with dissipative source term. *Numer. Algorithms*, 53(2):293–307, 2010.

Project: Finite element methods for coupled volume-surface reaction-diffusion problems

This project deals with the development of asymptotic preserving numerical schemes for the simulation of reaction-diffusion processes acting in the volume and at the boundary simultaneously. Such applications arise in the modeling of biological systems, e.g., in cell metabolism. A key ingredient in the design of proper numerical schemes is the conservation of mass and the guarantee of positivity on the discrete level. Based on analytical considerations, long-term stability and exponential convergence to equilibrium can be obtained.

Partner: Tang Quoc Bao and Klemens Fellner (KFU Graz)

Support: Project within IGDK 1754, Munich/Graz

Contact: H. Egger

References

[1] T. Q. Bao, K. Fellner, and S. Rosenberger. A reaction-diffusion system modelling asymmetric stem-cell division: existence, uniqueness, numerical simulation and rigorous quasi-steady-state approximation. Technical report, KFU Graz, 2014.

Project: On finite element methods for modified Allen-Cahn equations

This project deals with the numerical simulation of modified Allen-Cahn equations that arise in the modelling of phase transitions in elastic bodies. The main goal is to devise stable numerical schemes that obey an energy dissipation law which is valid, at least for simplified models, on the continuous level. Convergence and asymptotic stability of the schemes are investigated.

Contact: A. Böttcher, H. Egger

References

[1] H.-D. Alber and P. Zhu. Comparison of a rapidely converging phase field model for interfaces in solids with the Allen-Cahn model. *J. Elast.*, 111:153–221, 2013.

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

Project: Discontinuous Galerkin Trefftz approximations for Maxwell's equations

The project aims at the construction and numerical analysis of discontinuous Galerkin methods for the time-dependent Maxwell equations utilizing Trefftz polynomials. A systematic construction of a basis for the Trefftz polynomials is provided and a particular basis consisting of polynomial plane waves is constructed. The latter can be utilized to formulate new types of absorbing boundary conditions. Stability and convergence of the numerical schemes is investigated.

Partner: I. Tsukerman (Akron) and S. M. Schnepp (ETH Zürich)

Support: GSC 233 Computational Engineering, TU Darmstadt

Contact: H. Egger, F. Kretzschmar

References

[1] H. Egger, F. Kretzschmar, S. Schnepp, I. Tsukerman, and T. Weiland. Transparent boundary conditions in a discontinuous Galerkin Trefftz method. Technical report, TU Darmstadt, October 2014. arXiv:1410.1899.

[2] H. Egger, F. Kretzschmar, S. M. Schnepp, and T. Weiland. A space-time discontinuous Galerkin Trefftz method for time dependent Maxwell's equations. Technical report, TU Darmstadt, December 2014. arXiv:1412.2637.

[3] F. Kretzschmar, F. Ahmadi, N. Nowak, S. M. Schnepp, I. Tsukerman, H. Egger, and T. Weiland. Trefftz absorbing boundary conditions in analytical, discontinuous Galerkin and finite difference form. *ICEAA*, pages 176–177, 2014.

Project: Inverse problems in nonlinear diffusion processes

The project deals with identification of unknown parameter functions in non-linear parabolic and elliptic diffusion problems. Such inverse problems arise, e.g., in the modeling of biological systems, where the identification can be considered a learning process about the system under investigation. Questions of uniqueness and stability are discussed and numerical methods are proposed for a stable solution.

Partner: M. Schlottbom (Universität Münster)

Support: DFG PI 1073/1-1

Contact: H. Egger, J.-F. Pietschmann

References

[1] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of chemotaxis models with volume-filling. *SIAM J. Appl. Math.*, 75:275–288, 2014.

[2] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of nonlinear heat conduction laws. *J. Inv. Ill-Posed Probl.*, published online, 2014.

[3] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Numerical identification of a nonlinear diffusion law via regularization in Hilbert scales. *Inverse Problems*, 30:025004, 2014.

[4] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Simultaneous identification of diffusion and absorption coefficients in a quasilinear elliptic problem. *Inverse Problems*, 30:035009, 2014.

Project: Inverse free boundary value problems

Free boundary value problems arise in the modeling of various physical phenomena, e.g., in the melting of ice, in population dynamics, but also in biological applications like wound healing. The goal of this project is to utilize observations of the physical state in order to determine unknown model parameters, e.g., nonlinear diffusion or source terms. Questions of uniqueness and stability in the identification process are discussed and numerical methods are proposed for an efficient solution.

Partner: M. Yamamoto (University of Tokyo) and Yuki Kaneko (Waseda University, Tokyo)

Support: DFG IRTG 1529

Contact: H. Egger, J.-F. Pietschmann

References

[1] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Simultaneous identification of diffusion and absorption coefficients in a quasilinear elliptic problem. *Inverse Problems*, 30:035009, 2014.

[2] Y. Kaneko. Spreading and vanishing behaviors for radially symmetric solutions of free boundary problems for reaction-diffusion equations. *Nonlinear Anal. Real World Appl.*, 18:121–140, 2014.

[3] Y. Kaneko and Y. Yamada. A free boundary problem for a reaction-diffusion equation appearing in ecology. *Adv. Math. Sci. Appl.*, 21(2):467–492, 2011.

Project: Gibbs sampling for spatial probit models

Probit and logit models are basic tools in econometrics to describe observable quantities governed by an underlying market model. Spatial models take into account dependence of distance, e.g., between customers or companies. One of the key questions in spatial probit/logit is the inference of model parameters from indirect observations of the underlying process. This can be accomplished, e.g., in the framework of Bayesian inference. To obtain information about the posterior distributions of the parameters of interest, very high dimensional nonlinear problems have to be solved. This can be circumvented by stochastic sampling, i.e., by computing samples of the posterior in an efficient way. The aim of the project is to investigate Gibbs sampling strategies for Baysian inference in spatial probit and logit models.

Partner: P. Egger, M. Kesina (ETH Zürich)

Contact: H. Egger

References

[1] H. Badinger and P. Egger. Estimation of higher-order spatial autoregressive cross-section models with heteroscedastic disturbances. In *Papers in Regional Science*, volume 90, pages 213–235. Wiley Blackwell, 2011.

Project: FVM-BEM coupling for parabolic-elliptic interface problems

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. The next step will be to extend this methodology to problems of other types, 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 posteriori error estimates and adaptive mesh refinement for the coupling of the finite volume method and the boundary element method. *SIAM Journal on Numerical Analysis*, 51(3):1777–1804, 2013.

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 this diversity of elastic function is achieved by only one common building unit, that is the mineralized collagen fibril, but 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 in Darmstadt 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 (LIB), 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. 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? Technical report, accepted for publication in Acta Biomaterialia, 2014.

[2] S. Tiburtius, S. Schrof, F. Molnár, P. Varga, F. Peyrin, Q. Grimal, K. Raum, and A. Gerisch. On the elastic properties of mineralized turkey leg tendon tissue: multiscale model and experiment. *Biomechanics and Modeling in Mechanobiology*, 13(15):1003–1023, 2014.

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

Biological processes like the invasion of tissue by cancer cells, or the adhesion-driven reorganisation of tissue, or the cascade of steps in fracture healing can be modelled 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 Dundee, Scotland); K. J. Painter (Heriot-Watt University, Edinburgh, Scotland); L. Geris (University of Liège, Belgium)

Contact: A. Gerisch

References

[1] P. Domschke, D. Trucu, A. Gerisch, and M. A. J. Chaplain. Mathematical modelling of cancer invasion: Implications of cell adhesion variability for tumour infiltrative growth patterns. *Journal of Theoretical Biology*, 361:41–60, 2014.

[2] K. Painter, J. Bloomfield, J. Sherratt, and A. Gerisch. A nonlocal model for contact attraction and repulsion in heterogeneous populations. Technical report, submitted to Bulletin of Mathematical Biology, 2014.

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: Weizhang Huang (University of Kansas, USA); Lennard Kamenski (WIAS Berlin)

Contact: J. Lang

References

[1] W. Huang, L. Kamenski, and J. Lang. Adaptive finite elements with anisotropic meshes. In A. C. et al., editor, *Numerical Mathematics and Advanced Applications 2011: Proceedings of ENUMATH 2011, the 9th European Conference on Numerical Mathematics and Advanced Applications, Leicester, September 2011*. Springer, 2013.

[2] W. Huang, L. Kamenski, and J. Lang. Stability of explicit Runge-Kutta methods for finite element approximation of linear parabolic equations on anisotropic meshes. Technical Report 1869, WIAS Berlin, 2013.

Project: Large Eddy Simulation on Moving Meshes

This project is concerned with an automated adaptive mesh design approach for Large Eddy Simulation (LES) of turbulent flows. Based on a dynamic moving mesh partial differential equation (MMPDE), a fixed number of grid points is redistributed according to statistical quantities of interest (QoI) selected to capture certain mean flow properties. Physically motivated LES-specific QoI, as the time-averaged gradient of streamwise velocity and the production rate, as well as more general QoI derived from the dual weighted residual method (DWRM) for time-averaged statistics are investigated for a flow over periodic hills with Re = 10 595. The numerical results compared to a highly resolved LES reference solution show the high potential of moving mesh methods to efficiently improve the resolution of turbulent flow features.

Partner: Claudia Liersch (TU Dresden); Jochen Fröhlich (TU Dresden)

Support: DFG SPP 1276 MetStröm

Contact: J. Lang

References

[1] C. Hertel, M. Schümichen, J. Lang, and J. Fröhlich. Using a moving mesh pde for cell centres to adapt a finite volume grid. *Flow, Turbulence and Combustion*, 90:785–812, 2013.

[2] C. Liersch, M. Frankenbach, J. Lang, and J. Fröhlich. Recent progress in designing moving meshes for complex turbulent flows. *Meteorologische Zeitschrift*, 23:425–439, 2014.

[3] S. Ullmann, S. Löbig, and J. Lang. Adaptive large eddy simulation and reduced-order modeling. In J. Janicka, A. Sadiki, M. Schäfer, and C. Heeger, editors, *Flow and Combustion in Advanced Gas Turbine Combustors*, Fluid Mechanics and Its Applications. 2013.

Project: Adaptive Multilevel Methods for PDAE-Constrained Optimal Control Problems

The main goal of this project is to develop a fully adaptive optimization environment, suitable to solve complex optimal control problems of practical interest, which are restricted by partial differential algebraic equations (PDAEs) and pointwise constraints on control and state. The environment relies on continuous adjoint calculus, coupling our fully space- time adaptive PDAE solver KARDOS, highly efficient optimization techniques, and a multilevel strategy which tailors the grid refinement to the optimization progress. Controlling the inconsistencies caused by inexact reduction, the multilevel strategy ensures global convergence of the finite dimensional control iterates to a stationary point of the infinite dimensional problem.

Partner: Stefanie Bott (TU Darmstadt); Stefan Ulbrich (TU Darmstadt); Debora Clever (Ruprecht-Karls-Universität Heidelberg)

Support: DFG SPP 1253 "Optimization with Partial Differential Equations"

Contact: J. Lang, D. Schröder

References

[1] S. Bott, D. Clever, J. Lang, S. Ulbrich, C. Ziems, and D. Schröder. On a fully adaptive SQP method for PDAE-constrained optimal control problems with control and state constraints. In G. Leugering, P. Benner, S. Engell, A. Griewank, H. Harbrecht, M. Hinze, R. Rannacher, and S. Ulbrich, editors, *Trends in PDE Constrained Optimization*, International Series of Numerical Mathematics. Springer Basel AG, 2014.

[2] D. Clever, J. Lang, and D. Schröder. Model hierarchy based optimal control of radiative heat transfer. *International Journal of Computational Science and Engineering*, 9:509–525, 2014.

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

Project: 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 is 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: Roland Herzog (TU Chemnitz)

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

Contact: M. Lass (Vallejos)

References

[1] C. Gräser and R. Kornhuber. Multigrid methods for obstacle problems. *J. Comput. Math.*, 27(1):1–44, 2009.

[2] R. Herzog and C. Meyer. Optimal control of static plasticity with linear kinematic hardening. *Journal of Applied Mathematics and Mechanics*, 91(10):777–794, 2011.

[3] M. Hintermüller and I. Kopacka. A smooth penalty approach and a nonlinear multigrid algorithm for elliptic mpecs. *Comput. Optim. App.*, 50:111–145, 2011.

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

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

Contact: A. Lukassen, M. Kiehl

References

[1] S. Franz. *Modellierung und Simulation reaktionskinetischer Prozesse mit Hilfe dynamisch angepasster quasi-stationärer Zustände*. Logos Verlag Berlin, 2003.

Project: Global Error Estimation for Stiff Systems of Ordinary Differential Equations

Modern solvers for ordinary differential equations gain in efficiency by adaptively optimizing their grids based on local error control. However, the accuracy imposed by the user applies to the global error of the approximation. If the conditioning of the considered system is bad, a local error control alone should not be trusted and estimates on the global errors are required. In the literature, reliability of existing global error estimates from the theory on ordinary differential equations is proven only in the non-stiff case. Nevertheless, for the various examples of stiff systems, e.g., appearing subproblems in the method of lines for partial differential equations of parabolic type or equations describing chemical reactions, reliability of the estimates can be questioned. In this project we focus on efficient and reliable estimation and control of the global errors for stiff differential equations. We estimate the global errors by solving linearized error transport equations. For global error control we use the property of tolerance proportionality. Due to the stiffness of the considered problems, our strategies are based on the concepts of B-stability and B-convergence. We propose two choices of continuous extensions and give a proof for asymptotic correctness of the associated estimators.

Partner: K. Debrabant (University of Southern Denmark, Odense, Denmark)

Contact: A. Rath, J. Lang

References

[1] K. Debrabant and J. Lang. On global error estimation and control of finite difference solutions for parabolic equations. *ArXiv e-prints*, 2009.

[2] J. Lang and J. G. Verwer. On global error estimation and control for initial value problems. *SIAM Journal on Scientific Computing*, 29:1460–1475, 2007.

Project: Fully adaptive linearly implicit peer methods

In [1] linearly-implicit two-step peer methods are sucessfully applied in the numerical solution of time-dependent partial differential equations. The computations were performed adaptive in time, but on a fixed spatial grid. However problems like the propagation of flame fronts are solved more efficiently when solved both adaptive in time and space. This project addresses the fully adaptive solution of PDEs with linearly-implicit peer methods. We first discretize in time with linearly implicit peer methods and then discretize in space with linear finite elements. The error in time is estimated by an embedded solution of lower order, while the spatial error is estimated by the DLY error estimator based on hierarchical bases. It can be shown, that the derived spatial error estimator is efficient and reliable. Numerical experiments for several nonlinear test problems show the potential benefit of linearly-implicit two-step peer methods compared to traditional Rosenbrock methods.

Contact: D. Schröder, J. Lang

References

[1] A. Gerisch, J. Lang, H. Podhaisky, and R. Weiner. High-order linearly implicit two-step peer-finite element methods for time-dependent pdes. *Applied Numerical Mathematics*, 59:624 – 638, 2009.

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. Magnetic Resonance Velocimetry [1] allows to obtain fully three dimensional, time-averaged measurements of the flow field in a single measurement process. Like in many other measurement techniques, the measured flow fields are perturbed by a rather large amount of measurement noise which inhibits a direct 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 and can be used to deduce the required information. The reconstruction process is formulated as an inverse problem which can be cast into an optimization problem with pde constraints. This inverse problem is studied from a theoretical point of view, uniqueness and stability issues are investigated, but also numerical methods for its efficient solution are proposed and analyzed. The results obtained in this project will be used for the characterization of flow regimes and in the design of heat exchangers.

Partner: F. Wassermann, MRV Group, CSI, TU Darmstadt

Support: DFG IRTG 1529 and GSC 233

Contact: T. Seitz, H. Egger

References

[1] C. Elkin, M. Markl, N. Pelc, and J. Eaton. 4d magnetic resonance velocimetry for mean velocity measurements in complex turbulent flows. *Experiments in Fluids*, 34:494 – 503, 2003.

Project: Adaptive Large Eddy Simulation for Flexible Energy Converter

The aim of this project is to develop robust numerical methods for improving combustion technologies with respect to efficiency, emissions and stability of aircraft engines and gas turbines. Nowadays, the design of smart energy networks, electrical power systems and flexible energy converters strongly demands for accuracy and reliability of the modeled process. Such dynamic and multi-physics systems are usually modeled by coupled time-dependent PDEs and ODEs as well as algebraic equations on computational grids. Since multi-physics models exhibit a wide range of space and time scales, this kind of simulations is always time-consuming and in the worst case scenario the corresponding computations are not even capable using traditional numerical simulation algorithms. Therefore, adaptive discretization methods are commonly recognized as an effective approach in the numerical solution of such complex systems. To obtain a more accurate and robust result from the complicated simulations, our research will focus on recent developments in the field of adaptive moving mesh methods based on the dual weighted residual error estimation for the large eddy simulation of a chemical reactive flow.

Partner: C. Sehrt (TU Darmstadt); S. Ulbrich (TU Darmstadt); S. Doost (GSC Energy Science and Engineering, TU Darmstadt); J. Janicka (GSC Energy Science and Engineering, TU Darmstadt)

Support: DFG Excellence Initiative, Darmstadt Graduate School of Excellence Energy Science and Engineering (GSC 1070)

Contact: Z. Sun, J. Lang

References

[1] S. Ullmann, S. Löbig, and J. Lang. Adaptive large eddy simulation and reduced-order modeling. In J. Janicka, A. Sadiki, M. Schäfer, and C. Heeger, editors, *Flow and Combustion in Advanced Gas Turbine Combustors*, Fluid Mechanics and Its Applications. 2013.

Project: Reduced-order modeling for incompressible flows with stochastic boundary conditions

We investigate POD-Galerkin reduced-order modeling in the context of statistical estimation for incompressible flows with uncertain boundary data. The stochastic collocation on sparse grids is a standard method to solve such problems. The method relies on the numerical solutions of deterministic equations for a possibly large set of collocation points contained in a multi-dimensional parameter domain. By replacing a full-order finite element model with a reduced-order POD-Galerkin model a considerable acceleration can be achieved. In order to accurately represent the stochastic boundary data in the reduced-order model we provide an extension to previously available techniques.

Support: DFG SPP 1276 "MetStröm: Skalenübergreifende Modellierung in der Strömungsmechanik und Meteorologie", 2013; DFG Graduate School of Excellence Computational Engineering, TU Darmstadt, 2014

Contact: S. Ullmann, J. Lang

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 will be tested at the Rheinisch-Westfälischen Wasserwerkgesellschaft (RWW). A management system allows to compute optimal operation plans for the constructions of the water production, the water preparation and the water distribution. Additionally, the system should also manage to decide if self-generated energy is used or purchased from energy supply companies. Mathematically, we want to develop new dynamic simulation and optimization models for transport processes in water distributions under consideration of procedural constructions of the water supply with continuously dynamic multi-scale methods for time behaviour and modeling depth.

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

Contact: L. Wagner, J. Lang

References

[1] P. Domschke, O. Kolb, and J. Lang. Computational optimization and applications in engineering and industry. *Studies in Computational Intelligence, chapter Adjoint-based control of model and discretization errors for gas and water supply networks*, 359, 2011.

[2] O. Geissler, O. Kolb, J. Lang, G. Leugering, A. Martin, and A. Morsi. Mixed integer linear models for the optimization of dynamical transport networks. *Mathematical Methods of Operations Research*, 73, 339–362.

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

Often, in the numerical simulation of real world problems, e.g., arising from mechanics or biomechanics, precise information about the regularity of the solution cannot be obtained easily a priori. In fact, the solution may be more or less regular in different regions of the computational domain and even singularities may occur. In this case, increasing the number of degrees of freedom within or close to a critical region of low regularity can improve the overall accuracy of the numerically obtained approximation. The detection of such a critical region can be made feasible by using a posteriori error estimators which do not rely on any additional regularity assumptions. 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 the non-linearity. 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 different discretization methods.

Partner: A. Veeser (University of Milan, Italy); R. Krause (USI Lugano, Switzerland)

Contact: M. Walloth

References

[1] P. Hild and S. Nicaise. Residual a posteriori error estimators for contact problems in elasticity. *M2AN Math. Model. Numer. Anal.*, 41(5):897–923, 2007.

[2] 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.

[3] K. Moon, R. Nochetto, T. von Petersdorff, and C. Zhang. A posteriori error analysis for parabolic variational inequalities. *M2AN Math. Model. Numer. Anal.*, 41(3):485–511, 2007.

[4] A. Veeser. Efficient and reliable a posteriori error estimators for elliptic obstacle problems. *SIAM J. Numer. Anal.*, 39(1):146–167, 2001.

[5] M. Walloth. *Adaptive numerical simulation of contact problems: Resolving local effects at the contact boundary in space and time.* PhD thesis.

[6] 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. Springer, Berlin, Heidelberg, 2015.

Project: Discontinuous Galerkin methods for variational inequalities

This project deals with the numerical solution of variational inequalities by discontinuous Galerkin methods. Advantages and disadvantages of different methods are investigated and a-priori as well as a-posteriori error estimates are established. The application to obstacle and simplified friction problems will be investigated.

Contact: H. Egger, M. Walloth

References

[1] T. Gudi and K. Porwal. A posteriori error control of discontinuous Galerkin methods for elliptic obstacle problems. *Math. Comp.*, 83:579–602, 2014.

[2] F. Wang, W. Han, and X. Cheng. Discontinuous Galerkin methods for solving elliptic variational inequalities. *SIAM Journal of Numerical Analysis*, 48:709–733, 2010.

2 Collaborative Research Projects and Cooperations

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

2.1 Center of Smart Interfaces

The Center of Smart Interfaces (CSI) started as a Cluster of Excellence (EXC 259), funded by the German Research Foundation (DFG). The DFG funding period began in November 2008 and lasted until October 2014, having a total volume of about € 42 million. From November 2014 on, the Center of Smart Interfaces continues as one of the Research Clusters of the TU Darmstadt.

The CSI is an international center for interdisciplinary research, focusing on the scientific areas “static and dynamic wettability”, “heat and mass transfer enhancement”, “near wall reactive flows”, “near wall multiphase flows” and “drag and circulation control” with the aim to understand and design fluid boundaries.

The CSI has 24 Principal Investigators, combining the expertise of the departments of Mechanical Engineering, Physics, Chemistry, Mathematics, and Material Sciences at the TU Darmstadt with four non-University research institutes in Darmstadt and Mainz. In addition, six research professors and three young research group leaders were newly appointed at the Cluster of Excellence.

With the four Principal Investigators Reinhard Farwig, Matthias Hieber, Jens Lang and Stefan Ulbrich and the two newly appointed professors Dieter Bothe and Jürgen Saal, the Department of Mathematics is strongly involved in the CSI. Scientifically, mathematics also plays an eminent role for the fundamental research in all of the above mentioned areas which is performed at the CSI. The involved mathematical disciplines are Mathematical Modeling, Analysis of Partial Differential Equations, Numerical Analysis, and Optimization. This enables relevant contributions to the understanding of continuum mechanical flow models via their mathematical analysis, numerical simulation and the solution of inverse problems such as the optimization concerning complex model parameters.

In 2014, Jürgen Saal obtained and accepted an offer for a full professorship at the Heinrich-Heine Universität Düsseldorf. At least partly, this offer was due to the interdisciplinary expertise which Jürgen Saal had gained during his time at the CSI - a strong proof of the success of the interdisciplinary concept.

The CSI was also involved in several activities in mathematics, the most prominent one in the report period being the co-funding and co-organization of the International Conference on Numerical Methods in Multiphase Flows (ICNMMF-II) hold in Darmstadt June 2014. This outstanding event with main speaker including H. Jasak, D. Juric, S. Popinet, A. Prosperetti, M. Shashkov, M. Sussman, S. Takagi and B. van Wachem attracted about 150 participants.

2.2 Collaborative Research Centre Transregio TRR 154

The Collaborative Research Centre Transregio TRR 154 “Mathematical Modelling, Simulation and Optimization Using the Example of Gas Networks” was established in 2014. 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 contacts 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, and Ulbrich 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`.

2.3 Graduate School of Computational Engineering

Computational Engineering (CE) denotes computer based modeling, analysis, simulation, and optimization. It is a cost-effective, efficient and complementary approach to study engineering applications and to engineer new technical solutions when experimental investigations are too complex, risky, or costly. CE enables the creation of scalable models to support research, development, design, construction, evaluation, production, and operation of engineering applications which address key issues in future technology developments for the economy and society in areas such as energy, health, safety, and mobility. However, such engineering applications are becoming increasingly complex. Consequently, the theory and methodologies required to investigate corresponding systems become challenging.
With the Graduate School of Computational Engineering, TU Darmstadt was able to further strengthen its role in CE. The school enables highly talented PhD students to develop their scientific skills in a focused way, and to cooperate under optimal conditions in a highly

stimulating interdisciplinary environment based on the interaction of Computer Science, Mathematics, and Engineering Sciences. Partnerships with well established research organizations as well as cooperation with industry increase the impact of the Graduate School. Building on the well established interdepartmental expertise at TU Darmstadt, the Graduate School focusses on the following key research areas: modeling and simulation of coupled multi-physics problems, simulation based optimization, and hierarchical multi-scale modeling and simulation. The research efforts in the above fields are accompanied by corresponding developments of methods of visualization, simulated reality, high-performance computing, verification and validation, as well as software engineering and lifecycle research. The PhD students work together within research foci comprising one or more of the above topics. The joint research on specially defined use cases will further strengthen the interdisciplinary skills and cooperation.
Six professors of the Department of Mathematics are Principal Investigators within the Graduate School Computational Engineering (Aurzada, Bothe, Egger, Lang, Pfetsch, Ulbrich) with expertise in Probability Theory and Stochastic Analysis, Mathematical Modeling and Analysis, Numerical Analysis and Scientific Computing, Numerics of Partial Differential Equations, Discrete Optimization, and Nonlinear Optimization and Optimal Control. Three more members of the department are Research Group Leaders (Erath, Schwartz, Ullmann) with scientific focus on 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.

2.4 Graduate School of Energy Science and Engineering

The mission of the Darmstadt Graduate School of Energy Science and Engineering is to educate tomorrow's leading Energy Engineers in a multidisciplinary field of expertise needed to identify and master the most demanding scientific, engineering, economic and social challenges in an interdisciplinary approach. The main challenge is viewed to be a continuous transition from the carbon-based, non-renewable primary energy sources of today to renewable and environmentally friendly energy resources of tomorrow.
The optimal strategy to meet this challenge is on the one hand to improve conventional energy technologies and render them progressively more efficient, to meet the ever more stringent demands on pollutant emissions, and on the other hand to simultaneously develop innovative, advanced renewable energy technologies, which must be brought to a competitive technological readiness level and provide safe, reliable and cost-effective solutions.
Two professors of the Department of Mathematics are Principal Investigators within the Graduate School Energy Science and Engineering (Lang, Ulbrich) with expertise in Numerical Analysis, Nonlinear Optimization and Optimal Control.

2.5 International Research Training Group IRTG 1529

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

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

The principal investigators in Darmstadt are Volker Betz, Dieter Bothe, Herbert Egger, Reinhard Farwig, Matthias Geissert, 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 2013 and 2014 includes leading experts of the field, e.g., L. Brandolese, P. Constantin, R. Danchin, G. Galdi, M. Lopes Filho, G. Karch, J. Kelliher, Y. Maekawa, S. Monniaux, Š. Nečasová, P. Mucha, J. Prüss, L. Székelyhidi, E. Titi.

Highlights of the program were altogether 8 conferences or bigger workshops in 2013 and 2014, e.g., the “International Workshops on Mathematical Fluid Dynamics” at Waseda University, Tokyo, in June and November 2013 and the “Autumn School on Mathematical Fluid Dynamics” in Bad Boll in October 2014.

The “Information Days on Mathematical Fluid Dynamics” in December 2013 were selforganized by our PhD students and attracted other PhD students to apply for a PhD position within the IRTG.

A “Winter Seminar and Klausurtagung on Fluids and Snow” took place in January 2014 in La Clusaz, France.

2.6 Scientific and Industrial Cooperations

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

Pia Domschke

– Prof. Dr. O. Kolb (Universität Mannheim): Adjoint-Based Error Control for the Simulation and Optimization of Gas and Water Supply Networks.

– Dr. A. Gerisch (TU Darmstadt), Prof. Dr. M. A. J. Chaplain (University of Dundee, Scotland), Dr. D. Trucu (University of Dundee, Scotland): Mathematical Modelling of Cancer Invasion.

Herbert Egger

– Prof. Dr. A. Düster (TU Hamburg-Harburg): Domain Decomposition Solvers for the Finite Cell Method.

– Prof. Dr. P. Egger, M. Kesina (ETH Zürich): Efficient Gibbs Sampling for Spatial Probit Models.

– Dr. S. M. Schnepp (ETH Zürich), Prof. I. Tsukerman (Akron, US), F. Kretzschmar (TU Darmstadt): Discontinuous Galerkin Methods for Maxwell's Equations.

– Dr. M. Schlottbom (Universität Münster), Dr. J.-F. Pietschmann (TU Darmstadt): Identification of Chemotaxis Models with Volume Filling.

– Dr. M. Schlottbom (Universität Münster): Explicit Time Stepping Methods for Radiative Transfer.

– Prof. S. Arridge (UCL London), M. Schlottbom (TU Darmstadt): Fast Solvers for Optical Tomography.

– Prof. Dr. B. Wohlmuth (TU München), Prof. Dr. U. Rüde (Universität Erlangen-Nürnberg): Finite Element Methods for Corner Singularities.

– Yuki Kaneko (Waseda University Tokyo), J.-F Pietschmann (TU Darmstadt): Inverse Free Boundary Value Problems.

– Prof. K. Fellner, Bao Q. Tang (KFU Graz): Finite Element Methods for Surface-Volume Reaction-Diffusion Systems.

Christoph Erath

– Dr. Mark A. Taylor (Sandia National Laboratories, Albuquerque, NM, USA) and Ramachandran Nair (NCAR, CO, USA): Semi-Lagrangian scheme for the spectral element dynamical core.

– Prof. Dr. Ilaria Perugia (Universität Wien), Prof. Dr. Jens Markus Melenk and Prof. Dr. Dirk Praetorius (TU Wien): Coupling Discontinuous Galerkin Methods with Boundary Element Methods for the Helmholtz equation.

– Prof. Dr. Dirk Praetorius (TU Wien): Convergence of some adaptive finite volume methods.

– Dr. Günther Of (TU Graz): Non-symmetric coupling of finite volume methods and boundary element methods.

Sofia Eriksson

– Prof. Jan Nordström (Linköping, Sweden): Non-reflecting boundary conditions for finite difference methods.

Alf Gerisch

– Prof. Dr. M. A. J. Chaplain (University of Dundee, Scotland), Dr. D. Trucu (University of Dundee, Scotland), Dr. P. Domschke (TU Darmstadt): Mathematical Modelling of Cancer Invasion.

– Prof. Dr. K. Raum (Charité Universitätsmedizin Berlin), Prof. Dr. Q. Grimal (Biomedical Imaging Lab (LIB), UPMC Paris, France), Dr. R. Penta (TU Darmstadt): Multiscale structure-functional modelling of musculoskeletal mineralized tissues.

- Prof. Dr. J. Lang (TU Darmstadt), D. Schröder (TU Darmstadt), Prof. Dr. R. Weiner (Universität Halle-Wittenberg), Dr. H. Podhaisky (Universität Halle-Wittenberg): PEER methods and their application in the Finite Element system KARDOS.
- Prof. Dr. J. Lang (TU Darmstadt), Prof. Dr. F. Müller-Plathe (TU Darmstadt), Prof. Dr. M. 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. Rüdiger Weiner (Universität Halle-Wittenberg): Linearly implicit time integrators.
- Bodo Erdmann (ZIB, Berlin): Kardos programming.
- Prof. Dr. Jochen Fröhlich (TU Dresden): Large Eddy Simulation with Adaptive Moving Meshes, Supported by DFG SPP 1276 MetStröm, 2007-2014.

Jan-Frederik Pietschmann

- Group of Prof. Dr. Martin Burger (WWU Münster): Crowded Transport.
- Group of Prof. Dr. Zuzanna Siwy (UC Irvine): Simulation of Nanopores.

Matthias Schlottbom

- Prof. S. Arridge (UCL London), Prof. Dr. H. Egger (TU Darmstadt): Fast Solvers for Optical Tomography.
- Prof. M. Frank (RWTH Aachen), Prof. M. Herty (RWTH Aachen): Reduced Models in Radiotherapy.
- Prof. M. Burger (WWU Münster), O.L. Elvetun (Norwegian University of Life Sciences): Diffuse Domain Methods for Heart Imaging.

Mirjam Walloth

- Prof. Dr. R. Krause (USI Lugano, Switzerland): Adaptive finite element discretization methods for the numerical simulation of static and dynamic contact problems.
- Prof. Dr. A. Veeser (University of Milan, Italy): 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* (Member of the editorial board)

3.2 Monographs and Books

[1] M. Behr, A. Bode, M. Bücker, J. Lang, E. Rank, U. Rüde, and M. Schäfer. *Multiphysics Problems in Computational Engineering*, volume 9 of *Int. J. Comput. Science and Engineering*. Inderscience Enterprise Ltd, 2014.

3.3 Publications in Journals and Proceedings

3.3.1 Journals

[1] S. Arridge, H. Egger, and M. Schlottbom. Preconditioning of complex symmetric linear systems with applications in optical tomography. *APNUM*, 74:35–48, 2013.

[2] M. Burger, J.-F. Pietschmann, and M.-T. Wolfram. Identification of nonlinearities in transport-diffusion models of crowded motion. *Inverse Problems and Imaging*, 7(4):1157–1182, 2013.

[3] D. Clever, J. Lang, and D. Schröder. Model Hierarchy Based Optimal Control of Radiative Heat Transfer. *International Journal of Computational Science and Engineering*, 9:509–525, 2014.

[4] P. Domschke, D. Trucu, A. Gerisch, and M. A. J. Chaplain. Mathematical modelling of cancer invasion: Implications of cell adhesion variability for tumour infiltrative growth patterns. *Journal of Theoretical Biology*, 361:41–60, 2014.

[5] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of chemotaxis models with volume-filling. *SIAM J. Appl. Math.*, 75:275–288, 2014.

[6] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Identification of nonlinear heat conduction laws. *J. Inv. Ill-Posed Probl.*, 2014. doi:10.1515/jiip-2014-0030.

[7] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Numerical identification of a nonlinear diffusion law via regularization in Hilbert scales. *Inverse Problems*, 30:025004, 2014.

[8] H. Egger, J.-F. Pietschmann, and M. Schlottbom. Simultaneous identification of diffusion and absorption coefficients in a quasilinear elliptic problem. *Inverse Problems*, 30:035009, 2014.

[9] H. Egger, U. Rüde, and B. Wohlmuth. Energy-corrected finite element methods with optimal convergence for corner singularities. *SIAM J. Numer. Anal.*, 52:171–193, 2013.

[10] H. Egger and M. Schlottbom. An L^p theory for stationary radiative transfer. *Applicable Analysis*, 93:1283–1296, 2013. doi:10.1080/00036811.2013.826798.

[11] H. Egger and M. Schlottbom. Diffusion asymptotics for linear transport with low regularity. *Asymptotic Analysis*, 89:365–377, 2014. doi:10.3233/ASY-14123.

[12] H. Egger and M. Schlottbom. Numerical methods for parameter identification in stationary radiative transfer. *Comput. Optim. Appl.*, 2014. doi:10.1007/s10589-014-9657-9.

[13] H. Egger and M. Schlottbom. Stationary radiative transfer with vanishing absorption. *M3AS*, 24:973–990, 2014.

[14] C. Erath. A new conservative numerical scheme for flow problems on unstructured grids and unbounded domains. *Journal of Computational Physics*, 245:476–492, 2013.

[15] C. Erath. A posteriori error estimates and adaptive mesh refinement for the coupling of the finite volume method and the boundary element method. *SIAM Journal on Numerical Analysis*, 51(3):1777–1804, 2013.

[16] C. Erath. A nonconforming a posteriori estimator for the coupling of cell-centered finite volume and boundary element methods. *Numerische Mathematik*, 2014.

[17] C. Erath. Comparison of Two Couplings of the Finite Volume Method and the Boundary Element Method. In J. Fuhrmann, M. Ohlberger, and C. Rohde, editors, *Finite Volumes for Complex Applications VII - Methods and Theoretical Aspects*, pages 255–263. Springer, 2014.

[18] C. Erath, S. Funken, P. Goldenits, and D. Praetorius. Simple error estimators for the Galerkin BEM for some hypersingular integral equation in 2D. *Applicable Analysis*, 92(6):1194–1216, 2013.

[19] C. Erath, P. Lauritzen, and H. Tufo. On Mass Conservation in High-Order High-Resolution Rigorous Remapping Schemes on the Sphere. *Monthly Weather Review*, 141(6):2128–2133, 2013.

[20] C. Erath and R. Nair. A conservative multi-tracer transport scheme for spectral-element spherical grids. *Journal of Computational Physics*, 256:118–134, 2014.

[21] T. Gamble, K. Decker, T. S. Plett, M. Pevarnik, J.-F. Pietschmann, I. Vlassiouk, A. Aksimentiev, and Z. S. Siwy. Rectification of ion current in nanopores depends on the type of monovalent cations: Experiments and modeling. *The Journal of Physical Chemistry C*, 118(18):9809–9819, 2014.

[22] C. Hertel, M. Schümichen, J. Lang, and J. Fröhlich. Using a Moving Mesh PDE for Cell Centres to Adapt a Finite Volume Grid. *Flow, Turbulence and Combustion*, 90:785–812, 2013.

[23] 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.

[24] K. Kuhn and J. Lang. Comparison of the asymptotic stability for multirate Rosenbrock methods. *Journal of Computational and Applied Mathematics*, 262:139–149, 2014.

[25] J. Lang and J. Verwer. W-methods in optimal control. *Numerische Mathematik*, 124:337–360, 2013.

[26] C. Liersch, M. Frankenbach, J. Lang, and J. Fröhlich. Recent Progress in designing moving meshes for complex turbulent flows. *Meteorologische Zeitschrift*, 23:425–439, 2014.

[27] R. Penta, D. Ambrosi, and R. Shipley. Effective governing equations for poroelastic growing media. *Q J Mechanics Appl. Math.*, 67:69–91, 2014.

[28] J.-F. Pietschmann, M.-T. Wolfram, M. Burger, C. Trautmann, G. Nguyen, M. Pevarnik, V. Bayer, and Z. Siwy. Rectification properties of conically shaped nanopores: consequences of miniaturization. *Phys. Chem. Chem. Phys.*, 15:16917–16926, 2013.

[29] B. Schieche and J. Lang. Uncertainty Quantification for Poiseuille Flow Using Stochastic Collocation. *International Journal of Computational Science and Engineering*, 9:465–477, 2014.

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

[31] M. Taffetani, C. de Falco, R. Penta, D. Ambrosi, and P. Ciarletta. Biomechanical modelling in nanomedicine: multiscale approaches and future challenges. *Archive of Applied Mechanics*, 84:1627–1645, 2014.

[32] S. Tiburtius, S. Schrof, F. Molnár, P. Varga, F. Peyrin, Q. Grimal, K. Raum, and A. Gerisch. On the elastic properties of mineralized turkey leg tendon tissue: multiscale model and experiment. *Biomechanics and Modeling in Mechanobiology*, 13(15):1003–1023, 2014.

[33] M. Vallejos. A comparison of smoothers for state-constrained optimal control problems. *Phil. Sci. Lett.*, 7:13–21, 2014.

3.3.2 Proceedings and Chapters in Collections

[1] S. Bott, D. Clever, J. Lang, S. Ulbrich, C. Ziems, and D. Schröder. On a fully adaptive SQP method for PDAE-constrained optimal control problems with control and state constraints. In G. Leugering, P. Benner, S. Engell, A. Griewank, H. Harbrecht, M. Hinze, R. Rannacher, and S. Ulbrich, editors, *Trends in PDE Constrained Optimization*, International Series of Numerical Mathematics. Springer Basel AG, 2014.

[2] K. Debrabant and J. Lang. On global error estimation and control of finite difference solutions for parabolic equations. In C. T. J. P. Moitinho de Almeida, P. Diez and N. Pares, editors, *Adaptive Modeling and Simulation 2013*, International Conference on Adaptive Modeling and Simulation. International Center for Numerical Methods in Engineering (CIMNE), Barcelona, Spain, 2013.

[3] S. Heinze, M. Joulaian, H. Egger, and A. Düster. Efficient computation of cellular materials using the finite cell method. *PAMM*, 14:251–252, 2014.

[4] W. Huang, L. Kamenski, and J. Lang. Adaptive finite elements with anisotropic meshes. In A. Cangiani et al., editor, *Numerical Mathematics and Advanced Applications 2011: Proceedings of ENUMATH 2011, the 9th European Conference on Numerical Mathematics and Advanced Applications, Leicester, September 2011*. Springer, 2013.

[5] F. Kretzschmar, F. Ahmadi, N. Nowak, S. M. Schnepp, I. Tsukerman, H. Egger, and T. Weiland. Trefftz absorbing boundary conditions in analytical, discontinuous Galerkin and finite difference form. In *2014 International Conference on Electromagnetics in Advanced Applications (ICEAA)*, pages 176–177. IEEE, 2014.

[6] R. Penta and D. Ambrosi. Poro-elastic modeling for biological tissues and human eye: Recent advances and future perspectives. In P. Causin, G. Guidoboni, R. Sacco, and A. Harris, editors, *Integrated Multidisciplinary Approaches in the Study and Care of the Human Eye*, chapter 11. Kugler Publications, 2014.

[7] B. Schieche and J. Lang. Adjoint error estimation for stochastic collocation methods. In J. Garcke and D. Pflüger, editors, *Sparse Grids and Applications - Munich 2012*, Lecture Notes in Computational Science and Engineering. Springer, 2014.

[8] S. Ullmann and J. Lang. POD-Galerkin modeling and sparse-grid collocation for a natural convection problem with stochastic boundary conditions. In J. Garcke and D. Pflüger, editors, *Sparse Grids and Applications - Munich 2012*, Lecture Notes in Computational Science and Engineering. Springer, 2014.

[9] S. Ullmann, S. Löbig, and J. Lang. Adaptive large eddy simulation and reduced-order modeling. In J. Janicka, A. Sadiki, M. Schäfer, and C. Heeger, editors, *Flow and Combustion in Advanced Gas Turbine Combustors*, Fluid Mechanics and Its Applications. 2013.

[10] 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. Springer, Berlin, Heidelberg, 2015.

3.4 Preprints

[1] M. Burger, O. Elvetun, and M. Schlottbom. Analysis of the diffuse domain method for second order elliptic boundary value problems. Technical report, WWU Münster, December 2014. arXiv:1412.5641.

[2] P. Domschke, O. Kolb, and J. Lang. Adjoint-based error control for the simulation and optimization of gas and water supply networks. Submitted, 2014.

[3] P. Domschke, D. Trucu, A. Gerisch, and M. A. J. Chaplain. Structured models of cell migration incorporating membrane reactions. Submitted, 2014.

[4] H. Egger, F. Kretzschmar, S. Schnepp, I. Tsukerman, and T. Weiland. Transparent boundary conditions in a discontinuous Galerkin Trefftz method. Technical report, TU Darmstadt, October 2014. arXiv:1410.1899.

[5] H. Egger, F. Kretzschmar, S. M. Schnepp, and T. Weiland. A space-time discontinuous Galerkin Trefftz method for time dependent Maxwell's equations. Technical report, TU Darmstadt, December 2014. arXiv:1412.2637.

[6] M. Granke, Q. Grimal, W. 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? Accepted, Acta Biomaterialia, 2014.

[7] S. Liu, A. Gerisch, M. Rahimi, J. Lang, M. Böhm, and F. Müller-Plathe. Robustness of a new molecular dynamics-finite element coupling approach for soft matter systems analyzed by uncertainty quantification. Accepted, Journal of Chemical Physics, 2014.

[8] R. Penta and D. Ambrosi. The role of the microvascular tortuosity in tumor transport phenomena. Accepted, Journal of Theoretical Biology, 2014.

[9] R. Penta, D. Ambrosi, and A. Quarteroni. Multiscale homogenization for fluid and drug transport in vascularized malignant tissues. Accepted, Math. Models Methods Appl. Sci., 2014.

3.5 Reviewing and Refereeing

Herbert Egger: Computational Methods in Applied Mathematics, ESAIM: Mathematical Modelling and Numerical Analysis, Journal of Mathematical Analysis and Applications, SIAM Journal on Scientific Computing, IMA Journal on Numerical Analysis, Applied Mathematics and Computation, SIAM Journal on Matrix Analysis and Applications, Mathematics and Computers in Simulation, Inverse Problems, Mathematical Methods in the Applied Sciences, IMA Journal of Applied Mathematics, Numerical Algorithms, SIAM Journal on Numerical Analysis, Journal of Applied Mathematics and Computing, Computers and Mathematics with Applications, Applicable Analysis

Christoph Erath: SIAM Journal on Numerical Analysis, Mathematical Reviews, Journal for Computational Physics, Geoscientific Model Development Discussion, Finite Volumes for Complex Applications VII

Alf Gerisch: Journal of Computational and Applied Mathematics, Engineering Computations, Journal of Theoretical Biology, Applied Mathematics and Computation, Biomechanics and Modeling in Mechanobiology, Mathematical Biosciences and Engineering, SIAM Journal on Scientific Computing

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

Matthias Schlottbom: Zentralblatt, Mathematical Reviews; Abstract and Applied Analysis, Computers and Mathematics with Applications

Sebastian Ullmann: Mathematical Modelling and Analysis

Mirjam Walloth: International Journal for Numerical Methods in Engineering, Journal of Computational and Applied Mathematics, SIAM Journal on Numerical Analysis

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

Contributor at TU Darmstadt: Pia Domschke, Jens Lang, Lisa Wagner

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 PDE's 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

4 Theses

4.1 PhD Dissertations

2013

Clever, Debora, *Adaptive Multilevel Methods for PDAE-Constrained Optimal Control Problems* (Jens Lang)

2014

Frankenbach, Matthias, *An Adjoint Based A Posteriori Error Estimator for Moving Meshes in Large Eddy Simulation* (Jens Lang)

Kuhn, Karen, *Stability and applications of higher-order multirate Rosenbrock and Peer methods* (Jens Lang)

Ullmann, Sebastian, *POD-Galerkin Modeling for Incompressible Flows with Stochastic Boundary Conditions* (Jens Lang)

4.2 Diplom Theses

2013

Schulz, Alexander, *Numerische Lösung der Black-Scholes PDE* (Jens Lang)

4.3 Master Theses

2013

Buschbacher, Alwin, *Adaptive Multilevel-Verfahren für die optimale Steuerung der Stahlhärtung* (Jens Lang)

Siebert, Sandra Maria, *Finite-Elemente-Methoden für konvektionsdominante Probleme* (Jens Lang)

2014

Kodja, Joe-Loic, *Simulation of fluid flow and heat transfer in a heat exchanger* (Herbert Egger)

Sieber, Jessica, *Konvergenzanalyse und Numerische Tests für die Prothero-Robinson-Gleichung* (Jens Lang)

4.4 Bachelor Theses

2013

Abt, Fabian Ferdinand Erich, *Projektionen zur Lösung von* ℓ_1*-Problemen* (Marc Pfetsch)

Adami, Thomas, *Robuste Portfoliooptimierung* (Stefan Ulbrich)

Aissa, Benjamin, *The Hasse principle and Selmer's counter example* (Nils Scheithauer)

Akman, Tugba, *Die Fouriertransformation und die Plancherel-Gleichung* (Matthias Hieber)

Beian, Abraham, *Der Kern eines kooperativen Spiels* (Werner Krabs)

Müller, Fabian, *Theoretische und numerische Untersuchungen an einem Modell der Lymphangionese* (Jens Lang)

2014

Althaus, Lea, *Modellierung kollektiver Zellbewegung* (Herbert Egger)

Lang, Florian, *Numerische Methoden zur Bestimmung der Karhunen-Loève-Entwicklung von Zufallsfeldern* (Alf Gerisch)

Ruppert, Simon Moritz, *Two Point Boundary Value Problems and the Shooting Method* (Herbert Egger)

Schneider, Moritz, *Finite element methods for the one dimensional obstacle problem* (Herbert Egger)

Zimmer, Petra, *Stabilität gewöhnlicher Differentialgleichungen* (Herbert Egger)

5 Presentations

5.1 Talks and Visits

5.1.1 Invited Talks and Addresses

Pia Domschke

12/05/2014 *Mathematical modelling of cancer invasion: Implications of cell adhesion variability for tumour infiltrative growth patterns*
International Workshop on Numerical Methods and Emerging Computational Challenges in Mathematical Biology 2014, Dundee

Herbert Egger

27/02/2013 *Explicit Time Stepping for Radiative Transfer based on Mixed Variational Formulations*
SIAM CSE, Boston

14/03/2013 *An explicit time stepping method for radiative transfer*
MIRAN Inverse Problems in Transport, Manchester

28/03/2013 *Optical Tomography: Models, Analysis, Numerics and Inverse Problems*
10 Years Johann Radon Institute, RICAM

17/04/2013 *Stabilität, Konsistenz, Approximation: Fehlerhaft Rechnen mit System*
Mathematisches Kolloquium, TU Darmstadt

28/06/2013 *Radiative Transfer: Analysis, Numerics and Inverse Problems*
Rhein-Main-Arbeitskreis, Universität Mainz

27/05/2014 *Inverse Probleme: Mathematische Antworten auf praktische Fragen*
Was steckt dahinter, TU Darmstadt

11/07/2014 *An inverse problem in nonlinear heat conduction*
Mathematisches Seminar, Universität Saarbrücken

12/09/2014 *A posteriori estimates for hybrid discontinuous Galerkin methods*
Workshop on Recent advances in discontinuous Galerkin methods, University of Reading

26/09/2014 *Computational Methods, Inverse Problems and Optimization in Radiative Transfer*
IPTA Recife

30/10/2014 *Computational Inverse Problems*
Toyota-CSI Workshop, TU Darmstadt

Christoph Erath

20/06/2013 *Advanced Finite Volume Methods - Theory and Practical Applications*
Numerik und Wissenschaftliches Rechnen, TU Darmstadt

20/05/2014 *Finite-Volume-Based Semi-Lagrangian Schemes for the Community Atmosphere Model CAM-SE*
Meteorological-Geophysical Kolloquium, Universität Wien

Alf Gerisch

08/11/2013 *Modellieren und passendes Simulieren*
Festkolloquium für Rüdiger Weiner, Martin-Luther-Universität Halle-Wittenberg

13/05/2014 *An adaptive stochastic collocation approach to uncertainty quantification*
ICMS Workshop on Numerical Methods and Emerging Computational Challenges in Mathematical Biology, Dundee

17/07/2014 *Numerical techniques for non-local models of cancer invasion*
Oberseminar der Numerik, Universität Mainz

14/10/2014 *Numerical challenges in models of tissue-scale tumour cell invasion*
Workshop Metastasis and Angiogenesis, Mathematical Biosciences Institute, Columbus, Ohio

Jens Lang

22/04/2013 *Higher Order and Adaptive Methods in Computational Fluid Dynamics*
Mathematical Seminar, CWI, Amsterdam

26/06/2013 *Adaptive Moving Meshes in Large Eddy Simulation for Turbulent Flows*
25th Biennial Numerical Analysis Conference, Glasgow

23/09/2013 *Convergence and Adaptivity at the PDE/Stiff ODE Interface*
26th Chemnitz FEM Symposium, Annaberg-Buchholz

22/05/2014 *Adaptivity in Numerical Methods for ODEs and PDEs*
Mathematical Seminar, Dundee

13/06/2014 *Adaptive Modelling, Simulation and Optimization of Water and Gas Supply Networks*
ECMI 2014, Taormina

22/07/2014 *Adaptive Surrogate Modelling in Unsteady Transport Systems*
World Congress of Computational Mechanics, Barcelona

29/09/2014 *On the design and Use of Adaptive PDAE Solvers*
Modelling, Simulation and Optimization Tools 2014, Berlin

02/10/2014 *Adaptive Moving Meshes in Large Eddy Simulation for Turbulent Flows*
Mathematical Seminar, WIAS Berlin

Raimondo Penta

16/12/2014 *An asymptotic homogenization approach for multiphase linear elastic composites with discontinuous material properties*
Biomox Seminar, Politecnico, Milan

Jan-Frederik Pietschmann

23/10/2014 *Motion and Size Exclusion - Derivation and Properties of non-linear Cross-Diffusion Models*
WIAS, Berlin

04/12/2014 *Identification of chemotaxis models with volume filling*
RICAM, Gruppe Dr. Wolfram, Linz

Matthias Schlottbom

14/03/2013 *Analysis of a forward problem in optical tomography*
MIRAN Inverse Problems in Transport, Manchester

02/07/2013 *Preconditioning of complex symmetric linear systems with applications in optical tomography*
Applied Inverse Problems, KAIST, Daejeon

05/07/2013 *Simultaneous identification of diffusion and absorption coefficients in a quasi-linear elliptic problem*
Applied Inverse Problems, KAIST, Daejeon

24/03/2014 *Numerical Methods for Parameter Identification in Stationary Radiative Transfer*
Seminar Talk, Universität Münster

06/08/2014 *Diffusion asymptotics for linear transport with low regularity*
Seminar Talk, RWTH Aachen

25/11/2014 *Analysis of the diffuse domain method for second order elliptic problems*
IRTG Seminar, TU Darmstadt

01/12/2014 *Simultaneous identification of diffusion and absorption coefficients in a quasi-linear elliptic problem*
Seminar talk, Universität Duisburg-Essen

Sebastian Ullmann

24/01/2013 *POD-Galerkin reduzierte Modelle für Strömungsprobleme mit stochastischen Randbedingungen*
Seminar Numerische Mathematik, WIAS Berlin

5.1.2 Contributed Talks

Pia Domschke

16/06/2014 *Modelling the role of adhesion in the heterogeneous dynamics of cancer invasion*
European Conference on Mathematical and Theoretical Biology (ECMTB) 2014, Göteborg

29/09/2014 *Adaptive Modelling and Simulation for the Optimization of Gas and Water Supply Networks*
Workshop MSO-Tools 2014, Berlin

Herbert Egger

19/02/2013 *Explicit Time Stepping for Radiative Transfer based on Mixed Variational Formulations*
Numa Workshop, Hirschegg, TU Darmstadt

18/07/2013 *Iterative methods for nonlinear tomography*
EUCCO, TU Chemnitz

Christoph Erath

11/02/2013 *New Finite Volume based Tracer Transport Schemes for CAM-SE*
Atmosphere Model Working Group (AMWG) meeting, Boulder, Colorado

27/02/2013 *A new multi-tracer-efficient semi-Lagrangian transport scheme for the Community Atmosphere Model*
SIAM Conference on Computational Science and Engineering (CSE13), Boston, Massachusetts

01/03/2013 *A conservative semi-Lagrangian transport scheme on spectral element cubed-sphere grids (SPELT)*
SIAM Conference on Computational Science and Engineering (CSE13), Boston, Massachusetts

05/03/2013 *Future tracer transport in CAM-SE: Finite Volume based Semi-Lagrangian schemes in HOMME*
CISL Seminar Series at the National Center for Atmospheric Research, Boulder, Colorado

27/05/2014 *Non-Conforming a Posteriori Estimates for the FVM-BEM Coupling*
Austrian Numerical Analysis Day 2014, Vienna

20/06/2014 *Comparison of two couplings of the finite volume method and the boundary element method*
7th International Symposium on Finite Volumes for Complex Applications, Berlin

Alf Gerisch

26/04/2013 *Mathematical modelling and numerical simulation in mechanobiology*
Treffen des MSB-Net Clusters Numerische Simulation, Hannover

08/05/2013 *Assessment of collagen fibril orientation in human lamellar bone with scanning acoustic microscopy and polarized Raman microscopy (presented by S. Schrof)*
5th European Symposium on Ultrasonic Characterization of Bone, Granada

14/05/2013 *Uncertainty Quantification Using Stochastic Collocation Method and Application in a Model of Mineralized Turkey Leg Tendon*
18th International Symposium on Computational Biomechanics, Ulm

16/06/2014 *Uncertainty quantification in a model of tumour invasion*
European Conference on Mathematical and Theoretical Biology (ECMTB) 2014, Göteborg

Jens Lang

27/08/2013 *Anisotropic Finite Element Meshes for Linear Parabolic Equations*
ENUMATH 2013, Lausanne

20/05/2014 *Transport in Wassernetzwerken*
EWAVE-Treffen Nürnberg

Michelle Lass (Vallejos)

20/06/2013 *A multigrid approach to PDE constrained optimal control problems*
The 10th Korean Women in Mathematical Sciences International Conference, Seoul

22/09/2014 *A multigrid approach to obstacle problems and to optimal control of obstacle problems*
27th FEM Symposium, TU Chemnitz

Raimondo Penta

04/09/2014 *The role of microvascular tortuosity in tumor transport phenomena*
CIME-CIRM course on Mathematical Models and Methods for Living Systems, Levico Terme

Jan-Frederik Pietschmann

04/04/2013 *Identification of non-linearities in transport-diffusion models of crowded motion*
Inverse Problems and Applications, Linköping

05/07/2013 *Identification of non-linearities in transport-diffusion models of crowded motion*
Applied Inverse Problem Conference

19/09/2014 *Identification of chemotaxis models with volume filling*
Chemnitz Symposium on Inverse Problems, Chemnitz

Matthias Schlottbom

02/04/2013 *Analysis of a forward problem in optical tomography*
Inverse Problems and Applications, Linköping

18/09/2014 *Identification of nonlinear heat conduction laws in heat transfer problems*
Chemnitz Symposium on Inverse Problems, TU Chemnitz

Dirk Schröder

18/07/2013 *Adaptive Multilevel Optimization of a 3D glass cooling problem with boundary control*
EUCCO 2013, Chemnitz

Tobias Seitz

14/05/2014 *Optimal Control of Navier-Stokes Equations: An Introduction*
Seminar Numerik, TU Darmstadt

27/08/2014 *Flow Reconstruction from MRV Measurements*
Particles in Flows Summer School and Workshop, Prague

28/10/2014 *Flow reconstruction from MRV measurements*
Autumn School and Workshop on Mathematical Fluid Dynamics, Bad Boll

Sara Tiburtius

23/01/2013 *Effektive elastische Eigenschaften muskuloskelettaler mineralisierter Gewebe - Sensitivitätsanalyse*
Seminar Numerik, TU Darmstadt

18/06/2013 *Finite element methods and numerical homogenization*
SPP 1420 PhD- and Postdoc-Workshop on theoretical and computational methods, TU Darmstadt

12/09/2013 *Elastic properties of the mineralized turkey leg tendon: experiment and model*
International Conference on Computational Bioengineering, Leuven

11/12/2014 *Homogenization for the multiple scale analysis of musculoskeletal mineralized tissues*
Seminar Numerik, TU Darmstadt

Sebastian Ullmann

26/02/2013 *Large-Eddy-Simulation mit adaptiven bewegten Gittern zur Lösung meterologischer Fragestellungen*
Metström Jahrestreffen, Berlin

26/05/2014 *POD-Galerkin Modeling for a Steady Thermally Driven Flow in a Cavity with Stochastic Boundary Conditions*
Workshop on Uncertainty Quantification in Computational Fluid Dynamics, Pisa

08/08/2014 *POD-Galerkin reduced-order modeling and stochastic collocation for natural convection under uncertainty*
Advances in Simulation-Driven Optimization and Modeling, Reykjavik

12/11/2014 *What is a finite element fictitious boundary method?*
Seminar "What is . . . ?", TU Darmstadt

Lisa Wagner

18/06/2014 *Optimal control in cancer therapy*
Seminar Numerik, TU Darmstadt

Mirjam Walloth

30/08/2013 *An efficient and reliable residual-type a posteriori error estimator for the Signorini problem*
ENUMATH 2013, Lausanne

03/09/2013 *Adaptive numerical simulation of contact problems. Resolving local effects at the contact boundary in space and time*
ECCOMAS YIC 2013, Bordeaux

13/03/2014 *Residual-type a posteriori error estimators for Signorini problems*
GAMM 2014, Erlangen

5.1.3 Visits

Pia Domschke, University of Dundee, September 2013 - September 2014

Herbert Egger, RICAM Linz, March 2013

Herbert Egger, TU München, September 2013

Herbert Egger, ETH Zürich, December 2013

Herbert Egger, ETH Zürich, July 2014

Herbert Egger, University Reading, September 2014

Jens Lang, CWI, Amsterdam, The Netherlands, April-May 2013

Jens Lang, University of Dundee, Scotland, May 2014

Jan-Frederik Pietschmann, UC Irvine, March 2013

Jan-Frederik Pietschmann, University of Cambridge, March 2014

Jan-Frederik Pietschmann, UC Irvine, November 2014

Jan-Frederik Pietschmann, RICAM Linz, Dezember 2014

Tobias Seitz, UC Irvine, US, November 2014

Sebastian Ullmann, WIAS Berlin, January 2013

Mirjam Walloth, USI Lugano, March 2014

Mirjam Walloth, University of Milan, March 2014

5.2 Organization and Program Commitees of Conferences and Workshops

Herbert Egger

– Summerschool *Reduced Basis Methods – Fundamentals and Applications*, September 16–19, 2013, TU München

6 Workshops and Visitors at the Department

6.1 Guest Talks at the Department

22/05/2013 Alexey Chernov (University of Reading), *Multilevel Monte Carlo FEM and application for random obstacle problems* (Herbert Egger)

18/06/2013 Prof. Dr. Quentin Grimal (Biomedical Imaging Lab (LIB), UPMC Paris), *Modelling of in-situ strain fields in cortical bone tissue* (Alf Gerisch)

29/10/2013 Bao Q. Tang (KFU Graz), *Existence and convergence to equilibrium for a class of reaction diffusion system* (Herbert Egger)

29/10/2013 Yikan Liu (University of Tokyo), *Initial-boundary value problems for multiterm time-fractional diffusion equations with positive constant coefficients* (Herbert Egger)

19/11/2013 Prof. Dr. Bastian von Harrach (Universität Stuttgart), *Inverse coefficient problems and shape reconstruction* (Jan-Frederik Pietschmann)

09/12/2013 Prof. Dr. Roland Griesmaier (Universität Leipzig), *Enhanced approximate cloaking by optimal change of variables* (Jan-Frederik Pietschmann)

28/04/2014 Prof. Dr. Günther Of (TU Graz), *Coupling of Finite and Boundary Element Methods: Applications and New Developments* (Herbert Egger)

03/07/2014 Michelle Vallejos (TU Chemnitz), *A multigrid approach to optimal control of obstacle problems* (Herbert Egger)

31/07/2014 Daniel Akrapovic (TU Kaiserslautern), *Modellreduktion mithilfe der Proper Orthogonal Decomposition im Bereich des Strahlungstransports* (Herbert Egger)

11/11/2014 Bao Q. Tang (Universität Graz), *Well posedness, numerics and quasi-steady-state approximation for a volume-surface reaction-diffusion system* (Herbert Egger)

11/11/2014 Yuki Kaneko (Waseda University Tokyo), *Spreading and vanishing for a free boundary problem in population ecology* (Herbert Egger)

04/12/2014 Dr. Dumitru Trucu (University of Dundee, Scotland), *Novel perspectives in multiscale modelling and analysis: the novel concept of three-scale convergence* (Pia Domschke, Alf Gerisch)

6.2 Visitors at the Department

Dr. Dumitru Trucu (University of Dundee, Scotland), December 2014.

Bao Q. Tang (Universität Graz), August – October 2013.

Yikan Liu (University of Tokyo), October – December 2013.

Bao Q. Tang (Universität Graz), October – December 2014.

Yuki Kaneko (Waseda University Tokyo), October – December 2014.

Prof. Dr. Quentin Grimal (Biomedical Imaging Lab (LIB), UPMC Paris, France), June 2013.

6.3 Workshops and Conferences at the Department

- DFG SPP1420 Summer School *Theoretical & Computational Methods*, June 17-18, 2013 (organized by Sara Tiburtius and Alf Gerisch)

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.

Activities for secondary school students and prospective students

- Presentation of the department and its study programmes at the university information day, TUDay, every May: with talks by the student advisor, sample lectures and tutorial classes, meetings with students of the department; about 90 participants over the course of the day in 2014 (lectures from the field of Numerical Analysis in 2014 and from the fields of Logic and Optimization in 2015). In 2014, the TUDay coincided with the Schülerinnen- und Schülernachmittag zur Mathematik (see below).

- Support of the annual organization of the Mathematikolympiade Hessen (third level) in cooperation with the Zentrum für Mathematik, 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. Bokowski (2013) and Prof. Kiehl and Prof. Ziegler (2014).

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

8 Contact

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