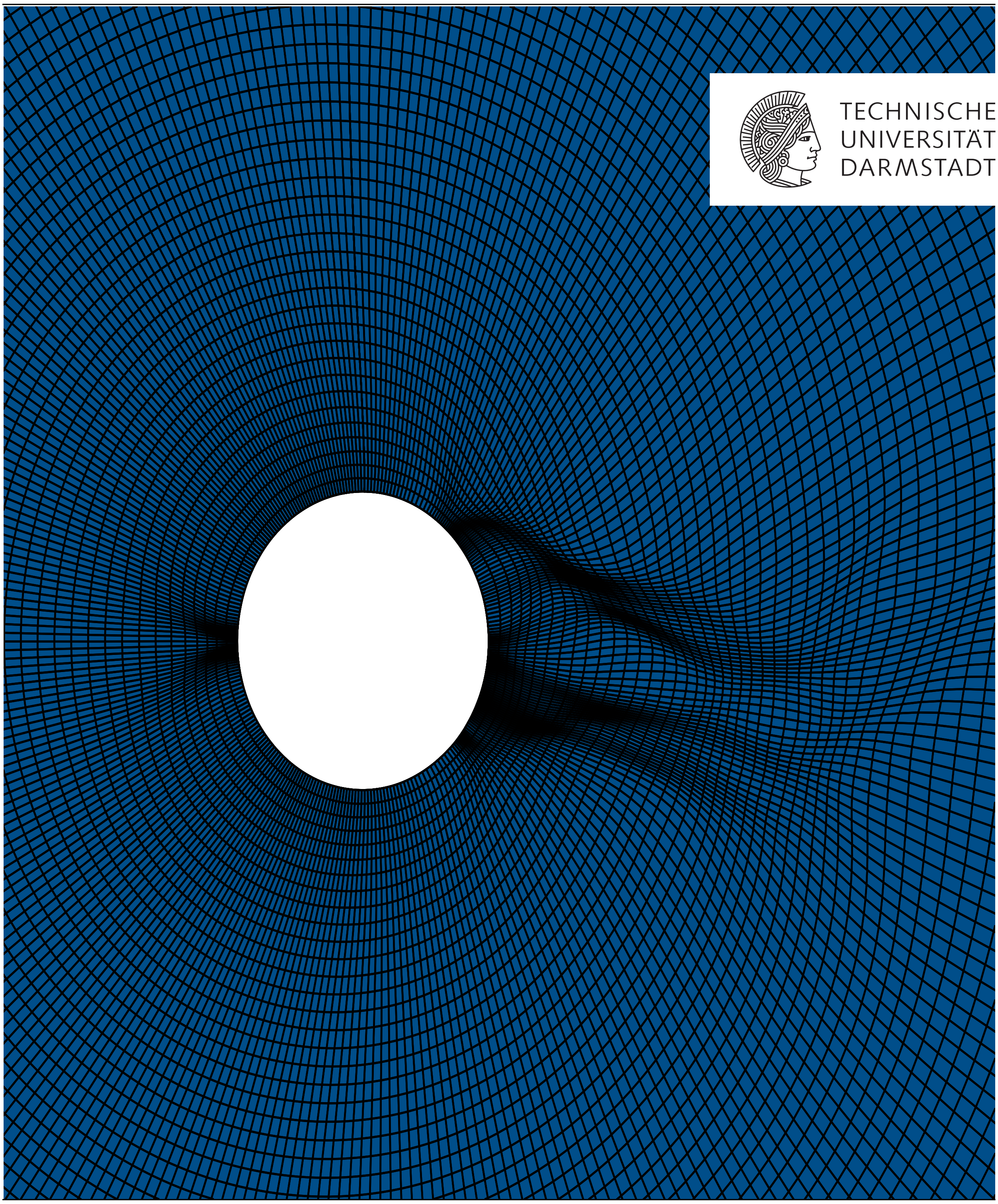
Biannual Report

Department of Mathematics
Research Group Numerical Analysis and Scientific Computing
2011 and 2012



Contents

General Remark

This document contains a subset of the information of the biannual report of the Department of Mathematics at TU Darmstadt for 2011 and 2012. 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, March 2013

1 Research

1.1 Overview

Besides the research done in the eight research groups, 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.

1.1.1 Center of Smart Interfaces

The Center of Smart Interfaces (CSI) is a Cluster of Excellence (EXC 259), funded by the German Research Foundation (DFG). The initial funding period started in November 2008 and runs until October 2014, having a total volume of about 42 Million EUR. The CSI is an international center for interdisciplinary research, focusing on the scientific areas “static and dynamic wettability”, “heat 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 enabled 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.

The CSI was involved in several activities in mathematics. Both in 2011 and 2012, a section on Interfacial Flows was co-organized by members of the mathematical group from the CSI. At the CSI, the seminar series on experiments, modeling and theory of contact line dynamics was continued. Furthermore, together with the IRTG ”Mathematical Fluid Dynamics” and the Graduate School ”Computational Engineering”, the International Workshop on Modeling, Simulation and Optimization of Complex Fluid Flows was organized by Bothe, Lukacova, Schäfer and Ulbrich in June 2012. With main speakers including Y. Bazilevs, K. Kunisch, R. Kupfermann, R. Löhner, A. Reusken, M. Tabata, Y. Teramoto, and S. Turek, this was an outstanding international event. Another highlight was the 7$^{\text{th}}$ International OpenFOAM Workshop with more than 300 participants from all over the world. Finally, the CSI was strongly involved in the organization of the GAMM annual meeting 2012.

1.1.2 Collaborative Research Centre SFB 568

The Collaborative Research Centre SFB 568 “Flow and Combustion in Future Gas Turbine Combustion Chambers" started in 2001 and aims at the formulation of an integral model for the development and optimization of new gas turbine combustion chamber concepts which make more efficient use of rare resources in the conversion of energy compared to today’s technology. The main points that have to be considered are the occuring and highly complex coupled and interacting physico-chemical processes such as turbulent transport, two- or multi-phase flows, materials transport, chemical reactions/combustion and radiation. The integral model comprises four main elements:

1. submodels of physical/chemical mechanisms and interactions
2. suitable numerical methods
3. consideration of basic conditions and neighboring components and interactions
4. implementation of targeted validation experiments

The Department of Mathematics contributes to the SFB 568 within two subprojects (Lang, Ulbrich). The topics under investigation are the control of errors of the numerical simulation, model reduction techniques and the numerical optimization of gas turbine relevant problems. To control and estimate errors of the complex numerical simulations, grid refinement strategies based on suitable error estimators are investigated. To reduce the cost of the simulations, model reduction techniques are further developed to account for turbulence (Lang). Since the simulation itself is a challenging task, new mathematical techniques for the optimization have to be developed that make optimization applicable in reasonable time (Ulbrich).

1.1.3 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 often 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 is becoming challenging. With the Graduate School of Computational Engineering, the 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 (Egger, Joswig, Lang, Pfetsch, Stannat, Ulbrich) with expertise in Discrete Algortihmic Mathematics, Numerical Analysis, Discrete Optimization, Stochastics, Nonlinear Optimization and Optimal Control. They supervise more than 10 interdiciplinary PhD projects within the Graduate School in close cooperation with a co-supervisor from Engineering or Computer Science.

1.1.4 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.

1.2 Research Groups

1.2.1 Numerical Analysis and Scientific Computing

The particular strength of the Numerical Analysis and Scientific Computing group is in the development of novel, efficient, and accurate numerical methods that are capable of tackling complex problems of practical interest. Our broad long-term goal is to provide good software for the solution of differential equations and optimization problems - one of the main modelling tools in science and engineering. We are currently engaged in the following specific application areas: computational medicine and meteorology, simulation and optimal control of gas and water networks, inverse problems, radiative transport, optical tomography, modelling and simulation of ion channels and nanopores, and computational biology.

Project: Adaptive Multilevel Methods for PDAE-Constrained Optimal Control Problems With Application to Radiative Heat Transfer

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 a fully space-time adaptive PDAE solver (e.g. Kardos [4]), highly efficient optimization techniques (e.g. a generalized SQP method [3]), 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.
Within this project, the environment is used to solve an optimal boundary control problem arising in glass manufacturing during the cooling process. The physical behavior of the cooling process is modeled by radiative heat transfer and simplified by spherical harmonics resulting in systems of partial differential algebraic equations. The performance of the environment and the results of the optimization are studied at basis of several models of different complexity in two and three spatial dimensions [2, 1].
Numerical experiments show that, together with the multilevel strategy, the coupling of continuous adjoint calculus with full space-time adaptivity has the great potential to solve complex optimal control problems of practical interest.

Partner: S. Bott, S. Ulbrich, C. Ziems

Support: German Research Association (DFG), priority program 1253

Contact: D. Clever, J. Lang, D. Schröder

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[1] D. Clever. *Adaptive Multilevel Methods for PDAE-Constrained Optimal Control Problems*. PhD thesis, TU Darmstadt, 2013. Verlag Dr. Hut, ISBN 978-3-8439-0878-8.

[2] D. Clever and J. Lang. Optimal control of radiative heat transfer in glass cooling with restrictions on the temperature gradient. *Optimal Control Applications and Methods*, 33(2):157–175, 2012.

[3] D. Clever, J. Lang, S. Ulbrich, and J. C. Ziems. Generalized multilevel SQP-methods for PDAE-constrained optimization based on space-time adaptive PDAE solvers. *Constrained Optimization and Optimal Control for Partial Differential Equations*, 160:37–60, 2012.

[4] B. Erdmann, J. Lang, and R. Roitzsch. KARDOS-User's Guide. Manual, Konrad-Zuse-Zentrum Berlin, 2002.

Project: Adjoint-based Control of Model and Discretization Errors for Gas and Water Supply Networks

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.

Contact: P. Domschke, J. Lang

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[1] P. Domschke, O. Kolb, and J. Lang. Adjoint-based control of model and discretization errors for gas flow in networks. *International Journal of Mathematical Modelling and Numerical Optimisation*, 2(2):175–193, 2011.

[2] P. Domschke, O. Kolb, and J. Lang. Adjoint-based error control for the simulation of gas and water supply networks. In D. Aubry, P. Diez, B. Tie, and N. Pares, editors, *Adaptive Modeling and Simulation 2011*, pages 183–194. CIMNE, Barcelona, Spain, 2011.

[3] P. Domschke, O. Kolb, and J. Lang. *Computational Optimization and Applications in Engineering and Industry*, volume 359 of *Studies in Computational Intelligence*, chapter Adjoint-Based Control of Model and Discretization Errors for Gas and Water Supply Networks, pages 1–18. Springer, 2011.

Project: Domain-decomposition preconditioners for the Finite-Cell Method

The finite cell method is a framework that allows to utilize high order finite element methods on complicated geometries. The geometry and boundary conditions are taken into account by appropriate integration. The resulting linear systems are highly ill-conditioned and typically solved via direct solvers. In order to deal with large scal problems arising from applications in structural mechanics, we consider iterative solvers with additive Schwarz preconditioners based on overlapping domain decompositions. Mesh independent convergence can be proven under mild assumptions on the underlying geometry.

Partner: A. Düster, M. Joulaian; TU Hamburg-Harburg

Contact: H. Egger

Project: Numerical Methods for Optical Tomography

Optical Tomography is a non-invasive medical imaging technique that allows to probe biological tissue via near infrared light. For the simulation of light propagation, we consider high order Galerkin approximations and approriate preconditioned iterative solvers. The inverse problem is tackled by adequate regularization methods that allow to take into account a-priori information about the optical parameters in the object under investigation.

Partner: S. Arridge, UCL London

Contact: H. Egger, M. Schlottbom

References

[1] S. Arridge, H. Egger, and M. Schlottbom. Preconditioning of complex symmetric linear systems with applications in optical tomography. Preprint, TU Darmstadt, 2012.

[2] H. Egger and M. Schlottbom. A mixed variational framework for the radiative transfer equation. 22:1150014, 2012.

[3] H. Egger and M. Schlottbom. On unique solvability for stationary radiative transfer with vanishing absorption. Preprint, TU Darmstadt, 2012.

Project: Discontinuous Galerkin Methods for Incompressible Flow

For the approximation of incompressible flow problems, we consider discontinous Galerkin approximations of high order on unstructured meshes. Such discretizations are well-suited for adaptivity and a stable treatment of the convective terms by upwind mechanisms. Particular emphasis is put on deriving stability estimates with explicitly known dependence on the polynomial approximation order. These allow for a systematic a-priori and a-posteriori *hp* error analysis on locally refined and non-conforming hybrid meshes.

Partner: C. Waluga, TU München

Contact: H. Egger

References

[1] H. Egger and C. Waluga. hp-analysis of a hybrid DG method for Stokes flow. *IMA J. Numer. Anal.*, 2012.

[2] H. Egger and C. Waluga. A hybrid mortar method for incompressible flow. *IJNAM*, 9:793–812, 2012.

[3] C. Waluga and H. Egger. An implementation of hybrid discontinuous Galerkin methods in DUNE. In A. Dedner, B. Flemisch, and R. Klöfkorn, editors, *Advances in DUNE*. Springer, 2012.

Project: Finite Element Methods for Corner Singularities

The regularity of solutions of elliptic partial differential equations on polygonal domains is limited by the maximal interior angle. Following an idea of Zenger et al, we investigate a modification of the finite element method in a vicinity of the singularity that allows to obtain optimal convergence in weighted norms. Also other important quantities like *stress intensity factors* can be computed with optimal accuracy.

Partner: B. Wohlmuth, TU München

Contact: H. Egger

References

[1] H. Egger, U. Rüde, and B. Wohlmuth. Energy-corrected finite element methods for corner singularities. Preprint, TU München, 2012.

Project: Unique Solutions for Prices in Dixit-Stiglitz and Eaton-Kortum Models of Trade

We consider the existence of the key vector of endogenous variables, namely (goods or factor) prices, in Dixit-Stiglitz-type or Eaton-Kortum-type new trade models with arbitrarily many countries. Most quantitative (calibrated or estimated) models rely on such type of models. Provided existence and uniqueness of prices, it can be shown that the vector of prices can be determined numerically. But general results on existence and uniqueness are not available to date.

Partner: P. Egger, ETH Zürich

Contact: H. Egger

Project: Stability estimates for the Raviart-Thomas projector

Polynomial approximation estimates play a key role in the a-priori and a-posteriori error analysis of finite element methods. We consider *hp* estimates of the Raviart-Thomas projector for simplicial and rectangular elements in standard an non-standard norms. Such estimates are required, e.g. for the error analysis of mixed formulations of elliptic problems, for the analysis of a-posteriori error estimators based on flux reconstruction, but also for the stability analysis of novel discretizations for incompressible flow problems.

Partner: A. Chernov, Universität Bonn

Contact: H. Egger

Project: Quality Assessment for Large-Eddy-Simulations

In numerical simulations of flow problems or other engineering models governed by systems of partial differential equations, mesh adaptivity has become a major feature securing the quality of the solution of a simulation. For modeling turbulent flows with Large-Eddy-Simulations, locally large solution variations are best resolved by a high concentration of mesh points while in domains with less solution activity fewer mesh points are sufficient. We equip a common flow solver with a Mesh-Moving-PDE, which is able to redistribute grid points while keeping the data structure. So called monitor functions measure the importance of certain domains by user defined criteria and support the Mesh-Moving-PDE with the needed information where grid points are mostly desired. These criteria are usually physically motivated like the turbulent kinetic energy.

To compare these physically motivated monitor functions with mathematically motivated ones, we add adjoint-based information. For time averaged quantities of interest, we derived an adjoint-based a posteriori error estimator using a stationary adjoint equation. This new error estimator will help to improve mesh quality and also allows to focus on scalar quantities of interest, like for example drag and lift coefficients. Furthermore, a separation of the discretization and the modeling error is in the focus of our research, which will result in more accurate solutions for turbulent flows.

Partner: C. Hertel (TU Dresden), M. Schümichen (TU Dresden), J. Fröhlich (TU Dresden), Rolls-Royce Deutschland

Support: German Research Association (DFG) doctorate program GRK1344 “Instationäre Systemmodellierung von Flugtriebwerken”, Graduate School of Computational Engineering (CE).

Contact: M. Frankenbach, J. Lang

References

[1] C. Hertel, M. Schümichen, S. Löbig, J. Fröhlich, and J. Lang. Adaptive large eddy simulation with moving grids. *Theoretical and Computational Fluid Dynamics*, pages 1–25, 2012.

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: Prof. Dr. K. Raum (Charité Universitätsmedizin Berlin), Prof. Dr. Q. Grimal (Pierre-and-Marie-Curie University (Paris VI), France)

Support: DFG grants GE1894/3 and Ra1380/7

Contact: S. Tiburtius, A. Gerisch

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[1] M. Granke, Q. Grimal, A. Saïed, P. Laugier, F. Peyrin, A. Gerisch, and K. Raum. Contributions of pore volume fraction and mineralized matrix elasticity to millimeter-scale cortical bone elastic coefficients. In C. Hellmich, M. H. Hamza, and D. Simsik, editors, *IASTED Biomedical Engineering, 15.-17.02.2012, Innsbruck, Austria*, pages 764–133. ACTA Press, 2012.

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[3] K. Raum, Q. Grimal, P. Laugier, and A. Gerisch. Multiscale structure-functional modeling of lamellar bone. *Proceedings of Meetings on Acoustics*, 9:020005, 2011.

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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. Chaplain (University of Dundee, Scotland), L. Geris (University of Liége, Belgium)

Contact: A. Gerisch

References

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[2] L. Geris and A. Gerisch. Mathematical modelling of cell adhesion in tissue engineering using continuum models. In A. Gefen, editor, *Cellular and Biomolecular Mechanics and Mechanobiology*, volume 4 of *Studies in Mechanobiology, Tissue Engineering and Biomaterials*, pages 431–450. Springer Berlin Heidelberg, 2011.

[3] V. Peiffer, A. Gerisch, D. Vandepitte, H. Van Oosterwyck, and L. Geris. A hybrid bioregulatory model of angiogenesis during bone fracture healing. *Biomech Model Mechanobiol*, 10:383–395, 2011.

Project: Autumn School for High-School Pupils in Mathematical Modelling

40 pupils and 16 teachers and teacher students work together in 8 groups for one week. Each group has to solve a different problem from a different application. The problem has to be transferred into a mathematical problem (modeling), it has to be solved and the solution has to be documented (report) and presented in a final talk. The pupils were in the last year before graduation an had been selected by a countrywide competition in mathematics. The aim is to further motivate these pupils for further egagement in mathmatics. The teacher should experience mathematics as an universal instrument for reasonable decisions in all parts of our live and supply them with authentic examples, so that they can act as multipliers and spread the knowledge about the importance of mathematics in a modern industrial community.

Contact: M. Kiehl

References

[1] M. Kiehl. Bedeutung von Mathematik erfahrbar machen – Modellierungswochen für Schüler und Lehrer. To appear.

Project: Mathematical modeling integrated in the discussion of function classes

Mathematical modeling is a newly formulated requirement for the education in school. Nevertheless, there are very few hints, to tell the teacher, how they can meet these requirements. In this project we will develope a set of mini-projects, and prepare solutions and programming environments so that not much extra time is needed in class nor for preparation by the teacher. The projects should not only teach the basics of modelling, but also promote the understanding of mathematics as a universal tool and at the same time support a better an deeper understanding of functions and the meaning of their parameters and stimulate a critical handling with empirical results.

Contact: M. Kiehl

References

[1] M. Kiehl. Modellieren mit Funktionen im Rahmen der Curriculumsspirale. To appear.

Project: Mathematical models of the chemical evolution of t-RNA

Evolution as we know it today consists of an media (m-RNA) that can store information and preserve it over long time, because it is a very inert molecule, that does hardly react itself. It can also be copied (reproduction) with the chance of misstakes (mutation). Because m-RNA hardly reacts, a translation mechanism (t-RNA) is needed, that converts the information into very reactive molecules (proteins) that can help the compartment (cell), that also includes the information, to survive (selection) and so promote the spread of the according information. The question of how such a system could evolve leads to the classical dilemma of "which came first, the chicken or the egg?". In more detail, the question is, why should there be only a very special set of t-RNA, to translate special triplets of a m-RNA into a special sequence of amino acids, as long as there is no meaningful m-RNA and why should there be any m-RNA that might be meaningful, if it would be translated into a sequence of amino acids when using the right code, before there is a fixed set of t-RNA that provides with the according translation? In the project we develope models for this initial evolution process.

Contact: M. Kiehl

References

[1] M. Kiehl and F. Knapp. Fast computation of a realistic secondary structure of RNA by local minimization of the Zuker-free-energy inspired by models of the real folding process in vitro. To appear.

Project: Discrete-Continuous Optimization of Gas and Water Supply Networks

Today's demands in the management of gas and water supply networks require the close collaboration between industry and scientists from engineering and applied mathematics. The aim of this project is to tackle recent problems in gas and water management with state-of-the-art numerical methods and to develop new adapted algorithms.
The given tasks include the solution of hyperbolic partial differential algebraic equations on networks as well as discrete-continuous optimal control problems. The numerical methods for the solution of the underlying partial differential algebraic equations and continuous optimization problems are implemented in our software package ANACONDA. Discrete decisions can be (partially) given a-priori or determined via a penalization approach.

Partner: K. Klamroth (Universität Wuppertal), G. Leugering (Universität Erlangen-Nürnberg), A. Martin (Universität Erlangen-Nürnberg), M. Oberlack (TU Darmstadt), M. Ostrowski (TU Darmstadt), Hessenwasser GmbH & Co. KG, Siemens AG

Support: Federal Ministry of Education and Research (BMBF)

Contact: O. Kolb, J. Lang

References

[1] A. Martin, K. Klamroth, J. Lang, G. Leugering, A. Morsi, M. Oberlack, M. Ostrowski, and R. Rosen, editors. *Mathematical Optimization of Water Networks*, volume 162 of *International Series of Numerical Mathematics*. Birkhäuser Basel, 2012.

Project: Higher-order multirate methods for transient multi-physics problems

Many physical phenomena can be described by a set of coupled ordinary differential equations (ODEs) in time. A normal singlerate time integrator solves all ODEs with the same time step sizes, which are determined by taking all the components into account. This might produce very small time steps that also have to be applied to components with much less activity. The idea of multirate methods is to use different time step sizes for different components, depending on the individual activity of the solution, which means there will be a differentiation between active and latent components. The coupling can be managed by interpolation/extrapolation. Multirate methods using Rosenbrock-methods are well known in literature, but have the problem that due to the order reduction phenomenon of one step methods in the case of stiff problems, higher-order methods are difficult to obtain. To gain higher-order multirate methods the idea of this project is the development of multirate methods using two-step Peer-methods. Since for Peer-methods no order reduction was observed in the singlerate case, a similar behaviour in the multirate case is expected. Also stability investigations of multirate Rosenbrock- and multirate Peer-methods are part of this project.

Support: Graduate School of Computational Engineering, TU Darmstadt (DFG)

Contact: K. Kuhn, 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. *Appl. Numer. Math.*, 59:624–638, 2009.

[2] K. Kuhn and J. Lang. Comparison of the asymptotic stability for multirate Rosenbrock methods. submitted 2012 to Journal of Computational and Applied Mathematics.

Project: KARDOS - Software Package for Solving Nonlinear Evolution Problems

The code KARDOS was originally developed at ZIB Berlin to solve systems of non-linear mixed parabolic-elliptic partial differential equations by means of adaptive space and time discretizations. Linearly implicit one-step methods of Rosenbrock type are coupled with standard finite elements of various orders. KARDOS uses unstructured grids in one, two, and three space dimensions.

A large proportion of the current work is carried out in close collaboration with ZIB Berlin. Extensions that we are working on include: incorporation of computational fluid dynamics (CFD), electromagnetics, optimisation, uncertainty quantification and moving finite elements.

Although this software is mainly used for scientific and educational purposes, we are interested in cooperations with external organisations (industry, goverment research laboratories, etc) or other university departments (particularly engineering departments).

Partner: P. Deuflhard, B. Erdmann, R. Roitzsch (ZIB)

Contact: J. Lang

Project: W-methods for Optimal Control

We have developed W-methods of linearly implicit structure for the numerical approximation of optimal control problems within the first-discretize-then-optimize approach. Following the concept of transformed adjoint equations, we analyzed the approximation order and derived novel order that have to be satisfied by the coefficients of the W-methods so that the Taylor expansions of the continuous and discretize state and costate solutions match to order three. The W-methods are remarkably robust with respect to varying approximations of the Jacobian matrix. This allows for partitioning to treat stiff and nonstiff components more efficiently in the linear algebra. Most notable for the W-methods is their structural advantage when they are applied within a gradient approach to solve state and costate equations separately. Only a sequence of linear equations with one and the same system matrix has to be solved to compute the stages values. We expect that this property will become even more important for the numerical solution of large scale PDE-constrained optimal control problems.

Partner: J. Verwer (CWI, Amsterdam)

Support: German Research Association (DFG)

Contact: J. Lang

References

[1] J. Lang and J. Verwer. W-methods for optimal control. Preprint, TU Darmstadt, 2011.

Project: Stabilized Finite Elements for Transient Flow Problems

We proposed a way to circumvent artificial pressure oscillations for transient flow problems discretized with stabilized finite elements which may arise due to mesh changes for the projection. Instead of using the velocities of the previous time step in the right hand side of the new time level, a divergence-free projected velocity should be used. This projected velocity is the solution of a corresponding discrete Darcy problem with its own stabilization. It turns out that additional terms should be considered in the discrete equations in order to get a consistent scheme. We analyzed the corresponding Stokes system and proved bounded discrete pressure for arbitrary small time steps. The type of stabilization is quite general.

Partner: M. Braack, N. Taschenberger (Universität Kiel)

Contact: J. Lang

References

[1] M. Braack, J. Lang, and N. Taschenberger. Stabilized finite elements for transient flow problems on varying spatial meshes. *Computer Methods in Applied Mechanics and Engineering*, 253:106–116, 2012.

Project: Forward and Inverse Problems in Non-Linear Drift-Diffusion

Non-linear drift diffusion models are a specific class of partial differential equations. They appear in a large number of applications ranging from the dynamics of single molecules in an ion channel or the movement of cells up to the collective behaviour of animals or even humans. In their most general form these equations raise a large number of mathematical problems, such as whether there exists a solution (direct problem) or the determination of unknown parameters in the equation using measurements of a given solution (inverse problem). Due to the diversity of questions this project focuses on some numerical and analytical aspects as well as inverse problems related to these models with a special emphasis on their connection. We examine the inverse problem both analytically and numerically, which includes the development of robust numerical discretisations for the direct problem. Furthermore, we will consider an alternative geometric interpretation, yielding to the concept of gradient flows. This reformulation gives additional information about the solutions, which will help us to evaluate the numerical algorithms, cf. [1]. As a final step we shall apply these results to real data in the context of ion channels and nanopores.

Partner: Deutsche Forschungsgemeinschaft (DFG), The Daimler and Benz Foundation (PostDoc stipend)

Contact: J.-F. Pietschmann

References

[1] M. Burger, J.-F. Pietschmann, and M.-T. Wolfram. Identification of nonlinearities in transport-diffusion models for size exclusion. *UCLA CAM report*, 11-80, 2011.

Project: New mathematical methods and models for an improved understanding of synthetic nanopores

Synthetic nanopores are an important element in nanotechnology with applications in the medical and pharmaceutical industry. However, existing linear models, such as the Poisson-Nernst-Planck equations, can only explain part of the experimental observations. Thus, in this project we will introduce new, nonlinear models including finite size effects. Continuing previous work, cf. [1, 2], we shall perform extensive numerical simulations and compare the results with experimental data from our collaborators, the Siwy research lab at the University of California, Irvine. In a second step, methods from the scope of inverse problem will be applied to reconstruct properties of the pore that cannot be observed experimentally. A prominent example is the surface charge inside the pore.

Partner: German Academic Exchange Service (DAAD), PPP-Project

Contact: J.-F. Pietschmann

References

[1] M. Burger, M. Di Francesco, J.-F. Pietschmann, and B. Schlake. Nonlinear cross-diffusion with size exclusion. *SIAM Journal on Mathematical Analysis*, 42(6):2842–2871, 2010.

[2] M. Burger, P. A. Markowich, and J.-F. Pietschmann. Continuous limit of a crowd motion and herding model: analysis and numerical simulations. *Kinet. Relat. Models*, 4(4):1025–1047, 2011.

Project: Global Error Estimation for Finite Element Methods for Parabolic Differential Equations

Modern solvers for partial differential equations of parabolic type gain in efficiency by adaptivly optimizing their grids based on local error control. However, the accuracy imposed by the user applies to the global error of the approximation. In this project we focus on efficient and reliable estimation and control of the global errors in finite element methods.

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 appearing subproblems in the method of lines our strategies are based on the concepts of B-stability and B-convergence.

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

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.

Project: Unsteady Adaptive Stochastic Collocation Methods on Sparse Grids

This project incorporates uncertain quantities arising in nature or processes into numerical simulations. By doing so, computational results become more realistic and meaningful. Underlying mathematical models often consist of Partial Differential Equations (PDEs) with input data, that specify the describing system. If these input parameters are not explicitly known or subject to natural fluctuations, we arrive at PDEs with random parameters. We focus on random parameters that can be described by correlated random fields. A parametrization into finitely many random variables yields problems with possibly high dimensional parameter space, that has to be discretized beside the deterministic dimensions. To this end, we use adaptive, anisotropic stochastic collocation on sparse grids. Similar to a Monte Carlo simulation, this approach decouples and hence parallelizes the stochastic problem into a set of deterministic problems. By means of fluid flow examples, we show impressively that the method is able to resolve a stochastic parameter space of up to $20-50$ dimensions. Moreover, we extend the adjoint approach to stochastic collocation methods in order to derive error estimates for stochastic quantities of interest.

Contact: B. Schieche, J. Lang.

Support: German Research Foundation (DFG): Graduate School of Computational Engineering, TU Darmstadt.

References

[1] B. Schieche. Adaptive stochastic collocation on sparse grids. In H.-D. Alber, N. Kraynyukova, and C. Tropea, editors, *Proceedings in Applied Mathematics and Mechanics*, pages 653–654. WILEY, Weinheim, 2012.

[2] B. Schieche and J. Lang. Adjoint error estimation for stochastic collocation methods. Preprint, TU Darmstadt, 2012.

[3] B. Schieche and J. Lang. Uncertainty quantification for thermo-convective poiseuille flow using stochastic collocation. *Int. J. Computational Science and Engineering*, to appear.

Project: Stability and consistency of discrete adjoint peer methods

In optimal control of differential equations there are essentially two approaches to generate an discrete optimality system. The first-optimize-then-discretize approach means that the continuous optimality system is discretized, wheras the first-discretize-then-optimize approach solves the optimality system generated from the discretized optimal control problem. It is advantageous in optimal control, if the two approaches are interchangeable. Therefore it is important that the discrete adjoint of a time discretization is consistent with the continuous adjoint equation.

Implicit peer methods are sucessfully applied in the numerical solution of stiff ordinary differential equations and time time-dependent partial differential equations. We derived additional consistency order conditions for constant stepsizes, such that the discrete adjoint method is consistent with the continuous adjoint. Furthermore, we analyzed the stability of the discrete adjoint method. Stable methods of order two and three with a consistent discrete adjoint were constructed and the theoretical order was tested on a selection of ODE test problems. It was shown that in terms of consistency order of the method and its discrete adjoint implicit peer methods can not be better than backward differentiation formulas.

Contact: D. Schröder, J. Lang

References

[1] D. Schröder, J. Lang, and R. Weiner. Stability and Consistency of Discrete Adjoint Implicit Peer Methods. *submitted to Journal of Computational and Applied Mathematics*, 2012.

Project: Reduced-order modeling of incompressible flow problems

Reduced-order models promise speed-up of orders of magnitude for applications where flow problems are solved multiple times for different parameters, under the condition that the solution can be represented by a linear combination of a small number of global basis functions. In this project, models based on the proper orthogonal decomposition (POD) and the centroidal Voronoi tessellation (CVT) are explored as means of order reduction.

The number of degrees of freedom necessary to compute flow fields accurately is increasing quickly with a rising Reynolds number, which makes direct numerical simulations of turbulent flows expensive in terms of computational cost. The large-eddy simulation (LES) tackles this problem by resolving only the larger scales of the flow and modeling the effect of the sub-grid scales, e.g. by introducing an artificial eddy viscosity. It is investigated how reduced-order models for the coherent structures of the flow field can be improved using LES modeling techniques.

Flow problems with uncertain boundary conditions are considered as another field of application for reduced-order models. 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 multidimensional parameter domain. The goal of the project is to save computational time by replacing full-order finite element computations with reduced-order computations at the collocation points.

Support: DFG Collaborative Research Centre (SFB) 568 “Flow and Combustion in Future Gas Turbine Combustion Chambers”, 2008-2011. DFG Cluster of Excellence (EXC) 259: “Center of Smart Interfaces”, 2012. DFG Schwerpunktprogramm (SPP) 1276: “MetStröm: Skalenübergreifende Modellierung in der Strömungsmechanik und Meteorologie”, 2012

Contact: S. Ullmann, J. Lang

References

[1] S. Ullmann and J. Lang. A POD-Galerkin reduced model with updated coefficients for Smagorinsky LES. In J. C. F. Pereira, A. Sequeira, and J. M. C. Pereira, editors, *Proceedings of the V European Conference on Computational Fluid Dynamics ECCOMAS CFD 2010*, Lisbon, Portugal, June 2010.

[2] S. Ullmann and J. Lang. POD and CVT Galerkin reduced-order modeling of the flow around a cylinder. In H.-D. Alber, N. Kraynyukova, and C. Tropea, editors, *Proceedings in Applied Mathematics and Mechanics*, pages 697–698. Wiley-VCH, 2012.

[3] S. Ullmann and J. Lang. POD-Galerkin modeling and sparse-grid collocation for a natural convection problem with stochastic boundary conditions. In *Sparse Grids and Applications*. Springer, 2013.

[4] 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*, pages 349–378. Springer, 2013.

1.3 Memberships in Scientific Boards and Committees

Alf Gerisch

- European Society of Mathematical and Theoretical Biology
- Gesellschaft Deutscher Naturforscher und Ärzte e.V.
- Society of Industrial and Applied Mathematics

Martin Kiehl

- Chairman of the supervisory board of: Zentrum für Mathematik, Bensheim

Jens Lang

- Member of board of directors of the research centre Computational Engineering, TU Darmstadt, since 2004
- Member of board of deans of the DFG Graduate School of Excellence, TU Darmstadt, since 2008
- Member of the DFG Cluster of Excellence Smart Interfaces: Understanding and Designing Fluid Boundaries, TU Darmstadt, 2008 - 2012
- Member of the DFG Graduate School of Excellence Energy Science and Engineering, TU Darmstadt, since 2012

1.4 Awards

Awards

Pia Domschke: Ruth-Moufang-Price (Fachbereich Mathematik, TU Darmstadt), May 25, 2011

2 Publications

2.1 Co-Editors of Publications

2.1.1 Editors of Journals

Jens Lang

– *Applied Numerical Mathematics* (Editor)

2.1.2 Editors of Proceedings

Martin Kiehl

– *Proceedings on Mathematische Modellierung mit Schülern – Die Projekte der Modellierungswoche, 9.-14.10.2011, Weilburg*

– *Proceedings on Mathematische Modellierung mit Schülern – Die Projekte der Modellierungswoche, 14.-19.10.2012, Fuldatal*

2.2 Monographs and Books

[1] A. Martin, K. Klamroth, J. Lang, G. Leugering, A. Morsi, M. Oberlack, M. Ostrowski, and R. Rosen. *Mathematical Optimization of Water Networks*, volume 162 of *International Series of Numerical Mathematics*. Birkhäuser, 2012.

2.3 Publications in Journals and Proceedings

2.3.1 Journals

[1] V. Andasari, A. Gerisch, G. Lolas, A. P. South, and M. A. J. Chaplain. Mathematical modeling of cancer cell invasion of tissue: biological insight from mathematical analysis and computational simulation. *J. Math. Biol.*, 63:141–171, 2011.

[2] M. Braack, J. Lang, and N. Taschenberger. Stabilized finite elements for transient flow problems on varying spatial meshes. *Computer Methods in Applied Mechanics and Engineering*, 253:106–116, 2012.

[3] D. Clever and J. Lang. Optimal control of radiative heat transfer in glass cooling with restrictions on the temperature gradient. *Optimal Control Applications and Methods*, 33(2):157–175, 2012.

[4] D. Clever, J. Lang, and D. Schröder. Model hierarchy based optimal control of radiative heat transfer. *Accepted to International Journal of Computational Science and Engineering*, 2012.

[5] D. Clever, J. Lang, S. Ulbrich, and J. C. Ziems. Generalized multilevel SQP-methods for PDAE-constrained optimization based on space-time adaptive PDAE solvers. *Constrained Optimization and Optimal Control for Partial Differential Equations*, 160:37–60, 2012.

[6] 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. on Computing*, 23(4):605–617, Oct. 2011.

[7] P. Domschke, O. Kolb, and J. Lang. Adjoint-based control of model and discretization errors for gas flow in networks. *International Journal of Mathematical Modelling and Numerical Optimisation*, 2(2):175–193, 2011.

[8] H. Egger and M. Schlottbom. A mixed variational framework for the radiative transfer equation. *Math. Mod. Meth. Appl. Sci.*, 22:1150014–1150043, 2012.

[9] H. Egger and C. Waluga. hp-analysis of a hybrid DG method for Stokes flow. *IMA J. Numer. Anal.*, 2012.

[10] H. Egger and C. Waluga. A hybrid mortar method for incompressible flow. *IJNAM*, 9:793–812, 2012.

[11] M. Frank, J. Lang, and M. Schäfer. Adaptive finite element simulation of the time-dependent simplified PN equations. *Journal of Scientific Computing*, 49(3):332–350, 2011.

[12] B. 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, 2011.

[13] Q. Grimal, K. Raum, A. Gerisch, and P. Laugier. A determination of the minimum sizes of representative volume elements for the prediction of cortical bone elastic properties. *Biomech Model Mechanobiol*, 10:925–937, 2011.

[14] C. Hertel, M. Schümichen, S. Löbig, J. Fröhlich, and J. Lang. Adaptive large eddy simulation with moving grids. *Theoretical and Computational Fluid Dynamics*, pages 1–25, 2012.

[15] V. Peiffer, A. Gerisch, D. Vandepitte, H. Van Oosterwyck, and L. Geris. A hybrid bioregulatory model of angiogenesis during bone fracture healing. *Biomech Model Mechanobiol*, 10:383–395, 2011.

[16] K. Raum, Q. Grimal, P. Laugier, and A. Gerisch. Multiscale structure-functional modeling of lamellar bone. *Proceedings of Meetings on Acoustics*, 9:020005, 2011.

[17] D. Rohrbach, S. Lakshmanan, F. Peyrin, M. Langer, A. Gerisch, Q. Grimal, P. Laugier, and K. Raum. Spatial distribution of tissue level properties in a human femoral cortical bone. *Journal of Biomechanics*, 45:2264 – 2270, 2012.

[18] B. Schieche and J. Lang. Uncertainty quantification for thermo-convective poiseuille flow using stochastic collocation. *Int. J. Computational Science and Engineering*, to appear.

2.3.2 Proceedings and Chapters in Collections

[1] D. Clever. *Adaptive Multilevel Methods for PDAE-Constrained Optimal Control Problems*. PhD thesis, TU Darmstadt, 2012. To appear in Verlag Dr. Hut, ISBN 978-3-8439-0878-8.

[2] D. Clever and J. Lang. Multilevel optimization for PDAE-constrained optimal control problems - pointwise constraints on control and state. *Proc. Appl. Math. Mech.*, 12:689–690, 2012.

[3] P. Domschke, O. Kolb, and J. Lang. Adjoint-based error control for the simulation of gas and water supply networks. In D. Aubry, P. Diez, B. Tie, and N. Pares, editors, *Adaptive Modeling and Simulation 2011*, pages 183–194. CIMNE, Barcelona, Spain, 2011.

[4] P. Domschke, O. Kolb, and J. Lang. *Computational Optimization and Applications in Engineering and Industry*, volume 359 of *Studies in Computational Intelligence*, chapter Adjoint-Based Control of Model and Discretization Errors for Gas and Water Supply Networks, pages 1–18. Springer, 2011.

[5] L. Geris and A. Gerisch. Mathematical modelling of cell adhesion in tissue engineering using continuum models. In A. Gefen, editor, *Cellular and Biomolecular Mechanics and Mechanobiology*, volume 4 of *Studies in Mechanobiology, Tissue Engineering and Biomaterials*, pages 431–450. Springer Berlin Heidelberg, 2011.

[6] M. Granke, Q. Grimal, A. Saïed, P. Laugier, F. Peyrin, A. Gerisch, and K. Raum. Contributions of pore volume fraction and mineralized matrix elasticity to millimeter-scale cortical bone elastic coefficients. In C. Hellmich, M. H. Hamza, and D. Simsik, editors, *IASTED Biomedical Engineering, 15.-17.02.2012, Innsbruck, Austria*, pages 764–133. ACTA Press, 2012.

[7] O. Kolb and J. Lang. *Mathematical Optimization of Water Networks*, chapter Simulation and Continuous Optimization, pages 17–33. Birkhäuser Basel, 2012.

[8] O. Kolb, A. Morsi, J. Lang, and A. Martin. *Mathematical Optimization of Water Networks*, chapter Nonlinear and Mixed Integer Linear Programming, pages 55–65. Birkhäuser Basel, 2012.

[9] B. Schieche. Adaptive stochastic collocation on sparse grids. In H.-D. Alber, N. Kraynyukova, and C. Tropea, editors, *Proceedings in Applied Mathematics and Mechanics*, pages 653–654. WILEY-VCH, Weinheim, 2012.

[10] S. Ullmann and J. Lang. POD and CVT Galerkin reduced-order modeling of the flow around a cylinder. In H.-D. Alber, N. Kraynyukova, and C. Tropea, editors, *Proceedings in Applied Mathematics and Mechanics*, pages 697–698. Wiley-VCH, 2012.

[11] S. Ullmann and J. Lang. POD-Galerkin modeling and sparse-grid collocation for a natural convection problem with stochastic boundary conditions. In *Sparse Grids and Applications*. Springer, to appear.

[12] 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*, pages 349–378. Springer, 2013.

[13] C. Waluga and H. Egger. An implementation of hybrid discontinuous Galerkin methods in DUNE. In A. Dedner, B. Flemisch, and R. Klöfkorn, editors, *Advances in DUNE*. Springer, 2012.

2.4 Preprints

[1] S. Arridge, H. Egger, and M. Schlottbom. Preconditioning of complex symmetric linear systems with applications in optical tomography. Preprint, TU Darmstadt, 2012.

[2] D. Clever. Analysis for an SP_1-N_ν-band model in radiative heat transfer. Preprint 2658, TU Darmstadt, 2012.

[3] H. Egger, U. Rüde, and B. Wohlmuth. Energy-corrected finite element methods for corner singularities. Preprint, TU München, 2012.

[4] H. Egger and M. Schlottbom. On unique solvability for stationary radiative transfer with vanishing absorption. Preprint, TU Darmstadt, 2012.

[5] J. Lang and J. Verwer. W-methods for optimal control. Preprint, TU Darmstadt, 2011.

[6] B. Schieche and J. Lang. Adjoint error estimation for stochastic collocation methods. Preprint, TU Darmstadt, 2012.

2.5 Refereeing

Herbert Egger: Applicable Analysis, Applied Mathematics Letters, Applied Numerical Mathematics, Computers and Mathematics with Applications, Inverse Problems, Inverse Problems in Imaging, Mathematics and Computers in Simulation, Numerical Algorithms, Numerische Mathematik, SIAM Journal on Numerical Analysis, SIAM Journal on Scientific Computing

Alf Gerisch: Applied Mathematics Letters, Bulletin of Mathematical Biology, Discrete and Continuous Dynamical Systems–B, PLoS ONE, Research Foundation – Flanders (Fonds Wetenschappelijk Onderzoek – Vlaanderen, FWO), SIAM Multiscale Modeling and Simulation, Journal of the Royal Society Interface

Martin Kiehl: Jugend forscht

Oliver Kolb: Workshop on Computational Optimization, Modelling and Simulation within ICCS 2011 and ICCS 2012

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

Jan-Frederik Pietschmann: Proceedings of the Royal Society A

2.6 Software

ANACONDA: *Solving Hyperbolic Partial Differential Algebraic Equations on Networks*
ANACONDA is a software package to solve hyperbolic partial differential algebraic equations on networks. Particularly, it is designed to solve simulation and optimal control tasks for gas and water supply networks. The software is jointly developed by Oliver Kolb, Björn Geißler and Antonio Morsi (all TU Darmstadt).

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. The software is jointly developed by Bodo Erdmann, Rainer Roitzsch (both ZIB) and Jens Lang, TU Darmstadt. For more information, see `www.zib.de`

donlp2: *Solving general smooth nonlinear optimization problems, version October 2012*
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. Four commercial licenses have been sold during this period and 57 academic licenses were given. For more information contact the author spellucci(_at_)mathematik.tu-darmstadt.de or see `http://www.mathematik.tu-darmstadt.de/fbereiche/numerik/staff/spellucci/DONLP2/index.html`

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. Each application comes with predefined test cases which can be used without programming knowledge at all. In the period under review the English version became fully operable. This version has been extended by 9 newly implemented methods and some other implementations were completely redesigned. There were about 6000 visits in 2011 and 12000 visits in 2012. Numawww meanwhile attracts attention internationally. For more information see `numawww.mathematik.tu-darmstadt.de`

Contributor at TU Darmstadt: Peter Spellucci

3 Theses

3.1 PhD Dissertations

2011

Domschke, Pia, *Adjoint-Based Control of Model and Discretization Errors for Gas Transport in Networked Pipelines* (Jens Lang)

Kolb, Oliver, *Simulation and Optimization of Gas and Water Supply Networks* (Jens Lang)

2012

Schieche, Bettina, *Unsteady Adaptive Stochastic Collocation Methods on Sparse Grids* (Jens Lang)

3.2 Diplom Theses

2011

Guo, Zhihong, *Numerical estimation of model parameters for a detailed industrial robot dynamics* (Oskar von Stryk / Martin Kiehl)

Kaspar, Larissa, *Metrikbasierte anisotrope Gitterverfeinerung* (Jens Lang)

Niederhöfer, Florian, *Zeitintegrationsverfahren höherer Ordnung in der Molekulardynamik* (Jens Wackerfuß / Jens Lang)

Schröder, Dirk, *Adaptive Multilevel-Verfahren für das Thermistor-Problem* (Jens Lang)

Steplavage, Martin Frank, *Konvergenzrate des Galerkin-Verfahrens für eine Klasse von stochastischen elliptischen Differentialgleichungen* (Klaus Ritter / Jens Lang)

2012

Brück, Sascha, *Development and analysis of a Discountinous Galerkin method on staggered grids for high frequency problems* (Erion Gjonaj / Jens Lang)

3.3 Master Theses

2012

Wolf, Melanie, *Druckstabilisierung bei adaptiver Diskretisierung der Stokes Gleichung* (Jens Lang)

3.4 Staatsexamen Theses

2011

Schwebel, Miriam, *Modellierung coexistierender Symbionten und Parasiten* (Martin Kiehl)

2012

Bott, Sebastian, *Projektions- und Rekonstruktionsmethoden für dreidimensionale Objekte* (Martin Kiehl, Regina Bruder (Zweitgutachter))

3.5 Bachelor Theses

2011

Kopp, Sonja, *Effiziente Gradienten- und Hesse-Matrix Berechnung bei gradientenbasierten numerischen Optimierungsverfahren angewandt auf atomistische molekulare Simulation* (Martin Kiehl)

2012

Knapp, Fabian, *Effiziente Ermittlung der RNA Sekundärstruktur durch lokale Optimierung auf Basis der freien Energie nach Zuker* (Martin Kiehl)

Lettmann, Michael, *Vorkonditionierung bei der iterativen Lösung linearer Gleichungssysteme* (Alf Gerisch / Jens Lang)

Lukassen, Axel Ariaan, *Stückweise kubische Rekonstruktion und deren Gradient von linearen Finite Element-Approximationen auf einer Triangulierung* (Alf Gerisch / Jens Lang)

Will, Karsten, *Implementierung und Test von Multirate-Rosenbrock-Verfahren* (Alf Gerisch / Jens Lang)

4 Presentations

4.1 Talks and Visits

4.1.1 Invited Talks and Addresses

Herbert Egger

10.10.12 *Analysis and Numerical Methods for Fluorescence Diffuse Optical Tomography*
Oberseminar Angewandte Mathematik, Universität Münster

24.10.12 *Numerical Realization of Tikhonov Regularization*
Workshop on Computational Inverse Problems, Oberwolfach

Alf Gerisch

05.04.11 *Fast evaluation of integral terms in a nonlocal PDE model of cellular adhesion*
Spring School on Evolution Equations, Universität Konstanz

13.11.12 *Mathematical modelling and numerical simulation of mechanical properties of muskuloskeletal mineralized tissues*
Conference and Workshop on Modelling and Computation in Musculoskeletal Engineering (MCME), Brisbane

Martin Kiehl

26.02.2011 *Die Mathematik im Puzzlestein – Warum Mathematiker ein Leben lang spielen?*
Mathematikolympiade Hessen, Darmstadt

26.03.2011 *Die Mathematik im Puzzlestein – Warum Mathematiker ein Leben lang spielen?*
Tag der Mathematik, Reinheim

25.02.2012 *Gier – Manchmal ein Weg zum Erfolg*
Mathematikolympiade Hessen, Darmstadt

10.03.2012 *Gier – Manchmal ein Weg zum Erfolg*
Tag der Mathematik, Reinheim

Oliver Kolb

06.09.12 *Combination of Linear and Nonlinear Programming Techniques for the Solution of Mixed Integer Optimization Problems in Water Supply Networks*
Conference on Modelling, Simulation and Optimization in Applications, Darmstadt

Jens Lang

15.01.11 *W-Methods for Optimal Control*
Jan Verwer's 65th Birthday - Farewell Conference, CWI Amsterdam

28.01.11 *Model Reduction in Unsteady Transport Systems*
Workshop on Model Order Reduction, WIAS Berlin

08.11.11 *Linearly Implicit Methods for Optimal Control Problems*
Mathematical Seminar, Geneva

01.04.12 *Linearly Implicit Time Integrators for Optimal Control Problems*
AMS Meeting, Lawrence

26.04.12 *Adaptive Time Integrators in Computational Fluid Dynamics*
Workshop on Adaptive Methods with Applications in Fluid Dynamics, WIAS Berlin

07.05.12 *Model Reduction in Unsteady Transport Systems*
Mathematical Seminar, Geosciences Department, Frankfurt

21.05.12 *Adaptive Multilevel Methods for Large-Scale Optimal Control Problems*
Mathematical Seminar, Leuven

10.07.12 *Adaptive Moving Meshes in Large Eddy Simulation for Turbulent Flows*
World Congress of Computational Mechanics, Special Session in Honor of J. Tinsley Oden's 75th Birthday, Sao Paulo

10.08.12 *Surrogate Modelling in Unsteady Transport Systems*
Workshop on Surrogate Modelling and Space Mapping for Engineering Optimization, Reykjavik

4.1.2 Contributed Talks

Debora Clever

16.05.11 *Model Hierarchy Based Multilevel SQP-Methods for PDAE-Constrained Optimal Control Problems with Application to Radiative Heat Transfer*
SIAM Conference on Optimization, Darmstadt

26.09.11 *Adaptive Multilevel SQP-Methods for PDAE-constrained Optimization*
Joint talk with J.C. Ziems, Annual Meeting - SPP1253, Kloster Banz

04.10.11 *Model Hierarchy Based Multilevel SQP-Methods for PDAE-Constrained Optimal Control Problems - Application to Radiative Heat Transfer in 2d and 3d*
2nd International Conference on Computational Engineering, Darmstadt

26.03.12 *Multilevel Optimization for PDAE-Constrained Optimal Control Problems - Pointwise Constraints on Control and State*
83rd Annual Meeting of the International Association of Applied Mathematics and Mechanics, Darmstadt

23.07.12 *Towards a Fully Space-Time Adaptive Multilevel Optimization Environment*
Workshop on Adaptivity and Model Order Reduction in PDE Constrained Optimization, Hamburg

Pia Domschke

18.05.11 *Optimization of Gas and Water Supply Networks*
SIAM Conference on Optimization OP11, Darmstadt

07.06.11 *Adjoint-based error control for the simulation of gas and water supply networks*
International Conference on Adaptive Modeling and Simulation (ADMOS) 2011, Paris

Alf Gerisch

18.01.11 *Fast evaluation of integral terms in a nonlocal PDE model of cellular adhesion*
Verwer65 Meeting, CWI, Amsterdam, The Netherlands

18.07.11 *A Micromechanical Model of the Mineralized Collagen Fibril Bundle with Application to Mineralized Turkey Leg Tendon Data (poster)*
ICIAM 2011, Vancouver, Canada

19.07.11 *Modelling and Simulation of Cellular Adhesion: the Impact on Spatio-temporal Patterns in Cancer Cell Invasion*
ICIAM 2011, Vancouver, Canada

27.10.11 *Numerical homogenization in multi-scale models of musculoskeletal mineralized tissues*
Comsol Conference, Stuttgart

16.11.11 *Numerical homogenization in multi-scale models of musculoskeletal mineralized tissues*
ACOMEM 2011, University of Liège, Belgium

02.05.12 *Tissue Scale Modelling and Simulation of Cell Adhesion*
SYNMIKRO Conference on Mathematical Modelling of Microbiological Systems, Universität Marburg

07.08.12 *Prediction of Effective Elastic Properties of Osteons by Means of Multiscale Models and Homogenization Methods (poster)*
SIAM Conference on the Life Sciences, San Diego, USA

11.09.12 *On the positivity in nonlocal PDE models of cell adhesion*
NUMDIFF-13, Universität Halle-Wittenberg

Oliver Kolb

14.04.12 *Optimization of Gas and Water Supply Networks*
Workshop on Numerical Methods for Optimal Control and Inverse Problems (OCIP) 2012, München

Karen Kuhn

24.07.12 *Stability analysis for multirate Rosenbrock- and Peer-methods*
ECMI, Lund

13.09.12 *Stability analysis for multirate Rosenbrock- and Peer-methods*
NUMDIFF-13, Halle

Jens Lang

13.07.11 *Linearly Implicit Methods for Optimal Control Problems*
SCiCADE 2011, Jan Verwer Memorial, Toronto

20.07.11 *Large Eddy Simulation with Adaptive Moving Meshes*
ICIAM 2011, Vancouver

06.09.11 *Adaptive Finite Elements with Anisotropic Mesh Refinement*
ENUMATH 2011, Leicester

26.06.12 *Adaptive Moving Meshes in Large Eddy Simulation for Turbulent Flows*
3rd European Seminar on Computing, Pilsen

10.09.12 *Adaptive Two-Step Peer Methods in Computational Fluid Dynamics*
NUMDIFF13, Halle

24.09.12 *Adaptive and Higher Order Methods in Computational Fluid Dynamics*
25th Chemnitz FEM Symposium 2012

Bettina Schieche

04.10.11 *Adjoint Error Estimation for Stochastic Collocation Methods*
2nd International Conference on Computational Engineering, Darmstadt

29.03.12 *Adaptive Stochastic Collocation on Sparse Grids*
GAMM, Darmstadt

02.04.12 *Adjoint Error Estimation for Stochastic Collocation Methods*
SIAM Conference on Uncertainty Quantification, Raleigh, North Carolina

26.06.12 *Analysis and Application of PDEs with Random Parameters*
European Seminar on Computing, Pilsen

05.07.12 *Analysis and Application of PDEs with Random Parameters*
2nd Workshop on Sparse Grids and Applications, Garching

Dirk Schröder

10.09.12 *Adjoint Consistent Implicit Peer Methods*
Numerical Solution of Differential and Differential-Algebraic Equations (NUMDIFF-13), 10-14 September 2012, Universität Halle-Wittenberg

Sara Tiburtius

30.06.11 *A multiscale model of mineralized fibril bundles - a homogenization approach*
ECMTB, Krakow

26.08.11 *A multiscale model of mineralized turkey leg tendon - a homogenization approach*
SimOrtho, Rostock

24.03.12 *SPP 1420 Project VI: Multiscale structure functional modeling of musculoskeletal tissues*
SPP 1420 Winter School, Golm

10.08.12 *Prediction of effective elastic properties of osteons by means of multiscale models and homogenization methods*
SIAM Conference on the Life Sciences (poster), San Diego

06.12.12 *Project VI: Multiscale structure-functional modeling of musculoskeletal mineralized tissues*
SPP 1420 project meeting, Düsseldorf

Sebastian Ullmann

27.03.12 *POD and CVT Galerkin reduced modeling of the flow around a cylinder*
GAMM 2012, Darmstadt

21.11.12 *POD-Galerkin-Modellierung thermo-konvektiver Strömungen*
Metström Bündeltreffen Adaptivität, Darmstadt

4.1.3 Visits

Herbert Egger, ETH Zürich, 11.-14.09.2012

Herbert Egger, TU München, 27.-28.09.2012

Herbert Egger, Universität Münster, 10.-11.10.2012

Herbert Egger, Oberwolfach, 21.-27.10.2012

Herbert Egger, Universität Linz, 9.-10.11.2012

Herbert Egger, TU München, 11.-12.11.2012

Jens Lang, University of Kansas, March-April 2012

Jan-Frederik Pietschmann, KTH Royal Institute of Technology, 19.-24. November 2012

Bettina Schieche, Universität Linz, December 2011

Sara Tiburtius, Pierre-and-Marie-Curie University (Paris VI), Laboratoire d'Imagerie Paramétrique, February - March 2011

Sara Tiburtius, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, 06.12.2012

4.2 Organization of Conferences and Workshops

Martin Kiehl

- Mathematikolympiade Hessen (Landesentscheid), 25.-26.02.2011, Darmstadt (jointly with Zentrum für Mathematik, Bensheim)
- Autumn School for Pupils; Mathematische Modellierungswoche, 9.-14.10.2011, Weilburg (jointly with Zentrum für Mathematik, Bensheim)
- Mathematikolympiade Hessen (Landesentscheid), 24.-25.02.2012, Darmstadt (jointly with Zentrum für Mathematik, Bensheim)
- Autumn School for Pupils; Mathematische Modellierungswoche, 14.-19.10.2012, Fuldatal (jointly with Zentrum für Mathematik, Bensheim)

Jens Lang

– 2nd International Conference on Computational Engineering, Marek Behr, Jens Lang, Ernst Rank, Michael Schäfer, October 2011, Darmstadt

– Workshop on Mathematics of Computation, Jens Lang and Stefan Ulbrich, Februray 2012, Darmstadt

5 Workshops and Visitors at the Department

5.1 Seminar Talks

14.03.12. Dr. Stefan Görtz (Deutsches Zentrum für Luft- und Raumfahrt, Braunschweig), *Reduzierte Modelle für aerodynamische Berechnungen*

5.2 Visitors

Prof. Dr. Gabriel Wittum (Universität Frankfurt), June 2011.

Jun.-Prof. Dr. Roland Pulch (Universität Wuppertal), April-October 2011.

Dr. Nilles (BASF Ludwigshafen), October 2011.

Prof. Dr. Rüdiger Weiner (Universität Halle-Wittenberg), February 2012.

Dr. Oswald Knoth (Leibnitz Institute for Tropospheric Research Leipzig), February 2012.

Prof. Dr. Willem Hundsdorfer (CWI Amsterdam), June 2012.

Prof. Dr. Martin Gander (University of Geneva), October 2012.

5.3 Workshops and Conferences

– International Project Meeting *Multiscale structure-functional modeling of musculoskeletal mineralized tissues*, TU Darmstadt, 10.-12.01.11 (organized by Alf Gerisch)

5.4 Scientific and Industrial Cooperations

Debora Clever

– Stefanie Bott, Prof. Dr. Stefan Ulbrich, Dr. Carsten Ziems (TU Darmstadt): Adaptive multilevel SQP-methods for PDAE-constrained optimization with restrictions on control and state. Supported by DFG, SPP 1253.

Herbert Egger

– Prof. S. Arridge, PhD (University College London): Numerical Methods for Optical Tomography.

– Prof. Dr. A. Chernov (Universität Bonn): Stability estimates for the Raviart-Thomas projector.

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

- Prof. Dr. P. Egger (ETH Zürich): Unique Solutions for Prices in Dixit-Stiglitz and Eaton-Kortum Models of Trade.
- Dr. C. Waluga (TU München): Hybrid DG Methods for Incompressible Flow.
- Prof. Dr. B. Wohlmuth (TU München), Prof. Dr. U. Rüde (Universität Erlangen-Nürnberg): Finite Element Methods for Corner Singularities.

Alf Gerisch

- Prof. Dr. K. Raum (Charité Universitätsmedizin Berlin) and Prof. Dr. Q. Grimal (Pierre-and-Marie-Curie University (Paris VI), France): Multiscale structure-functional modeling of musculoskeletal mineralized tissues.
- Prof. Dr. M. Chaplain (University of Dundee, Scotland): Mathematical modeling and simulation of cancer invasion.
- Prof. Dr. J. Lang (TU Darmstadt), Prof. Dr. R. Weiner, and Dr. H. Podhaisky (Universität Halle-Wittenberg): PEER methods and their application in the Finite Element system KARDOS.
- Prof. Dr. L. Geris (University of Liége, Belgium): Modeling and simulation of fracture healing and angiogenesis and in tissue engineering.

Oliver Kolb

- Prof. Dr. Kathrin Klamroth (Universität Wuppertal), Prof. Dr. Jens Lang (TU Darmstadt), Prof. Dr. Günter Leugering (Universität Erlangen-Nürnberg), Prof. Dr. Alexander Martin (Universität Erlangen-Nürnberg), Prof. Dr. Martin Oberlack (TU Darmstadt), Prof. Dr. Manfred Ostrowski (TU Darmstadt), Hessenwasser GmbH & Co. KG, Siemens AG: Diskret-kontinuierliche Optimierung komplexer dynamischer Wasserver- und -entsorgungssysteme. Supported by BMBF, 2007-2010.

Jens Lang

- Prof. Dr. Jan Verwer (University of Amsterdam and CWI): W-Methods for optimal control.
- Prof. Dr. Weizhang Huang (University of Kansas): Anisotropic mesh methods.
- Jun.-Prof. Dr. Oliver Kolb (Universität Mannheim): Simulation and optimization of gas and water networks.
- Prof. Dr. Malte Braack (Universität Kiel): Stabilized finite elements for transient flow problems.
- Prof. Dr. Rüdiger Weiner (Universität Halle-Wittenberg): Linearly implicit time integrators.
- Bodo Erdmann (ZIB): Kardos programming.

- Prof. Dr. Günter Leugering, Prof. Dr. A. Martin (Universität Erlangen-Nürnberg): Modelling, Analysis, Simulation and Optimal Control of Gas Transport in Networked Pipelines. Supported by DFG, 2007-2011.

- SFB 568: "Flow and Combustion in Future Gas Turbines". Speaker Prof. Dr.-Ing. Johannes Janicka (Department of Mechanical Engineering, TU Darmstadt). Supported by DFG, 2007-2011.

- GK 1344: "Instationary System Modelling of Aircraft Turbines", Speaker Prof. Dr.-Ing. Johannes Janicka (Department of Mechanical Engineering, TU Darmstadt). Supported by DFG, 2006-2014.

- SPP 1253: Optimization with PDEs. Supported by DFG, 2009-2012, jointly with Prof. Dr. Stefan Ulbrich (TU Darmstadt).

- Prof. Dr. Jochen Fröhlich (TU Dresden): Large Eddy Simulation with Adaptive Moving Meshes, Supported by DFG, Metstroem, 2007-2013.

- Dr. Nilles, BASF: Numerical Simulation, Modelling and Optimization of Multi-Phase and Multi-Scale Combustion Processes.

Jan-Frederik Pietschmann

- Prof. Dr. Martin Burger (Universität Münster): Flow Characteristics in a Crowded Transport Model.

- Dr. Marie-Therese Wolfram (Universität Wien): Numerical simulation and inverse problems related to ion channels.

- Prof. Dr. Zuzanna Siwy (University of California, Irvine): Modeling and simulation of nanopores.

- Prof. Dr. Henrik Shahgholian (KTH Royal Institute of Technology Stockholm): Numerical discretization of Hele-Shaw flow problems.

Sara Tiburtius

– SPP 1420: “Biomimetic Materials Research: Functionality by Hierarchical Structuring of Materials”. Supported by the German Research Foundation (DFG), 2012-2013, joint project of Dr. Alf Gerisch (Department of Mathematics, TU Darmstadt) and Prof. Dr. Kay Raum (Julius Wolff Institute and Berlin-Brandenburg School for Regenerative Therapies, Charité-Universitätsmedizin Berlin).

5.5 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

- Support of the annual organization of the Mathematikolympiade Hessen (third level) in cooperation with the Center for Mathematics Bensheim for all grades (about 25 participants per grade each year) (Prof. Kiehl, academic staff and students).
  As part of the final rounds in 2011 and 2012, mathematical afternoon lectures were delivered by Prof. Kiehl and Prof. Scheithauer.
- Organization of the Mathematical Modeling Week for secondary school students in grade 12 in cooperation with Center for Mathematics Bensheim each October (40 participants each year) (Prof. Kiehl).