# Österreichische Akademie der Wissenschaften

# Jahresbericht 2013

# Johann Radon Institute for Computational and Applied Mathematics (RICAM)

BERICHTSZEITRAUM:                    1.1.2013 – 31.12.2013

INSTITUTSDIREKTOR/IN :               Prof. Dr. Ulrich Langer
                                     (1.1.-31.3.2013)
                                     Prof. Dr. Ronny Ramlau
                                     (1.4.-31.12.2013)

ADRESSE                              Altenberger Straße 69,
                                     4040 Linz

# Inhalt

## 1. Mission Statement

The Johann Radon Institute for Computational and Applied Mathematics

- carries out basic research in computational and applied mathematics according to highest international standards
- obtains the motivation for its research topics also from challenges in other scientific fields and industry
- emphasizes interdisciplinary cooperation between its workgroups and with institutions with similar scope and universities world-wide
- cooperates with other disciplines in the framework of special semesters on topics of major current interest
- wishes to attract gifted PostDocs from all over the world and to provide an environment preparing them for international careers in academia or industry
- cooperates with universities by involving PhD-students into its research projects
- promotes, through its work and reports about it, the role of mathematics in science, industry and society

Das Institut verfügte 2013 über folgende Arbeitsgruppen:

- Arbeitsgruppe „Computational Methods for Direct Field Problems", Gruppenleiter: Prof. Dr. Ulrich Langer
- Arbeitsgruppe „Inverse Problems", Gruppenleiter: Prof. Dr. Otmar Scherzer
- Arbeitsgruppe „Symbolic Computation", Gruppenleiter: Prof. Dr. Josef Schicho
- Arbeitsgruppe „Analysis for Partial Differential Equations", Gruppenleiter: N.N.
- Arbeitsgruppe „Optimization and Optimal Control", Gruppenleiter: Prof. Dr. Karl Kunisch
- Arbeitsgruppe „Mathematical Imaging", Gruppenleiter: Prof. Dr. Otmar Scherzer
- Arbeitsgruppe „Mathematical Methods in Molecular and Systems Biology", Gruppenleiter: Prof. Dr. Christian Schmeiser, Prof. Dr. Philipp Kügler
- Transfergruppe,  Gruppenleiter: Prof. Dr. Ronny Ramlau
- Forschungsprojekt „Applied Discrete Mathematics and Cryptography", Projektleiter Doz. Dr. Arne Winterhof
- START-Project "Sparse Approximation and Optimization in High Dimensions", Projektleiter Prof. Dr. Massimo Fornasier

## 2. Wissenschaftliche Tätigkeit 2013 (Kurzfassung)

Im Folgenden wird kurz über die wissenschaftliche Tätigkeit der einzelnen Arbeitsgruppen berichtet. Details und Informationen über die Zusammenarbeit zwischen den einzelnen Gruppen sowie über die sonstigen wissenschaftlichen Tätigkeiten sind dem Abschnitt 6 zu entnehmen.

Die Forschungsarbeiten der **Computational Mathematics Group (CMG)** konzentrierten sich 2013 auf die Entwicklung, die Analyse sowie die Implementierung effizienter und robuster numerischer Methoden zur Lösung partieller Differentialgleichungen bzw. von Systemen gekoppelter partieller Differentialgleichungen wie sie in vielen Anwendungsfeldern entstehen. Typische Anwendungsbereiche sind Diffusionsphänomene in heterogenen Medien, Probleme aus der Festkörper- und Strömungsmechanik, Fluid-Struktur-Kopplungen, Elektromagnetik etc. Die CMG hat 2013 ganz wesentliche Beiträge zur Isogeometrischen Analysis (IGA) geleistet. Das ist ein relativ neues, weltweit boomendes Forschungsgebiet sowohl in den Ingenieurwissenschaften als auch in der Mathematik mit einem zu erwartendem hohen Impact in allen Bereichen der Computational Sciences sowie mit vielen Industrieanwendungen. Zwei Forschungsprojekte der CMG wurden 2013 vom FWF gefördert: Das IGA Software-Projekt G+SMO ist dabei ein Kooperationsprojekt verschiedener Gruppen im nationalen Forschungsnetzwerk NFN S117 „Geometry & Simulation".

Die Arbeitsgebiete der **Inversen Probleme Gruppe** sind traditionell sehr breit gefächert: Wir beschäftigen uns mit nichtlinearer Regularisiungstheorie, und, dazu in Verbindung stehend, mit der Entwicklung von Lernalgorithmen, die unter anderem zur Diabetes-Behandlung eingesetzt werden. Zu diesem Themenbereich gibt es in der Gruppe ein mathematisches FWF-Projekt P25424 „Data-driven and problem-oriented choice of the regularization space", welches von S. Pereverzyev geleitet wird. Wir beschäftigen uns zudem mit tomographischen Methoden, die in der Photoakustik verwendet werden. Dieses Thema wird durch den FWF im Rahmen des Nationalen Forschungsnetzwerks „Photoacoustic Imaging in Biology and Medicine" gefördert. Derzeit beschäftigen wir uns hier mit der Photoakustischen Bildgebung in einer stochastischen Umgebung. Des weiteren untersucht die Gruppe inverse Streuprobleme, ein klassisches Gebiet der Inversen Probleme.

Die Arbeitsgruppe **Symbolisches Rechnen** beschäftigte sich im Themenbereich der konstruktiven algebraischen Geometrie insbesondere mit der Parametrisierung von algebraischen

Kurven durch Radikale, die im Rahmen eines FWF Projektes sowie im vom FWF und dem Land Oberösterreich geförderte Doktoratskolleg "Computational Mathematics" zusammen mit mathematischen Instituten der Kepler Universität durchgeführt wurden.

In Kooperation mit H.-P. Schröcker von der Universität Innsbruck und Gabor Hegedüs (vormals RICAM, jetzt an der Universität von Obuda, Ungarn) ergaben sich Anwendungsmöglichkeiten im Bereich der Kinematik mit unerwarteten Durchbrüchen. Ein weiteres Gebiet, in dem die Gruppe schon länger tätig ist, ist die symbolische Funktionalanalysis, wo sowohl Algorithmen verbessert werden konnten als auch für die Bewertung von Versicherungsrisiken angewandt werden konnten. Ein Gebiet, in welchem die Gruppe erst seit 2012 einen weiteren Forschungsschwerpunkt hat, ist die algorithmische Kombinatorik. In diesem Jahr wurden mit dieser Methode Erfolge in der Knotentheorie und in der Theorie der Spline-Räume erzielt.

Die Forschung der Gruppe **Optimization and Optimal Control** konzentrierte sich auf die Analysis und die Entwicklung numerischer Verfahren von Optimalen Steuerungsproblemen bei partiellen Differentialgleichungen, unter besonderer Berücksichtigung von Gleichungen, welche Wellenausbreitungen beschreiben. Eine besondere Bedeutung wurde auch der Optimalen Steuerung der Bidomaingleichungen, welche die elektrokardio-graphische Beschreibung der Herzaktivität darstellen, eingeräumt. Im Bereich der Optimalsteuerung bei Gleichungen in der Fluidmechanik wurden einerseits Kontrollierbarkeitsprobleme und andererseits Gebietoptimierungsprobleme analysiert. Darüber hinaus wurde eine mittelfristige Neuausrichtung der Gruppe von open- auf closed loop Probleme begonnen.

Die **Imaging Gruppe** beschäftigte sich im Berichtzeitraum mit der Analyse und numerischen Implementierung von Orts-Zeit Algorithmen für parabolische Evolutionsgleichungen und der Parameterschätzung in Transportgleichungen, die in Imaging Problemen auftreten. Unsere Arbeiten auf dem Gebiet hoher Wellen von inkompressiblen Flüssigkeiten, einem freiem Randwertproblem, führte zu einem neuen, zum ersten Mal nicht stochastischen, numerischen Algorithmus. Erhebliche Effizienzgewinne dieses Algorithmus konnten durch analytische Überlegungen zur Berechnung besserer Startwerte erzielt werden. Diese neuen Überlegungen waren für die wissenschaftliche Community überraschend, da sie nicht mit der mathematischen Intuition von der Anzahl der unabhängigen Parameter korreliert.

Gemeinsam mit Kollegen der Max F. Perutz Laboratorien hat die **Bio-Gruppe** an der Stressantwort der Hypothalamus-Hypophyse-Nebennierenrinde-Achse zur Cortisolproduktion geforscht. Hypocortisolismus kann als defekter bistabiler Schalter des zugrundeliegenden

Reaktionsnetzwerks aufgefasst werden, am RICAM entwickelte Methoden zur Bifurkationskontrolle liefern mit der zunächst weiteren Reduktion des Cortisolniveaus einen Therapieansatz entgegen der medizinischen Intuition. Durch die Integration eines erst kürzlich experimentell entdeckten Glucocorticoidrezeptors in der Membran der Hypophysezellen in das mathematische Modell der Rückkopplungsmechanismen ist es nun auch möglich, das Krankheitsbild des Hypercortisolismus und entsprechende Therapiemaßnahmen zu simulieren. In einer Zusammenarbeit mit dem Institute for Molecular Biotechnology (ÖAW) gab es große Fortschritte beim Verständnis aktingetriebener Zellmotilität, wobei eine erste Erklärung für die Form von Lamellipodien und die detaillierte Beschreibung der intrazellulären Fortbewegung von Baculovirus hervorzuheben sind.

Ziel der 2011 gegründeten **Transfer Gruppe** ist die Überführung von aktuellen mathematischen Forschungsergebnissen in die Industrie. Daher erfolgen die Forschungsarbeiten der Mitarbeiter der Gruppe immer in Kooperation mit Unternehmen oder anderen außeruniversitären Einrichtungen. Im vergangenen Jahr wurden insbesondere Forschungskooperationen mit der Europäischen Südsternwarte ESO (Garching), der AVL List GmbH (Graz), der uni software plus GmbH (Linz), Siemens VAI Metals Technologies GmbH, der voestalpine Grobblech GmbH, der MathConsult GmbH (Linz) sowie mit der Bachmann GmbH (Feldkirch) durchgeführt. Für die ESO wurden im Rahmen eines österreichischen InKind Projektes mathematische Algorithmen und Software für die Adaptive Optik – Systeme des derzeit in Planung befindlichen European Extremely Large Telescopes (E-ELT) entwickelt. Dieses Projekt wurde in 2013 erfolgreich evaluiert und abgeschlossen. In den Reports wurde uns bestätigt, dass es in den vergangenen 4 Jahren gelungen ist, eine weltweit führende Gruppe im Bereich der Algorithmenentwicklung für Adaptive Optik Systeme in Linz aufzubauen.

Mit der AVL werden Methoden zur Modellierung und Simulation von Motorkomponenten mit dem Ziel einer Lösermodularisierung entwickelt. Im Rahmen der Kooperation in der Finanzmathematik mit der MathConsult und der uni software plus werden schnelle Löser für stochastische Differentialgleichungen und für spezifische partielle Differentialgleichungen sowie Methoden zur Identifikation von Parametern in diesen Differentialgleichungen entwickelt, insbesondere unter Berücksichtigung geänderter Marktbedingungen wie etwa sehr niedriger Zinsen. Die Kooperation mit Siemens VAI hat zum Ziel, existierende Methoden zur Simulation von Sinterprozessen signifikant zu beschleunigen. Mit der voestalpine Grobblech wurden schnelle thermomechanische Ersatzmodelle erarbeitet.

Zusammen mit der Bachmann Monitoring GmbH arbeiteten wir schon längere Zeit an der Entwicklung von Methoden zur Unwuchtüberwachung in Windenergieanlagen. Lag der

Focus bisher auf der Untersuchung von Anlagen, die mit konstanter Drehzahl betrieben werden, so werden in einem Folgeprojekt, gefördert von der FFG, Methoden für variable Drehzahlen untersucht.

Die Vielfalt der bearbeiteten Probleme erfordert den Einsatz und die Entwicklung unterschiedlichster mathematischer Techniken. Der Schwerpunkt der entwickelten mathematischen Methoden lag im Bereich der Inversen Probleme, der Signalverarbeitung sowie der Entwicklung von schnellen und stabilen Lösern für partielle Differentialgleichungen.

Das Forschungsprojekt **Applied Discrete Mathematics and Cryptography** konzentriert sich auf Anwendungsgebiete wie Kryptographie, Kodierungstheorie und die Analyse von Pseudo-zufallszahlen, wobei Methoden aus der diskreten Mathematik wie z.B. Exponentialsummen-techniken oder Diophantische Gleichungen vielversprechend sind. Eine besondere Betonung liegt auf endlichen Körpern und ihren Anwendungen, insbesondere Folgen in Kryptographie und numerischer Integration.

Ein Höhepunkt 2013 war das unter Führung dieses Projekts durchgeführte Special Semester über Anwendungen von Algebra und Zahlentheorie. Darüber hinaus wurde ein FWF Projekt gestartet und ein Teilprojekt im Rahmen eines SFBs genehmigt.

Das START Projekt „**Sparse Approximation and Optimization in High Dimensions**" beschäf-tigt sich mit der „sparsen" Optimierung und Anwendungen insbesondere bei der Dimensions-reduktion von komplexen Problemen. Die Dimension von zu verarbeitenden Daten aus Prob-lemstellungen unserer modernen Gesellschaft ist mittlerweile sehr groß. Um aus dieser Menge von Daten nur die wesentlichen Information zu extrahieren und zu interpretieren, ist die Etablierung eines neuen Fachgebietes der Natur- und Ingenieurwissenschaften vonnö-ten. Die Durchführung numerischer Simulationen basierend auf diesen Daten ist eine enorm wichtige Aufgabe im 21. Jahrhundert. Bemerkenswerte Vorstöße in diese Richtung in der modernen Datenanalyse und in numerischen Simulationen basieren auf der Erkenntnis, dass oft nur ein paar wenige führende Komponenten benötigt werden, um die Dynamik des gan-zen Problems zu beschreiben. Eine Reduktion der Dimensionalität kann hierbei durch die Forderung, dass das Ergebnis dünn besetzt (englisch "sparse") bzw. komprimierbar ist, er-reicht werden. Um die relevanten Freiheitsgrade des Ergebnisses zu identifizieren, werden effiziente Optimierungsmethoden benötigt. In diesem Zusammenhang beschäftigte sich das Start Projekt mit der Entwicklung effizienter Algorithmen zur Berechnung optimaler dünn be-setzter Ergebnisse. Darüber hinaus beschäftigt sich die Gruppe mit neuen Anwendungen in

innovativen Gebieten wie dem automatisierten Lernen und der optimalen Steuerung von hochdimensionalen dynamischen Systemen.

## 3. Highlights 2013

- Das ESO InKind Projekt "Mathematical Algorithms and Software for E-ELT Adaptive Optics", ein Gemeinschaftsprojekt von RICAM, dem Institut für Industriemathematik und der MathConsult GmbH, wurde erfolgreich von einem internationalem Review Board evaluiert. Den Projektpartnern wurde bestätigt, dass in Linz ein auf dem Gebiet der Algorithmenentwicklung für die Adaptive Optik international führendes Forschungsteam aufgebaut wurde. Die Forschungsarbeiten wurden auch von der österreichischen Presse dokumentiert, siehe etwa

  http://derstandard.at/1392687110748/Schnelle-Algorithmen-fuer-klare-Blicke-ins-All

- Wissenschaftler des RICAM waren auch 2013 wieder sehr erfolgreich bei der Einwerbung von Drittmitteln: So wird etwa im Rahmen des neu bewilligten Spezialforschungsbereiches (SFB) "Quasi-Monte Carlo Methods – Theory and Applications" ein Teilprojekt am RICAM durchgeführt. Auch vom neu bewillgten Doktoratskolleg (DK) "Nano-Analytics of Cellular Systems (NanoCell)" wird ein Teilprojekt am RICAM durchgeführt. Zusammen mit den astronomischen Instituten der Universitäten Wien, Graz und Innsbruck gelang es dem RICAM, im Rahmen der Ausschreibung des Hochschulraumstrukturfonds Forschungsmittel für das Projekt „Beobachtungsorientierte Astrophysik in der E-ELT Ära" einzuwerben. Darüber hinaus wurden am RICAM im Jahr 2013 weitere 5 Einzelprojekte von FWF und FFG eingeworben.

- Dr. Marie-Therese Wolfram hat von der ÖAW Fördermittel zum Aufbau einer New Frontiers Group zum Thema „Multiscale modeling and simulation of crowded transport in life and social sciences". Die Gruppe arbeitet seit Februar 2014 am RICAM.

- Dr. Kügler hat einen Ruf auf eine W3-Professur an die Universität Hohenheim erhalten und diese auch angenommen. Dr. Kraus hat einen Ruf auf eine W3-Professur an der Universität Duisburg-Essen erhalten und auch angenommen. Univ.-Prof. Dr. Ramlau hat die Professur für Industriemathematik an der Kepler-Universität in Linz angetreten. Zusätzlich erhielt er einen Ruf auf eine W3-Professur an der Universität Siegen, den er aber ablehnte.

- Im Herbst 2013 wurde am RICAM das Special Semester „Applications of Algebra und Number Theory" durchgeführt. An den 4 Workshops und den angebotenen Tutorials und Special Lectures nahmen insgesamt 180 auswärtige Wissenschaftler teil.

- Im Rahmen des 10. Jahrestages der RICAM-Gründung sowie zum 60. Geburtstag des Gründungsdirektors des RICAM, Prof. Dr. Heinz Engl, wurden zwei Workshops durchgeführt.
- S. V. Pereverzyev and S. Lu (Fudan University, Shanghai, China) haben ein Buch mit dem Titel "Regularization Theory for Ill-Posed Problems. Selected Topics" bei De Gruyter publiziert, M. Aichinger und A. Binder sind Autoren des Buches "A Workout in Computational Finance", erschienen bei Wiley.

## 4. Scientific Activity 2013 (Abstract)

The Group **"Computational Methods for Direct Field Problems" (CMG)** has focused on the development, analysis and implementation of novel fast and robust computational methods for Partial Differential Equations (PDEs) or systems of PDEs arising in different fields of applications like diffusion in heterogeneous media, solid and fluid mechanics, fluid-structure interaction, electromagnetics, and others. The CMG has made important contributions to the Isogeometric Analysis (IGA), a relatively new research direction that certainly will have a major impact on Computational Sciences and Industrial Applications. Two research projects on IGA were supported by the FWF. The IGA software project G+SMO is a collaborative effort of several research groups within the NFN S117 on "Geometry & Simulation" that is a long-term research network.

Traditionally, the working area of the **Inverse Problems Group** is very broad: We are concerned with nonlinear regularization theory, and related fields such as meta learning. The latter is in particular applied to Diabetes treatment. Theoretical aspects of regularization theory are funded by the Austrian Science Fund, Project P25424 „Data-driven and problem-oriented choice of the regularization space", which is headed by S. Pereverzyev. We are also concerned with tomographical methods, which are applied in Photoacoustics. Diese topic is funded by the Austrian Science Fund within the excellence program NFN „Photoacoustic Imaging in Biology and Medicine". As a novelty we have started to analyse photoacoustic imaging in a random environment. Moreover, we investigate classical topics of Inverse Problems such as inverse scattering problems.

In the scientific area of Constructive Algebraic Geometry, the research of the **Symbolic Computation Group** has been focused on the radical parametrization of algebraic curves. The work has been carried out in the context of an FWF project as well as within the doctoral col-

lege "Computational Mathematics", which is funded by the FWF and the state of Upper Austria. The doctoral college is a joint project with the several mathematical institutes of the Kepler University. A cooperation with H.-P. Schröcker (University of Innsbruck) and G. Hegedus (Unversity of Obuda, Hungary; a former RICAM postdoc) lead to unexpected breakthroughs in theoretical kinematics.

In the topic of Symbolic Functional Analysis, which has been emphasized at RICAM for some time, algorithms could be improved and applied to insurance risk models. The topic of Algorithmic Combinatoric is new at RICAM; here, we could achieve results in knot theory and in the theory of spline spaces.

The research in the **Optimization and Optimal Control Group** focused on the analysis and development of numerical methods for optimization with partial differential equations as constraint. Special attention was paid to the control of wave phenomena and to the optimal control of the bidomain equations, which are the commonly accepted model for the electrical activity of the heart. In the area of fluid mechanics significant new insight was obtained into controllability problems to trajectories as well as to shape optimization problems. The group is in the progress of shifting its research focus from open to closed loop control.

The research of the **Imaging Group** has been concerned with the analysis of space-time algorithms for solving parabolic partial differential equations and the investigation of parameter identification problems for parameters in transport equations, which are relevant in imaging. Our research in free boundary problems concerns estimation of non trivial waves of large amplitude in an incompressible fluid. We developed a novel algorithm, which can be extremely improved by determining appropriate initial conditions, which are derived by a creative analysis. The analysis is based on a higher order expansion of the solutions. This was an unexpected result for the mathematical community, as it is somehow counter-intuitive to the number of free parameters available.

Jointly with colleagues at the Max F. Perutz Laboratories the RICAM **Bio Group** studied the stress response of the hypothalamic-pituitary-adrenal-axis for the production of cortisol. Hypocortisolism can be understood as a dysfunctional bistable switch of the underlying biochemical reaction network, bifurcation control methods developed at RICAM suggest to at first further reduce the blood cortisol level and hence yield a counterintuitive therapeutic strategy. By means of the integration of a recently experimentally found glucocorticoidic receptor in the pituitary cell membrane into the mathematical model of the feedback mechanisms it is now also possible to simulate the pathological condition of hypercortisolism along

with corresponding therapeutic measures. In a cooperation with the Institute for Molecular Biotechnology (Acad. of Sci.) great progress in the understanding of actin driven cell motility has been achieved, including a first explanation of the shape of lamellipodia and a detailed description of intracellular motility of Baculovirus.

The **Transfer Group**, installed in 2011, aims at the transfer of modern mathematical methods to industry. Therefore the research is always done in close cooperation with industrial or other scientific partners. Within the last year we have in particular worked with the European Southern Observatory (ESO, Garching), AVL List GmbH (Graz), uni software plus GmbH (Linz), Siemens VAI Metals Technologies GmbH, voestalpine Grobblech GmbH, MathConsult GmbH (Linz) and with Bachmann GmbH (Feldkirch).

In the framework of an Austrian InKind Project we developed for ESO mathematical algorithms and software for Adaptive Optics Systems for the future European Extremely Large Telescope (E-ELT). The project has been successfully completed and evaluated in 2013. The evaluation reports confirm that we have succeeded to establish in Linz one of the leading groups in the area of development of algorithms for Adaptive Optics.

With AVL, methods for modeling and simulation of engine components are developed. The aim is in particular to develop a solver modularization of the simulation system. In Finance, we cooperate with MathConsult and uni software plus in the development of fast numerical solvers for stochastic and specific partial differential equations and methods for the identification of parameters in these differential equations. In particular we take into account changed market conditions such as the currently low interest rates. Together with Siemens VAI we aim at a significant speedup of simulation methods for sinter processes, whereas the focus of our cooperation with voestalpine Grobblech is on the development of fast surrogate models thermomechanical processes.

The development of methods for condition monitoring of wind power plants is the topic of the cooperation with Bachmann. So far, the focus has been on the development of methods for wind power plants operating with constant rotational speed. Within a new FFG project, starting officially on January 1, 2014, we will now consider plants that operate with changing speed.

The variety of the considered applications requires the use of a whole range of different mathematical techniques. The focus of our mathematical work was on the development of new reconstruction methods for Inverse Problems, Signal Processing and on the development of fast and stable numerical solvers for partial differential equations.

The **Research Project "Applied Discrete Mathematics and Cryptography"** focuses on application areas as cryptography, coding theory and the analysis of pseudorandom numbers where methods from discrete mathematics as for example exponential sum techniques and Diophantine equations are very promising. A special emphasis is put on finite fields and their applications, in particular, in cryptography and numerical integration.

A highlight in 2013 was the special semester on applications of algebra and number theory, which was organized under the leadership of the project. Moreover, an FWF project (V. Ziegler) started and a sub-project of an SFB (A. Winterhof) was granted.

The **START Project** "Sparse Approximation and Optimization in High Dimensions" focused on the topics sparse optimization and dimensionality reduction in complex problems. The dimension scale of problems arising in our modern information society became very large. Therefore it is necessary to extract and interpret significant information from the collected data. Numerical simulations based at collected data will be one of the great challenges of the 21st century. Recent advances in data analysis and numerical simulation are based on the observation that in several situations, even for very complex phenomena, only a few governing components are required to describe the whole dynamics; a dimensionality reduction can be achieved by demanding that the solution be "sparse" or "compressible". Since the relevant degrees of freedom are not prescribed, and may depend on the particular solution, we need efficient optimization methods for solving the hard combinatorial problem of identifying them. In this context, the Start Project addresses the problem of designing efficient algorithms which allow to achieve sparse optimization in high-dimensions. Additionally, the Project works on applications of the developed methods in image processing, automatic learning of dynamical systems.

## 5. Highlights 2013

- The ESO InKind Project "Mathematical Algorithms and Software for E-ELT Adaptive Optics", a joint project of RICAM, the Industrial Mathematics Institute of the Kepler University and MathConsult GmbH, was successfully evaluated by an international review board. It was recognized that an international leading scientific team on the area of Adaptive Optics has been established in Linz. The scientific work also has been documented in the Austrian press, see http://derstandard.at/1392687110748/Schnelle-Algorithmen-fuer-klare-Blicke-ins-All

- The scientists at RICAM were successful in raising third party funds: In the framework of the newly granted Special Research Area (SFB) "Quasi-Monte Carlo Methods – Theory and Applications", a RICAM-lead subproject received funding. In addition, a subproject of the newly granted Doctoral School (DK) "Nano-Analytics of Cellular Systems (NanoCell)" also received funding to be hosted at RICAM. Together with the Astronomical Institutes of the Universities Vienna, Graz and Innsbruck, RICAM was successful in obtaining funds from the Hochschulraumstrukturfonds for the Project „Observation Oriented Astrophysics in the E-ELT Area". An additional 5 stand-alone projects were granted for RICAM from the Austrian Science Fund (FWF) and the Austrian Research Promotion Agency (FFG).

- Based on her research proposal, Dr. Marie-Therese Wolfram obtained funds from the Austrian Academy of Sciences for a „New Frontiers Group" for the topic „Multiscale modeling and simulation of crowded transport in life and social sciences". In February 2014, the research group began its work at RICAM.

- Dr. Kügler accepted a call for a W3-professorship at the University of Hohenheim. Dr. Kraus accepted a call for a W3-professorship at the University of Duisburg-Essen. Univ.-Prof. Dr. Ramlau accepted the call for the professorship for Industrial Mathematics at the Kepler-University at Linz. Additionally, he rejected a call for a W3 professorship at the University of Siegen.

- In fall 2013, RICAM hosted a Special Semester „Applications of Algebra und Number Theory". Highlights were the four workshops and several tutorials and special lectures with about 180 participants from all over the world.

- In spring 2013, RICAM celebrated its 10th anniversary and the 60th birthday of its founding director, Prof. Dr. Heinz Engl, with two workshops.

- S. V. Pereverzyev and S. Lu (Fudan University, Shanghai, China) published the book "Regularization Theory for Ill-Posed Problems: Selected Topics" (De Gruyter). M. Aichinger and A. Binder published "A Workout in Computational Finance" (Wiley).

## 6. Tätigkeitsbericht 2013

## 6.1. Group "Computational Methods for Direct Field Problems"

Group Leader:
o.Univ.-Prof. Dipl.-Ing. Dr. Ulrich Langer
Univ.-Prof. Dr. Bert Jüttler (Deputy Group Leader)

Researchers funded via ÖAW:

Dr. Qingguo Hong (from 1 December 2013)

PD Dr. Johannes Kraus

Dr. Clemens Pechstein (from 1 August until 31 December 2013)

Dr. Angelos Mantzaflaris

Dr. Satyendra Tomar

Dr. Jörg Willems (until 14 July 2013)

Dr. Huidong Yang

Researchers externally funded:

MSc Nadir Bayramov

MSc Krishan Gahalaut (until 30 June 2013)

Dr. Ivan Georgiev (until 31 May 2013)

Dr. Qingguo Hong (until 30 November 2013)

Dipl.-Ing. Stefan Kleiss (until 31 October 2013)

DI Stephen Edward Moore

Dr. Ioannis Toulopoulos (since 1 August 2013)

The "Computational Mathematics Group" (CMG) has focused on the development, analysis and implementation of novel fast computational methods for Partial Differential Equations (PDEs) or systems of PDEs arising in different fields of applications like diffusion in hetero-geneous media, solid and fluid mechanics, fluid-structure interaction, electromagnetics, and others. In the following, we present the main scientific activities and the most important achievements and results obtained in 2013:

**Robust Algebraic Multigrid, Multilevel, and Multiscale Methods**

The research on this topic was carried out within several sub-projects:

**(a) FWF-Research Project P22989** "*Subspace correction methods for nearly singular and indefinite problems with highly oscillatory coefficients*" (2010-2014) led by **J. Kraus** (2 Post-Docs: Qingguo Hong and I. Georgiev, and 1 PhD student: N. Bayramov).

For 2013, the scientific results of this project can be summarized as follows. In [1] we have considered IP-DG methods for linear elasticity problems in a primal (displacement) formula-

tion as they provide locking-free approximations. A natural splitting of the DG space has been exploited to derive uniform preconditioners. Recently, we have also investigated an H(div)-conforming DG method (of Nitsche type) in order to solve the Stokes problem via the augmented Uzawa method. The main results of this research are the construction and theoretical analysis of robust multigrid algorithms for solving linear elasticity equations discretized by this type of DG method using non-inherited bilinear forms, see [2]. Variable V-cycle and W-cycle methods have been studied and their convergence rate has been proven to be independent of the Lame parameters.

Further, in [3] we have presented the construction of a new class of multigrid methods in which coarse-grid correction (as used in standard MG algorithms) is replaced by auxiliary-space correction. The coarse-grid operators are obtained from additive Schur complement approximation (ASCA), see also [4], which can be computed in parallel from two-level block factorization of local (finite element stiffness) matrices associated with a partitioning of the domain into overlapping or non-overlapping subdomains. The two-level analysis relies on the fictitious space lemma and condition number estimates for both, the two-level preconditioner, as well as for the ASCA have been derived.

Moreover, an algebraic formula for estimating the convergence rate of an aggregation-based two-level method has been developed in [5]. We have shown that the formula can be used to obtain sharp estimates of the convergence rates in the special case where matching is used for aggregation. The nearly optimal convergence and complexity of the related algebraic multilevel iteration (AMLI) method has been established.

Further progress in the area of multigrid and AMLI methods has been made in the context of isogeometric analysis (IGA), see *[6], [7]* and Research Topic 2 on IGA below.


**(b) Collaborative Research Project** on *"Subgrid Discontinuous Galerkin Approximations of Brinkman Equation with Highly Heterogeneous Coefficients"* by **J. Willems** (RICAM) and R. Lazarov (TAMU) supported by the mutual NSF project DMS-1016525.


Robust Multilevel methods for anisotropic problems with highly heterogeneous coefficients have been discussed in *[8]*. A comparative study of recently proposed robust two-level Schwarz methods using spectrally constructed coarse spaces has been presented in *[9]*. A further paper on the topic "Robust Multilevel Methods for General Symmetric Positive Definite Operators" by J. Willems is meanwhile accepted and will be published in the *SIAM Journal on Numerical Analysis* in 2014 [10]. J. Willems was successful with his FWF project application on "*Robust Preconditioning and Upscaling of Problems with Inseparable Scales*" that was approved by the FWF under the grant P25976 at the FWF board meeting in

June 2013. Unfortunately, due to his movement to Germany, the project could not be started at RICAM.

**(c) Algebraic Multigrid and Multilscale Domain Decomposition Methods.**

**H. Yang** has been working together with **U. Langer** on fluid-structure interaction simulation with nonlinear hyperelastic models in hemodynamics, see [11]. Therein, we focus on handling the nonlinearity of the fluid and structure sub-problems, the near-incompressibility of materials, the stabilization of employed finite element discretization, and the robustness and efficiency of Krylov subspace and algebraic multigrid methods for the linearized algebraic equations. The submission of very ambitious FWF Project P25396 on *"Computational Fluid-Structure Interaction with Applications to Vocal Production"* by H. Yang was unfortunately not successful.

**C. Pechstein** published a monograph on *"Finite and Boundary Element Tearing and Interconnecting Solvers for Multiscale Problems"* [12]. In this monograph, he considered scalar multiscale problems, i.e., mainly diffusion problems with highly heterogeneous coefficients, see also journal publications [13], [14] and [15]. Vectorial elasticity problems with heterogeneous coefficients, in particular, nearly incompressible materials, are a new research topic, see [16]. The new BEMbasedFEM technology is discussed in [17] and [18]. The results of the cooperations with the tranfer group are published in [19].

**S.K. Tomar** developed Algebraic multilevel preconditioner for H(curl) and H(div) problems [20], [21].

**Isogeometric Analysis (IGA)**

The research work on this topic was organised in several sub-projects:

**(a) FWF-Research Project P21516** *"Isogeometric method for numerical solution of partial differential equations"* (2009-2013).

This project, led by **S.K. Tomar** with the two PhD students K.P.S. Gahalaut and S.K. Kleiss, has been completed (with final project report due in March 2014).

During 2013, K.P.S. Gahalaut and S.K. Tomar (together with J.K. Kraus) completed the development of an efficient (almost p-robust) algebraic multilevel method for solving linear systems of equations resulting from the isogeometric discretization of elliptic problems (RICAM report 2013-05). This paper has been published in CMAME [7]. K.P.S. Gahalaut defended his PhD thesis on 20.06.2013 [22]. Furthermore, with S.K. Kleiss we developed guaranteed,

sharp, robust, and fully computable a-posteriori error estimates for isogeometric discretization of elliptic PDEs [23]. In this work, by exploiting the extra regularity offered by IGA basis functions (in our work we focussed only on NURBS but this is applicable to any of the IGA basis functions which offers higher than zero order regularity), we developed an efficient approach to compute these estimates. It is noteworthy that such an approach to compute these estimates is not possible with zero order regularity offered by FEM basis functions. This work is under review for publication. S.K. Kleiss submitted his PhD thesis on 20.12.2013, and defended it on 06.02.2014 [24]. S.K. Tomar also visited his co-operation partner Prof. T.J.R. Hughes (University of Austin, Texas) during July 29-August 23, 2013.

**(b) NFN-Research Project S117-03** *"Discontinuous Galerkin Domain Decomposition Methods in IGA" led by* **U. Langer**.

This research project is a part of the National Research Network NFN S117 on *"Geometry & Simulation"* (speaker: **B. Jüttler**) supported by the FWF (2012 – 2016 – 2020). For the project, 1 PhD (S. Moore) and 1 PostDoc (I. Toulopoulos) were hired, both funded by the NFN. Beside these project employees, A. Mantzaflaris, C. Pechstein and S. Tomar from the basic staff have contributed to this project. Moreover, the software project *G+SMO* is a joint effort of the NFN, but it is led by **A. Mantzaflaris**. In particular, hierarchical B-spline bases have been extended to the 3D case, and the overall efficiency is greatly improved, e.g., by new fast generation techniques [25]. Available features currently include simulations using continuous and discontinuous Galerkin approximation of PDEs over conforming multi-patch computational domains. PDEs on surfaces as well as integral equations arising from elliptic boundary value problems are also supported. Boundary conditions may be imposed both strongly and weakly. In addition to advanced discretization and generation techniques, efficient solvers like multigrid iteration schemes are available. Finally, a preliminary Stokes implementation is available and is currently tested. **S. Moore** was invited to give a minisymposium talk about our new results on "DG multipatch IGA for elliptic PDEs on surfaces" on the 22nd Domain Decomposition Conference [26]. Moreover, he also gave a poster presentation on G+SMO. **I. Toulopoulos** has started to work on DG multipatch IGA for 3d elliptic boundary value problems with low-regularity solutions on non-matching meshes.
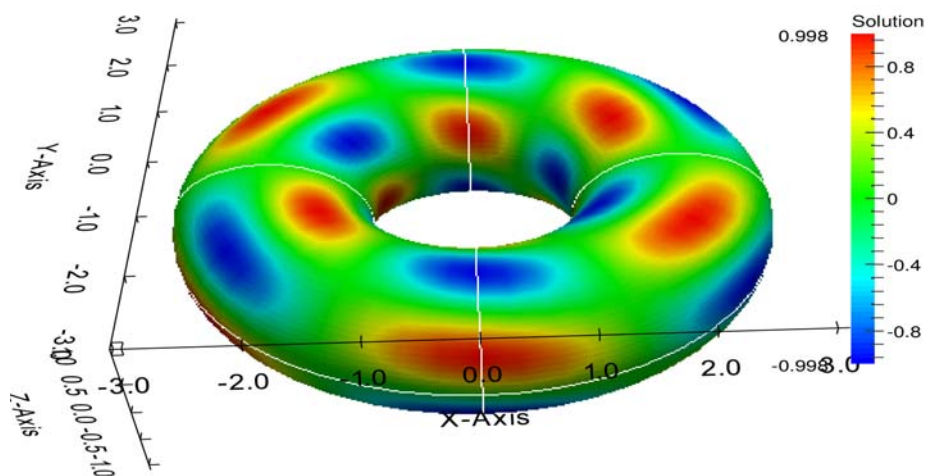
*Figure: DG multipach IGA solution of a diffusion problem on the torus.*

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[6] K. Gahalaut, J. Kraus, S. Tomar. Multigrid methods for isogeometric discretization. Computer Methods in Applied Mechanics and Engineering 253:413-425, 2013.

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[8] J. Willems. Robust Multilevel Solvers for High-Contrast Anisotropic Multiscale Problems. Journal of Computational and Applied Mathematics, 251:47-60, 2013.

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[14] C. Pechstein: Shape-explicit constants for some boundary integral operators. Applicable Analysis, 92 (5), 949-974, 2013.

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[27] J. Kraus, M. Wolfmayr. On the robustness and optimality of algebraic multilevel methods for reaction-diffusion type problems. Computing and Visualization in Science. (In Press).

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[33] I.G. Graham, U. Langer, J.M. Melenk, M. Sini, editors. Direct and Inverse Problems in Wave Propagation and Applications, Radon Series Comp. Appl. Math., vol.~14, Walter de Gruyter, Berlin/Boston, 2013.

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## 6.2. Group "Inverse Problems"

Group Leader:

Univ. Prof. Dr. Otmar Scherzer

Researchers funded via ÖAW/Upper Austrian government funds:

Dr. Ankik Giri

Dr. Valeriya Naumova (employed until 31.12.2013)

Dr. Rajesh Kumar (employed since 01.05.2013)

Prof. Dr. Sergei Pereverzyev

Priv. Doz. Dr. Mourad Sini

M.Sc. M.Tech. Durga Prasad Challa (employed since 10.11.2013)

Researchers externally funded:

M.Sc. M.Tech. Durga Prasad Challa (employed until 09.11.2013)

M.Sc. Manas Kar (employed until 09.11.2013)

MSc Pavlo Tkachenko (employed since 03.06.2013)

Traditionally the working area of the Inverse Problems group is very broad. The Inverse Problems Group has focused on the development and analysis of regularization methods for solving nonlinear inverse problems under stability conditions, computational inverse problems and applications to Diabetes treatment, scattering theory, and inverse problems with stochastic uncertainties, such as in random media. In the following we present the main scientific activities and the most important achievements and results obtained in 2013:

### Computational inverse problems

The research on this topic was carried out within several sub-projects led by **S. Pereverzyev**:

- We have studied the problem of Meta-learning and its application to Diabetes treatment. In this context a fundamental tool is multi-penalty regularization, which is analyzed in a Hilbert scales setting.
- Another research topic in this field is the analysis of regularization methods for the reconstruction of Earth gravitational potential.
- The FWF-Research Project P25424 "Data-driven and problem-oriented choice of the regularization space" (2013-2016) is led by S. Pereverzyev, and is concerned with theoretical justifications of learning.

## Inverse problems in wave propagation

The research on this topic has been carried out within several sub-projects guided by **M. Sini**:

- In this area the group provided a justification of the Foldy-Lax approximation of scattered waves taking into account the whole denseness of the cluster of scatterers.
- Moreover, we derived high frequency estimates of the scattering induced by interfaces and applied them to justify and quantify the convergence rates of the hopping type algorithms for reconstructing shapes from multi-frequency measurements.
- We studied the mathematically modeling of the diffusion by interfaces using the Krein resolvent method.

## Convergence rates of regularization methods for solving the nonlinear inverse problems based on stability estimates

- We have been considering Tikhonov regularization for solving nonlinear inverse problems. Unlike the previous analysis we do not assume source and nonlinearity conditions, but our analysis relies on stability estimates.
- Moreover, the interplay between source and other stabilization (Lipschitz) condition has been analysed. This work has been performed jointly by **A. Giri**, Lingyun Qui, M. deHoop, and **O. Scherzer**.

## Source localization in photoacoustic for a Gaussian random sound speed

- In the last 10 years members of the group have been working in the area of photoacoustic imaging. In particular we developed reconstruction algorithms and backprojection formulas within the National Research Network S105 „Photoacoustic Imaging in Biology and Medicine", funded by the FWF. Recent contributions are novel attenuation models and their use in photoacoustics. This is joint work of K. Kalimeris and O. Scherzer.
- R. Kumar has been working together with O. Scherzer on a new coherent interferometry algorithm to identify general source functions in a random environment for photoacoustical inverse problems.

<u>Publications</u> *(note that the publications of the group leader can be found in the bibliography list of the Mathematical Imaging group)*:

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harmonics Gravitational Field Modeling. International Journal on Geomathemat-ics, published online.

[3] H. N. Mhaskar, V. Naumova, and S. V. Pereverzyev. Filtered Legendre Expansion Method for Numerical Differentiation at the Boundary Point with Application to Blood Glucose Predictions. Applied Mathematics and Computation, vol. 224, 2013, pp. 835-847.

[4] Hui Cao, S. V. Pereverzyev, and E. Sincich. Discretized Tikhonov regularization for Robin boundaries localization. Applied Mathematics and Computation, vol. 226, 2013, pp. 374–385.

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[6] M. Fornasier, V. Naumova and S. Pereverzyev. Parameter Choice Strategies for Multi-Penalty Regularization. Submitted.

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[8] N. Honda, G, Nakamura and M. Sini. Analytic extension and reconstruction of obstacles from few measurements for elliptic second order operators. Math. Ann. 355 (2013), no. 2, 401-427.

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[15] M. Kar and M. Sini. Reconstruction of interfaces using CGO solutions for the Maxwell equations. Accepted by Journal of Inverse and Ill posed Problems.

[16] F. Al-Musallam, A. Boumenir and M. Sini. Detection of Multilayered Media in the Acoustic Waveguide. Appeared online in J. Math. Anal. Appl.

[17] G. Hu, A. Mantile and M. Sini. Direct and Inverse Acoustic Scattering by a Collection of Extended and Point-Like Scatterers. Revised to SIAM Journal on Multiscale Modeling and

Simulation.

[18] M. Kar and M. Sini. On the inverse elastic scattering by interfaces using one type of scattered waves. Accepted by Journal of Elasticity.

[19] M. Kar and M. Sini. Reconstruction of interfaces from the elastic farfield measurements using CGO solutions. Revised to SIAM J. Math. Anal.

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## 6.3. Group "Symbolic Computation"

Group Leader:
Ao. Univ.-Prof. Dr. Josef Schicho

Researchers funded via ÖAW/Upper Austrian government funds:
Dr. Nelly Villamizar (employed since 01.01.2013)
Dr. Anja Korporal (employed until 31.08.2013)
Dr. Christoph Koutschan
Dr. Georg Regensburger

Dr. Hamid Ahmadinezhad (employed since 01.09.2013))

In 2013, the group worked within three main research areas:

## Computational Algebraic Geometry

In 2012, the group came up with two new methods for the analysis of mechanical linkages with rotational joints, in a cooperation with H.-P. Schröcker (Univ. Innsbruck) and G. Hegedüs (Univ. Obuda, Hungary; a former RICAM postdoc): factorization of motion polynomials [1] and bond theory [2]. In 2013, these two concepts were further developed and applied for solving various previously open cases in the classification of mobile closed 6R linkages. Motion polynomials are univariate polynomials with coefficients in the skew ring of dual quaternions that parameterize motions of rigid bodies in 3D space. Since linear motions parameterize revolutions around a fixed axis, the factorization of a motion polynomial decomposes the parameterized motion into such revolutions, and the motion can be realized by a chain of rotational joints (see Figure 1). The factorization is not unique, so that one can realize the same motion by different chains, and this leads to the construction of closed linkages.
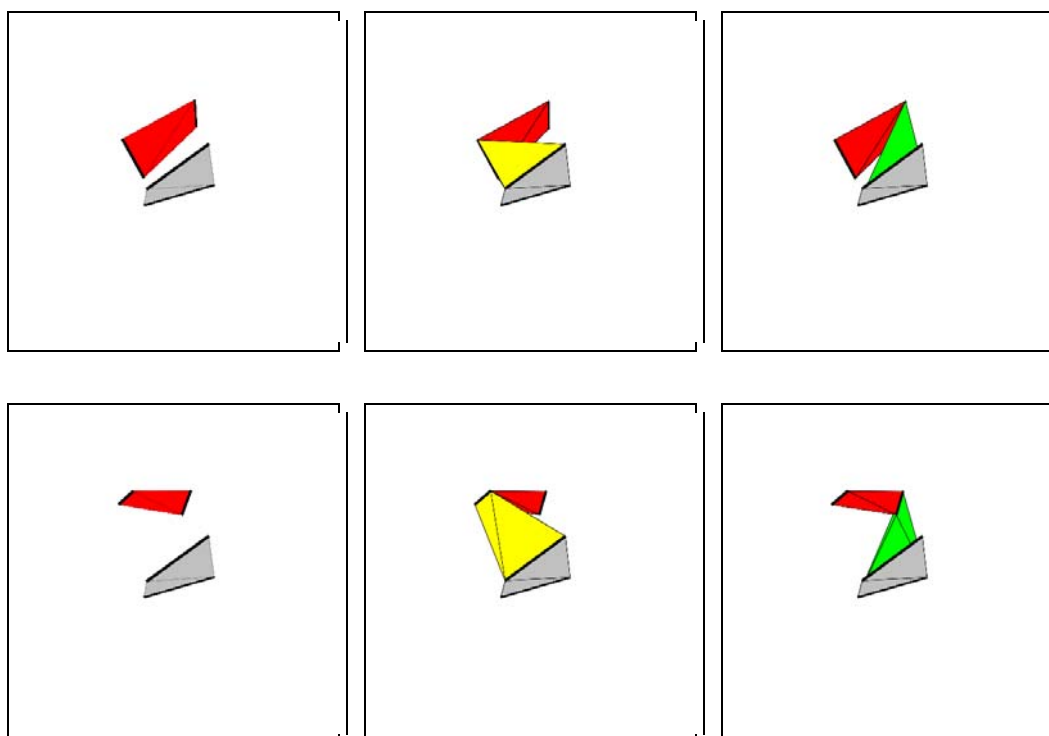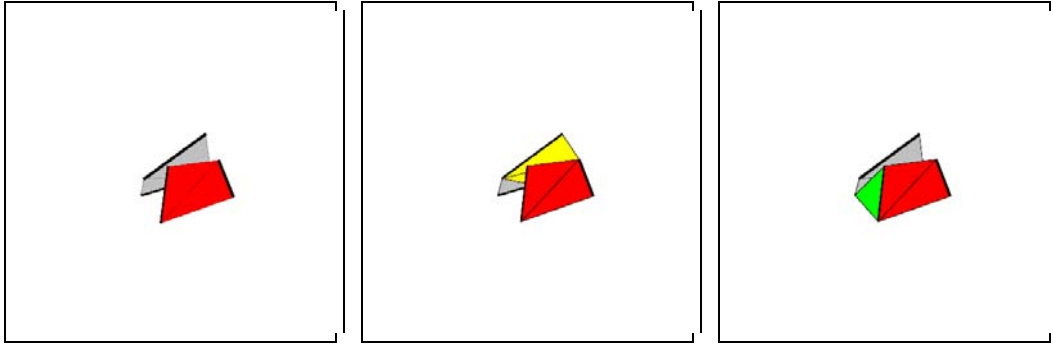
*Figure 1: The motion on the left can be decomposed in two ways (middle and right) into revolutions around fixed axes.*

The theory of bonds was introduced for the purpose of analyzing the algebraic structure of a closed linkage with revolute joints. As a proof-of-concept, the group gave an almost computation-free derivation [2] of the well-known classification of closed 5R linkages; the only proof known before makes extensive use of computations supported by a computer algebra system. Further results obtained with this method are the classification of two families of 6R linkages with specific properties, namely angle-symmetry [3] and the existence of parallel joint axes [4] (see also Figure 2).
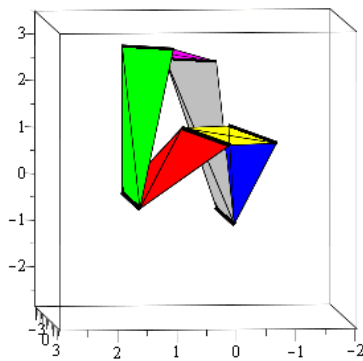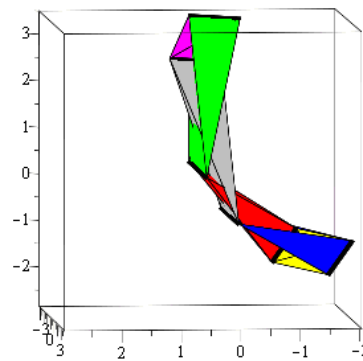


Fig. 2-1                    Fig. 2-2

*Figure 2: A new closed 6R linkage with three pairs of parallel lines.*

## Symbolic Functional Analysis

Algebras of integro-differential operators that are capable to express boundary problems have been defined and studied over the last years, in a cooperation with A. Korporal (INRIA Lille, France; former PhD student at RICAM) and M. Rosenkranz (University of Kent, Eng-

land; former postdoc at RICAM). Together with G. Li (Rutgers University), the group extended this approach by weights, in analogy to differential algebras [5]. This leads to an easier description of a basis.

Together with H.-J. Albrecher and C. Constantinescu (both from Univ. Lausanne, Switzerland), Z. Palmowksi (Univ. Wroclaw, Poland), and M. Rosenkranz, the group studied the algebraic structure of the Green's operator of a boundary problem modeling insurance risks [6]. This gave a good understanding of the asymptotic behavior of the solutions. In one important case (the compound Poisson risk model), closed-form solutions were obtained.

## Algorithmic Combinatorics

Together with B. Mourrain (INRIA at Sophia Antipolis, France), the group calculated the dimension of triangular spline spaces [7]. Since these dimensions are important for isogeometric analysis, this research will be continued together with A. Mantzaflaris from the group of Direct Field Problems.

Together with T. Thanatiponanda (RISC, Linz), the group proved three conjectures related to counting functions of plane partitions and rhombus tilings [8]; one of them was over 30 years old. Other results are the computation of differential equations for the lattice Green's functions of face-centered cubic lattices of dimension 4, 5, and 6 [9], and the minimal-order recurrence of the Jones polynomial of the 7/4 knot [10], together with S. Garoufaldis (Georgia Tech).

## Publications:

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with surplus-dependent premiums. SIAM Journal on Applied Mathematics, Bd. 73 (1), S. 47-66.

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[8] Koutschan, Christoph; Thanatipanonda, Thotsaporn (2013) Advanced Computer Algebra for Determinants. Annals of Combinatorics, Bd. 17 (3), S. 509-523

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## 6.4. Group "Optimization and Optimal Control"

Group Leader:
Prof. Dr. Karl Kunisch

Researchers funded via ÖAW:
Dr. Nagaiah Chamakuri
Dr. Henry Kasumba
Dr. Axel Kröner
Dr. Sérgio Rodrigues

The group has focused on the following topics:

**Large scale PDE constrained optimization of cardiac defibrillation** (N. Chamakuri)
Cardiac arrhythmias are recognized as a significantly challenging problem for clinical and theoretical research. In the optimal control approach to cardiac arrhythmias an applied electrical field is determined in such a way that defibrillation is achieved while optimizing a design objective. The aim of this work is the development and implementation of efficient numerical techniques to solve such complex multiscale and multiphysics optimal control problems arising in cardiac electrophysiology. We build upon ionic models for the cardiac action potential, [1], [2], which approximate well the restitution properties and spiral wave behavior of more complex ionic models of cardiac action potentials. Difficulties include the

appearance of state-dependent switching functionals in the Fenton-Karma model in the source terms. For this purpose a shape calculus based treatment of the sensitivities of the discontinuous source terms and a marching cubes algorithm for tracking the iso-surface of the excitation wave fronts were developed. While so far the focus was on 2D investigations, we are currently in the process of extending the optimal control approach to cardiac defibrillation in 3D geometries [3]. In this case the bidomain model includes cardiac tissue domain extracted from the histological images which is surrounded by an external bath domain, fiber rotation and anisotropic conductivity coefficients, which are axially symmetric around the fiber direction, see Figures 1 and 2.
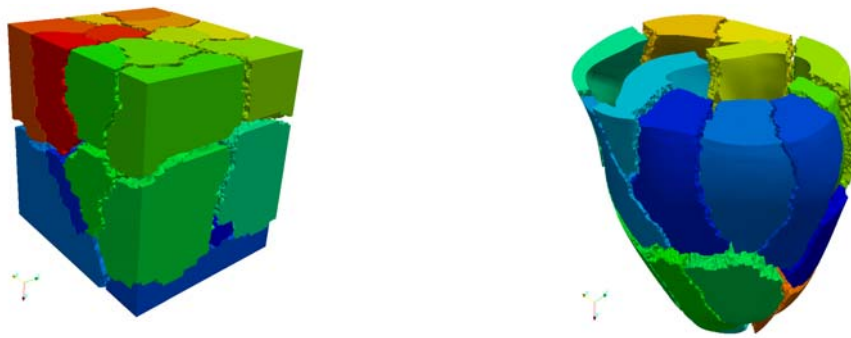


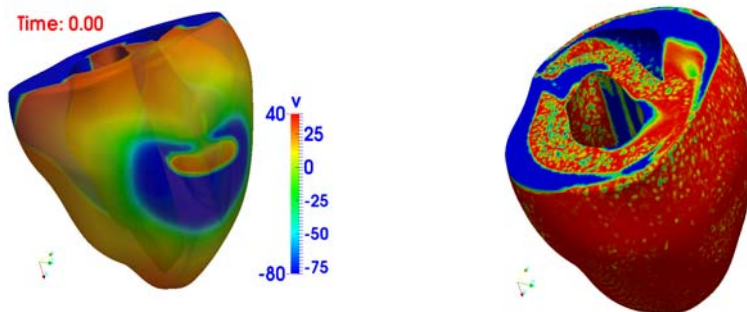Figure 1. *Domain decomposition of surrounding bath volume and cardiac tissue volume.*



Figure 2. *The state solution of transmembrane voltage and optimal state solution at time 4 msec.*

**Shape optimization with PDE constraints** (H. Kasumba)

The research is focussed on the optimal control of free boundary problems governed by the stationary Navier-Stokes equations. This problem has a significant room for novel ideas. To solve the free boundary problem, which appears as a state constraint in the optimal control problem, a fixed point method was developed in earlier work. In addition, the reformulation of free surface problems as shape optimization problems was proposed in [5]. This requires a systematic study of first and second order shape derivatives of the cost functionals [6]. It is in our future focus to extend the presentation in [6] to cost functionals introduced in [5].

Furthermore, a sensitivity analysis to the bilevel shape optimization problems was formally studied in earlier work. A first step towards a rigorous characterization of the shape sensitivity of a potential free surface flow was given in [4]. The extension of the results in [4] (c.f. Figure 3) to shape control of general free surface flows is work currently under investigation.

One of the characteristics of shape optimization problems is that they are ill posed, i.e., larger changes in the shape may have little effect on the cost criterion [5]. Thus, other control mechanisms (such as distributed or boundary control) may be effective in minimizing vortices in a free surface flow. A first attempt using potential free surface flows is in final stages of preparation for submission [7].
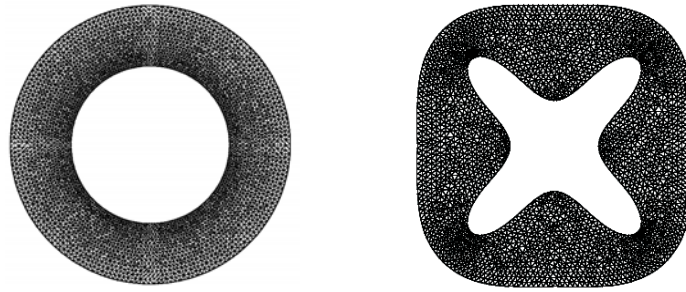


Figure 3. *Shape control of potential free surface flow.*
*(left) Initial flow domain with outer free boundary, (right) Controlled flow domain.*

### Nonsmooth optimal control problems for the wave equation (A. Kröner)

Optimal control problems of wave equations are important for applications arising in control of vibrations and propagation of (acoustic) waves. In comparison to optimal control of elliptic and parabolic equations this is a much less investigated subject. We analyzed the minimum effort problem for the wave equation, see [8], a nonsmooth optimal control problem where the nonsmoothness arises from the choice of the control cost term in the cost functional. To solve this problem a semi-smooth Newton method was applied and its superlinear convergence was shown. Furthermore, the theoretical results were confirmed by numerical examples.

### Optimal feedback control of partial differential equations (A. Kröner)

Optimal feedback control plays a crucial role in many applications since it leads to robust controls which allow to control and stabilize the underlying system also in case of disturbances and small errors. We considered optimal feedback control problems for partial differential equations based on a HJB approach, i.e. a semi-discrete formulation of the problem is considered whose value function can be characterized as the solution of a

Hamilton-Jacobi Bellman (HJB) equation. From the value function a feedback control can be derived. Since the number of basis functions used for the semi-discretization determines the dimension of the corresponding HJB equation, this requires solving high dimensional HJB equations. To address the curse of dimensionality a model reduction technique based on spectral elements was investigated in [9]. Moreover, we applied a HJB approach on a minimum time problem for an advection-diffusion-reaction system using balanced truncation for model reduction and incorporated a Luenberger observer to allow also local observations, see [10]. For optimal feedback stabilization to nonstationary trajectories for the 1D Burgers equation we used a Riccati based approach, see [11]. The main focus lies on an estimate for the dimension of a finite dimensional controller. Besides this we considered semi-Lagrangian schemes for Lp-penalized minimum time problems for dynamical systems, containing the case p=1, leading to sparse solutions, see [12].

To improve the accuracy of the feedback controls when using a HJB approach we started to work on advanced methods to solve high dimensional HJB equations. We started a collaboration with M. Nolte (University of Freiburg) on optimal feedback control within the highly parallelized C++ environment DUNE (www.dune-project.org) and with J. Garcke (University of Bonn) on solving HJB equations on sparse grids. In particular sparse grids is an interesting approach to reduce the storage consumption when solving HJB equations.


**Boundary stabilization to nonstationary solutions for the Navier–Stokes equations**
(S. Rodrigues)

The design of a robust stabilizing controller for the equations of fluid mechanics is important, because such a controller plays a crucial role in the suppression of instabilities that can occur in the dynamics of the fluid. The stabilization to a stationary (time independent) solution is by now well understood. The case of nonstationary solutions is equally important for applications, because we are often confronted with external forces that depend on time, but much less understood.

The main question is: given a (desired) reference trajectory û(t) for the Navier–Stokes system, and an initial velocity field û(0) (different from u(0)) can we find a control localized in a (given small) part of the boundary, finite-dimensional, and in feedback form such that the solution of the system, issued from u(0) at initial time t=0, will go exponentially to the reference trajectory, with a prescribed rate, as time increases? Notice that the above constraints on the control are important for applications purposes.

The answer is positive in the case of internal controls. Now, we can also say that a positive answer in the case of boundary controls is plausible. This conjecture is supported by some of the work that has been done during 2013: in [13], the existence of a boundary control

supported on a given subset of the boundary and driving the Navier–Stokes system issued from $u(0)$ at initial time to $û(T)$ at a given positive time $T>0$, was proven; from this result, truncated boundary observability inequalities, appropriated to deal with finite-dimensional controls as above, were derived for the adjoint Oseen–Stokes system (cf. [14]); finally, first computations strongly suggest that those inequalities will lead to the desired boundary stabilization result (ongoing research [15]).

Another important question concerns the dimension of the controller. In the case of internal controls, it is known that it is enough to take a big enough number $M$ of suitable controls. But no precise estimate for $M$ is known. Work in this direction was initiated in the last trimester of 2013 (ongoing research [11]).

Concerning this subject, the (externally funded) project P 26034-N25 entitled *"Stabilization to trajectories for equations of fluid mechanics"* was granted by the Austrian Science Fund (FWF) in June 2013, and started in December.

**Observer design for nonlinear systems with implicitly defined outputs** (S. Rodrigues)

The design of an observer providing an estimate $x_E$ of the state $x$ of a given real system, is important for many applications (e.g., feedback control design from given measured outputs $y$). For a "target" linear system up to output injection, $dz/dt=Lz+f(y)$, and with implicitly defined outputs, $Cz+z^TDy+Ey+F=0$ (for matrices $C$, $D$, $E$, and $F$, with suitable dimensions), it is known that an observer can be constructed; the same can be done for any system that is equivalent, up to a change of coordinates, to a system in this class. In [16, 17] necessary and sufficient conditions for that equivalence are given. The main difficulty/novelty was the fact that the outputs of the target system are not necessarily given as a linear function of the state.

<u>Publications:</u>

[1]    N. Chamakuri, K. Kunisch, and G. Plank: Application of optimal control to the cardiac defibrillation problem using a physiological model of cellular dynamics (submitted to Applied Numerical Mathematics journal)

[2]    N. Chamakuri, C. Engwer, and K. Kunisch: Boundary control of bidomain equations with state dependent switching source functions in the ionic model, Journal of Computational Physics (in revision)

[3]    N. Chamakuri, K. Kunisch, and G. Plank: PDE constrained optimization of electrical defibrillation in a 3D ventricular slice geometry (in progress)

[4]     H. Kasumba, K Kunisch, and  A. Laurain: A bilevel shape optimization problem for the exterior Bernoulli free boundary value problem. RICAM report 2012-18. (submitted).

[5]     H. Kasumba: Shape optimization approaches to free surface problems. International Journal of Numerical Methods in Fluids, (2014) DOI: 10.1002/fld.3876.

[6]     H. Kasumba and K. Kunisch: On computation of the shape Hessian of the cost functional without shape sensitivity of the state variable. Journal of Optimization theory and Appl.(2014) DOI: 10.1007/s10957-013-0520-4.

[7]     H. Kasumba: Boundary control of a Bernoulli free boundary problem, (in preparation)

[8]     A. Kröner and K. Kunisch: A minimum effort optimal control problem for the wave equation, Comput. Optim. Appl. 57 (2014), no. 1, 241-270.

[9]     A. Kröner, K. Kunisch, and Hasnaa Zidani: Optimal feedback control for the undamped wave equation by solving a HJB equation, (2013) submitted.

[10]    D. Kalise and A. Kröner: Reduced-order minimum time control of advection-diffusion-reaction systems via dynamic programming, (2013), submitted.

[11]    A. Kröner and S. S. Rodrigues: Remarks on the internal exponential stabilization to a nonstationary solution for 1D Burgers equations (in preparation).

[12]    M. Falcone, D. Kalise, and A. Kröner: A semi-Lagrangian scheme for Lp-penalized minimum time problems, (2013) submitted.

[13]    S. S. Rodrigues: Local exact boundary controllability of 3D Navier–Stokes equations, Nonlinear Anal.  95 (2014), 175–190.

[14]    S. S. Rodrigues: Boundary observability inequalities for the 3D Oseen–Stokes system and applications, RICAM-Report No. 2013-18, 2013.

[15]    S. S. Rodrigues: Boundary feedback exponential stabilization to a nonstationary solution for Navier–Stokes equations, (in preparation)

[16]    S. S. Rodrigues and A. P. Aguiar: On the linearization up to multi-output injection for a class of systems with implicitly defined outputs, IEEE Trans. Automat. Control (to appear), 2014. doi:10.1109/TAC.2013.2287728

[17]    S. S. Rodrigues and A. P. Aguiar: A new algorithm for linearization up to multi-output and multi-input injection for a class of systems with implicitly defined outputs, in Proceedings of the 2013 European Control Conference (ECC), Zurich, Switzerland, July 2013, 1734–1739.

[18]    K. Kunisch and L. Wang: Time optimal control of the heat equation with pointwise control constraints, ESAIM: COCV 19 (2013), 460–485.

[19]    K. Kunisch and L. Wang: Bang-bang property of time optimal controls of Burgers

equation, to appear in Journal Discrete and Continuous Dynamical System - A (2014).

[20]   K. Bredies, K. Kunisch and T. Valkonen. Properties of L1-TGV2: The one dimensional case. Journal of Mathematical Analysis and Applications, 398(1):438-454, 2013.

[21]   E. Casas, C. Clason, and K. Kunisch: Parabolic control problems in measure spaces with sparse solutions. SIAM Journal on Optimization and Control, 51(1), 28-63, 2013, doi: 10.1137/120872395

[22]   C. Clason and K. Kunisch: Multi-bang control of elliptic systems. Annales de l'Institut Henri Poincaré (C) Analyse Non Linéaire, 2013. Online, doi: 10.1016/j.anihpc.2013.08.005

[23]   K. Kunisch and X. Lu: Optimal control for an elliptic system with convex polygonal control constraints. IMA Journal of Numerical Analysis 33(3), 875-897, 2013.

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[25]   K. Kunisch and D. Wachsmuth: On time optimal control of the wave equation, its regularization and optimality system. ESAIM: Control, Optimisation and Calculus of Variations, 19(2), 317-336, 2013.

## 6.5. Group "Mathematical Imaging"

Group Leader:
Univ. Prof. Dr. Otmar Scherzer

Researchers funded via ÖAW funds:
Dr. Roman Andreev (employed since 01.09.2013)
Dr. Konstantinos Kalimeris

The Imaging group has focused on the development of algorithms for efficient determination of waves of large amplitude and the numerical solution of spatial-temporal variational formulations for imaging problems. In the following we present the main scientific activities and the most important achievements and results obtained in 2013 in the single working packages:

### Numerical calculation of waves of large amplitude

- We have introduced a novel iterative algorithm for calculating water waves of large amplitudes. This problem is a free boundary value problem, which can be transformed into a nonlinear partial differential equation where the solutions bifurcate. One branch of the bifurcation represents low flows, while the other branch represents the flows with high amplitude. We developed an algorithm based on an augmented Lagrangian technique, which is the first deterministic algorithm to approach this problem numerically. The existing algorithms by Strauss et al are stochastic and have a highly numerical complexity.

- In our algorithm, for the stable solution, we obtained novel asymptotic expansions of the solutions of the underlying equations. Such expansions have been an unexpected result in this field, and are expected to trigger a new fruitful research direction in highly amplitude waves research, because they allow for more efficient numerical solution.

This is joint work of A. Constantin, **K. Kalimeris** and **O. Scherzer**.

### Variational Methods on Manifolds

We are considering variational methods, which are defined on manifolds. Problems as such appear for instance in biological imaging, when cells are observed during early embriogenesis.
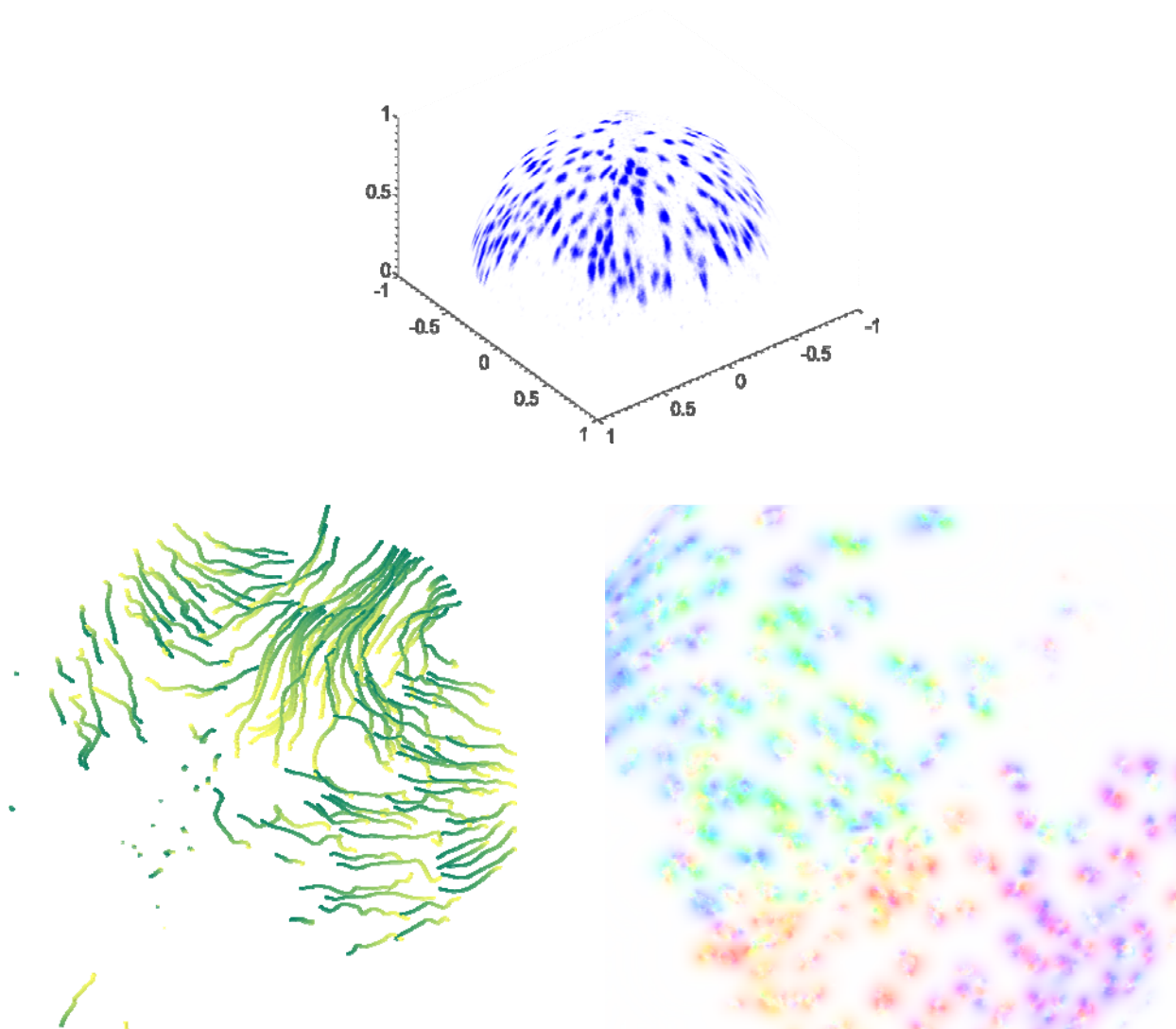
Cell data, trajectories of moving cells, and optical flow computation.

**Variational space-time problems and applications in Computer Vision**

In this field we have investigated the following research topics:

- We have been developing novel formulations of space-time optical flow problems appearing in Computer Vision and Cognitive Science. The novel features of these approaches are that they take into account one more dimension (the time component) and thus are highly numerically complex. Moreover, they are integro-differential equations, opposed to differential equations, which are normally used. This is joint work of **Roman Andreev** and **Otmar Scherzer**.

- We have been considering the development and analysis of space-time simultaneous discretization algorithms for two types of problems: parabolic evolution equations and the regularized equations of optical flow and related parameter identification problems

for transport equations.

- Moreover, R. Andreev and collaborators have been analyzing the classical collocation Runge-Kutta time-stepping schemes from the point of view of space-time simultaneous Petrov-Galerkin discretizations. It turns out that this discretization is stable in the Petrov-Galerkin sense if certain CFL-like conditions are respected.

Publications:

[1] C.J. Gittelson, R. Andreev, C. Schwab: Optimality of adaptive Galerkin methods for random parabolic partial differential equations. Journal of Computational and Applied Mathematics (online), 263:189-201, 2013.

[2] K. Kalimeris, O. Scherzer: Photoacoustic imaging in attenuating acoustic media based on strongly causal models, Mathematical Methods in The Applied Sciences, 16 (36), 2254-2264, 2013.

[3] A. S. Fokas, K. Kalimeris: Eigenvalues for the Laplace Operator in the Interior of an Equilateral Triangle, Computational Methods and Function Theory, DOI:10.1007/s40315-013-0038-7, 1-33, Springer, 2013.

[4] G. Bal, W. Naetar, O. Scherzer, J. Schotland: The Levenberg-Marquardt iteration for numerical inversion of the power density operator, Journal of Inverse and Ill-Posed Problems, vol. 21, no. 2, pp. 265–280, Feb. 2013.

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[9] M. Grasmair, O. Scherzer, A. Vanhems: Nonparametric instrumental regression with non-convex constraints, Inverse Problems, vol. 29, no. 3, p. 035006, 2013.

[10] M. Grasmair, M. Muszkieta, O. Scherzer, "An approach to the minimization of the Mumford–Shah functional using Γ-convergence and topological asymptotic expansion,

Interfaces and Free Boundaries, vol. 15, no. 2, pp. 141–166, 2013.

[11] G. Dong, M. Grasmair, S. H. Kang, O. Scherzer, Scale and Edge Detection with Topological Derivatives, in SSVM'13: Proceedings of the fourth International Conference on Scale Space and Variational Methods in Computer Vision, Berlin, Heidelberg, 2013, vol. 7893, pp. 404–415.

## 6.6. Group "Mathematical Methods in Molecular and Systems Biology"

<u>Group leaders:</u>

Prof. Dr. Philipp Kügler

Prof. Dr. Christian Schmeiser

<u>Researchers funded via ÖAW:</u>

Dr. Philipp Kügler (employed until 31.03.2013)

Dr. Stefan Müller (partially employed)

Dr. Dietmar Ölz (employed until 31.10.2013)

Dr. Wei Yang (employed until 30.09.2013)

MSc. Christoph Winkler (employed since 01.10.2013)

Dr. Stanislav Beyl (employed since 01.10.2013)

<u>Researchers externally funded:</u>

Mag. Stefanie Hirsch (employed until 28.02.2013)

Mag. Angelika Manhart (employed until 31.05.2013)

MSc. Christoph Winkler (employed until 31.01.2013)

In 2013 the group continued its work in the area of modeling and simulation of biochemical reaction networks. One focus was put on the study of how transitions from a healthy to a diseased state result from changes in genetic or environmental conditions. In that context the nonlinear inverse problem of inferring information about the Jacobian of a Langevin type network model from covariance data of steady state concentrations associated to two different experimental conditions was investigated. Under idealized assumptions on the Langevin fluctuation matrices it was proven that relative alterations in the network Jacobian can be uniquely identified when comparing the two data sets. Based on this result and the premise that alteration is locally confined to separable parts due to network modularity, a computational approach using hybrid stochastic-deterministic optimization was suggested for the de-

tection of perturbations in the network Jacobian using the sparsity promoting effect of lp-penalization. The approach was illustrated by means of published metabolomic and signaling reaction networks [3].

In collaboration with colleagues at the Max F. Perutz Laboratories, the hypothalamic-pituitary-adrenal axis (HPA axis) was studied [1]. It is a major part of the neuroendocrine system responsible for the regulation of the response to physical or mental stress and for the control of the synthesis of the stress hormone cortisol. Dysfunctions of the HPA axis characterized by either low (hypocortisolism) or increased (hypercortisolism) cortisol levels are implicated in various pathological conditions such as posttraumatic stress disorders or depression. Mass action and Michaelis Menten enzyme kinetics were used to provide a mechanistic description of the feedback mechanisms within the pituitary gland cells by which cortisol inhibits its own production. A recently found pituitary gland cell membrane receptor has been incorporated which mediates rapid non-genomic actions of glucocorticoids occurring on time scales of seconds to minutes which cannot be explained by interaction with intracellular receptors acting as ligand activated transcription factors. As a result the repertoire of qualitative nonlinear dynamics of the HPA axis model bas been significantly increased, now also capturing bistable behavior that is compatible with the scenario of hypercortisolism. The model has been validated against time resolved ACTH stress response data from in vitro AtT-20 pituitary tumour cells exposed to cortisol and CRH and enables the simulation of therapeutic strategies both for hypo- and hypercortisolism.

Joint with the institute for pharmacology and toxicology at the University of Vienna, the RICAM group analyzed effects of mutations of calcium channels on their voltage dependent gating properties [4]. Using macroscopic current recordings from voltage clamp experiments, equilibrium constants of the up- and downward voltage sensor movements and rate constants of pore transitions were estimated in terms of a circular four state (rest, activated, open, deactivated) channel model. Comparing wild type with mutant data, shifts in the activation curve of channelopathy mutations have been linked to transfers of the voltage sensor equilibrium towards activation. The inference algorithm is currently adapted in order to study drug channel interactions.

Jointly with the Symbolic Computation Group, the injectivity of families of generalized polynomial maps arising from chemical reaction networks was investigated [5]. The term generalized indicates that one considers polynomials with real exponents, which define maps on the positive orthant. As a main result, injectivity of generalized polynomial maps has been char-

acterized in terms of sign conditions [6]. As an immediate application, one obtains criteria for the uniqueness of steady states in chemical reaction networks with power-law kinetics. In the context of real algebraic geometry, the results reveal the first partial multivariate generalization of the classical Descartes' rule, which bounds the number of positive real roots of a univariate real polynomial in terms of the number of sign variations of its coefficients.

Furthermore the Bio and Symbolic groups studied constrained nonlinear optimization problems arising from kinetic metabolic networks. Clearly, the survival and proliferation of cells require a highly coordinated allocation of enzymes since the total enzymatic capacity for cellular metabolism is limited. While constrained optimization problems based only on stoichiometric information have been studied in the literature, the optimal solution of enzyme allocation problems was characterized in the RICAM collaboration with general kinetics, thereby using the theory of oriented matroids. In particular, it was shown that optimal solutions are elementary vectors or "elementary flux modes" in terms of stoichiometric network analysis [7]. This finding has significant consequences for the understanding of optimality in metabolic networks as well as for the identification of metabolic switches and the computation of optimal fluxes in kinetic metabolic networks.

In an ongoing cooperation with the group of J. Vic Small at the Institute for Molecular Biotechnology (IMBA) of the Austrian Academy of Sciences, the actin driven motility of cells and of intracellular pathogens has been studied [2]. A number of pathogens hijack actin monomers and a number of cytoskeletal proteins from their host cell, to build a motility machinery in the form of 'comet tails' consisting of filaments of polymerized actin. This mimics some of the processes in the cellular motility machinery. In a joint effort, detailed imaging of comet tails of baculovirus after fixation by electron tomography has been combined with simulations of a stochastic mathematical model of the comet tail dynamics. The amount of experimental data permitted not only a complete parameterization of the model, but also some tests of its predictive capacities. Convincing arguments for tethering of the filaments to the virus could be given, a question which had been a matter of controversy in the literature. The results have been published in PLoS Biology [9]. A second initiative is concerned with possible explanations of the flat shape of lamellipodia. Here a stochastic model of actin dynamics similar to the baculovirus study has been coupled to a model for the deformation of the cell membrane. The basic idea is that membrane proteins like IRSp53 mediate an interaction between membrane geometry and the actin filament nucleation and polymerization machinery. First successful simulations have been carried out, and two publications are in preparation [10, 11].

## Publications:

[1] Clemens A Zarzer, Martin Puchinger, Gottfried Köhler, Philipp Kügler (2013, online: 2013) Differentiation between genomic and non-genomic feedback controls yields an HPA axis model featuring Hypercortisolism as an irreversible bistable switch. Theoretical Biology and Medical Modelling.

[2] Koestler, S.A., Steffen, A., Nemethova, M., Winterhoff, M., Luo, N., Holleboom, J.M., Krupp, J., Jacob, S., Vinzenz, M., Schur, F., Schlueter, K., Gunning, P.W., Winkler, C., Schmeiser, C., Faix, J., Stradal, T.E.B., Small, J.V., Rottner, K. (2013) Arp2/3 complex is essential for actin network treadmilling as well as for targeting of capping protein and cofilin. Molecular Biology of the Cell, Bd. 24 (18), S. 2861-2875.

[3] Philipp Kügler, Wei Yang (2013, online: 2013) Identification of alterations in the Jacobian of biochemical reaction networks from steady state covariance data at two conditions. Journal of Mathematical Biology, Bd. DOI 10.1007/s00285-013-0685-3, S. 1-27.

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[7] Müller S, Regensburger G, Steuer R (2013) Enzyme allocation problems in kinetic metabolic networks: Optimal solutions are elementary flux modes. Bericht-Nr. arXiv:1308.0510 [q-bio.MN]; Cornell University: Ithaca .

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[9] J. Müller, J. Pfanzelter, C. Winkler, A. Narita, C. LeClainche, M. Nemethova, M.-F. Carlier, Y. Maeda, M.D. Welch, T. Ohkawa, C. Schmeiser, G.P. Resch, J.V. Small, Electron tomography and simulation of baculovirus actin comet tails support a tethered filament model of pathogen propulsion, PLoS Biol 12 (2014), e1001765.

[10] C. Winkler, C. Schmeiser, The flatness of lamellipodia explained by the interaction between actin dynamics and membrane deformation, in preparation.

[11] C. Winkler, C. Schmeiser, Numerics for stochastic lamellipodium modeling, in preparation.

## 6.7. Transfer Group

Group leader:
Prof. Dr. Ronny Ramlau

In the Transfer Group, all researchers are at least partially funded by external cooperation partners.

Researchers funded via ÖAW:
Dr. Michael Aichinger (50%)
Dr. Maximilian Emans (50% 01.01.-31.05.2013, 25% 01.06.-31.08.2013)
Dipl.-Ing. Johannes Fürst (50%)
Dipl.-Ing. Josef Haslinger (50%)
Dr. Roman Heinzle (50%)
DI Diana Hufnagl (50%)
Dipl.-Ing. Norbert Lorenz (50%)
Dr. Stefan Janecek (62.5%)

Researchers externally funded:
Dr. Jenny Niebsch (50% 01.01.-31.07.2013)
Dipl.-Ing. Mykhaylo Yudytskiy

The group focuses on the transfer of mathematical methods and numerical techniques to industrial and other scientific partners and develops algorithms and software prototypes for specific applications of the partners. Mathematically, the transfer group deals with the following fields:

- Inverse problems and optimization of systems described by integral and differential equations

- Fast and stable methods for (systems of) stochastic or partial differential equations arising from industrial applications.
- Model reduction and surrogate models

In 2013, the group worked on applications from the fields of Adaptive Optics, Automotive, Finance and Energy. The following results were achieved:

### Project „Mathematical Algorithms and Software for E-ELT Adaptive Optics"

The project "Mathematical Algorithms and Software for E-ELT Adaptive Optics" for the European Southern Observatory (ESO) is funded by the Austrian Ministry of Science. It is carried out in close cooperation between RICAM, the Industrial Mathematics Institute of the Kepler University Linz and the MathConsult GmbH. The aim of the project is the development of mathematical reconstruction methods for different types of adaptive optics systems for the planned European Extremely Large Telescope (E-ELT). The algorithms have to achieve a certain quality of reconstruction and the computations have to be carried out in real time.
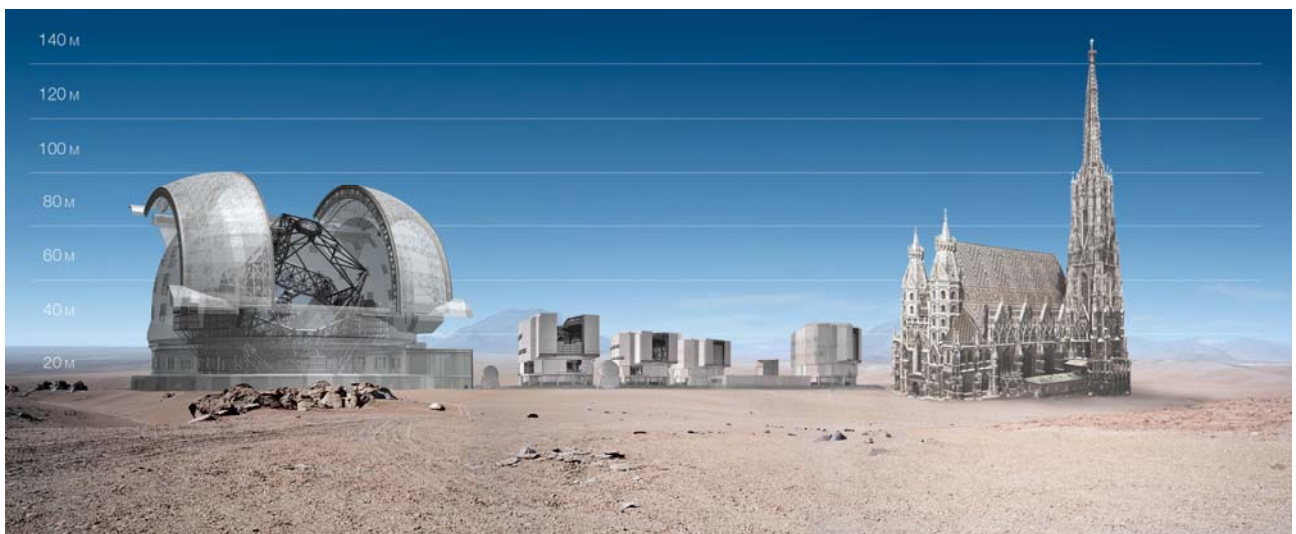


Fig. 1: A model of the planned European Extremely Large Telescope in comparison to the Very Large Telescope and the Stephansdom

In October 2013 the last of the four subprojects, Subproject AO3, has been successfully completed.  Subproject AO3 was concerned with development of reconstruction methods for Ground Layer Adaptive Optics (GLAO), Laser Tomography Adaptive Optics (LTAO) and Multi Object Adaptive Optics (MOAO).  The subproject passed the Final Review at ESO with excellent recommendations from the review board of the European Southern Observatory.

To quote the board report, "The Board unanimously recognized that the work carried out by the Project Team is fully in line with the statement of work and that the deliverables are compliant with the technical specifications. The Board firmly believes that the Project Team is to be commended for the quality and originality of the work performed."

The aim of Adaptive Optics (AO) is the correction of degraded images from ground based telescopes due to turbulence in the atmosphere. AO is a hardware-based technique for the correction of the phase of the incoming light. The correction is based on the reconstruction of the turbulence in the atmosphere from measurements in the direction of several guide stars, i.e., bright stars in the sky or artificially generated light sources using a laser. For each correction step, several subproblems have to be solved, where the essential subproblem is computation of a solution of the severely ill-posed atmospheric tomography problem, a variant of limited angle tomography.

In 2013 the research has been focused on LTAO and MOAO systems. At RICAM the emphasis has been on the development of fast and efficient algorithms for the atmospheric tomography subproblem, which plays a key role for the systems. LTAO and MOAO utilize several guide stars, each assigned to a wavefront sensor for atmospheric reconstruction. Further, the LTAO system uses one and MOAO several deformable mirror(s) for wavefront correction in the direction of one or multiple objects of interest. A sufficiently accurate reconstruction of the atmospheric turbulence over the telescope is vital for a good wavefront correction for the systems. Several methods have been developed, analyzed and implemented at RICAM, in particular the *Finite Element-Wavelet Hybrid Algorithm (FEWHA)* and three-step approach methods that solve the atmospheric tomography problem using a *Kaczmarz iteration* as well as gradient-based or conjugate gradient methods. The FEWHA was selected as the method of choice for implementation LTAO and MOAO systems.

The atmospheric tomography reconstruction in the FEWHA is obtained by solving the Bayesian maximum a-posteriori estimate with a preconditioned conjugated gradient algorithm coupled with a multi-scale strategy. In the hybrid algorithm, the turbulence layers of the atmosphere are discretized using a finite element and a wavelet basis simultaneously. A wavelet representation of layers has several advantages. First, wavelets have useful properties in the frequency domain, which allow for an efficient representation of turbulence statistics. Additionally, the operation of transforming the coefficients in the bilinear basis of finite elements to the coefficients in the wavelet basis, called the discrete wavelet transform (DWT), has a linear complexity and can be parallelized. Finally, wavelets have good approximative properties,

which means a turbulence layer can be well approximated using only a few wavelet coefficients. In contrast, the finite element representation of layers allows a very efficient representation of the atmospheric tomography operator. Due to these properties, the resulting finite element-wavelet hybrid algorithm for LTAO and MOAO delivers good qualitative performance, requires only a few iterations, and is computationally cheap due to its linear complexity and high level of parallelization.
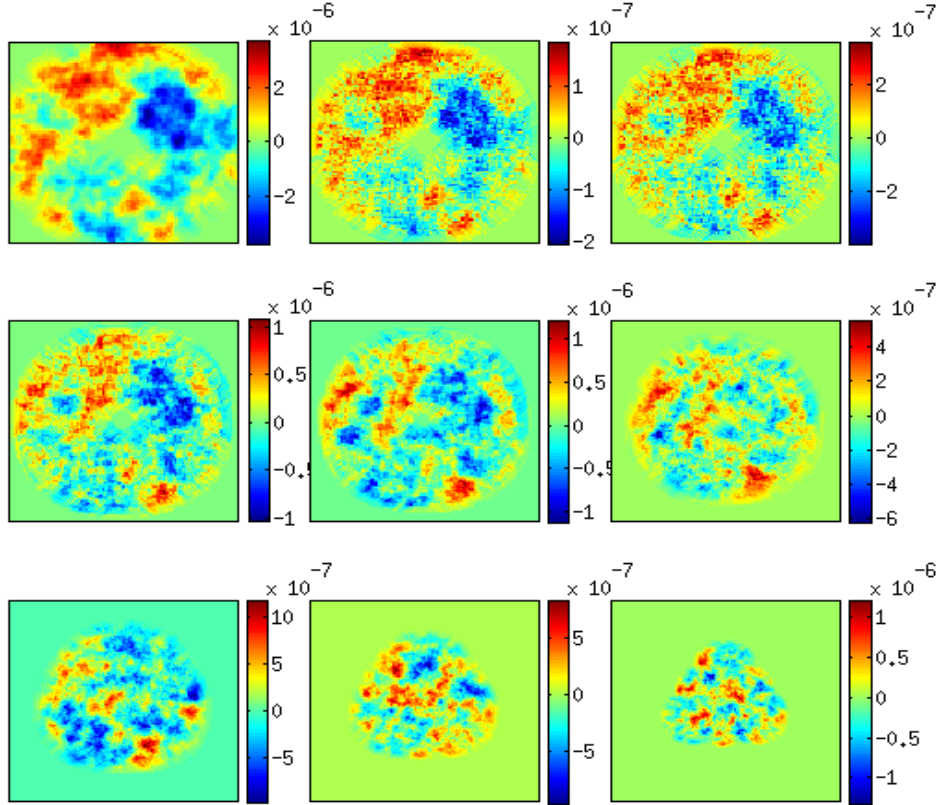


Fig. 2: Reconstructed turbulent layers in the atmosphere

The quality of the FEWHA was verified by simulations for the E-ELT on the ESO end-to-end simulation system OCTOPUS. The method was compared to the ESO version of the state of the art algorithm, the fractal iterative method (FrIM), and has shown to exceed the FrIM in almost all test cases. In terms of speed, a real-time computing (RTC) prototype of the algorithms showed that the method performs well on off-the-shelf hardware and has the potential to achieve the required reconstruction time of 1 millisecond on a dedicated RTC system. The FEWHA outperforms the matrix-vector-multiply (MVM) method of ESO, which serves as a benchmark in terms of speed, by a significant margin. Finally, the developed methods lead to significantly reduced costs for the required RTC hardware configuration, as now standard workstations can be used for the considered AO systems. The results were published in [1-7].

### Automotive

The work is carried out in cooperation with the company AVL List. In 2013, the group worked on several projects:

### System Engineering – Engine simulation tool in real-time

Topic of this project is, on the long run, to develop a multi-physic, multi-time scale and multi-domain over-all vehicle simulation tool on the basis of a software tool called AVL CRUISE M.The existing software tool captures all parts of the automotive vehicle including the engine, i.e., cooling and lubrication, chemical reactions as well as mechanical and electric parts.

In 2013 we worked in particular on the project "Solver Modularization" with the aim of efficiently coupling and simulating different physical domains (e.g., electric, and mechanic properties, the gas path, cooling and lubrication of the engine). A main goal of the project is to separate the physical modeling and its numerical treatment in order to simulate different physical domains with different numerical approaches and on different time scales. The concept for the modularization has been already developed. As a first physical domain, we started to adapt the cooling system to the new modular structure. Additionally, a solid wall component which separates different physical domains is now treated as a separate domain and thus can be evaluated on its own time domain, which reduces the calculation time for the full system.

Within a different project, the integration of hydraulic components into the system engineering tool was started. We developed a concept and finished the modeling of several components. The integration will be finished once the full modular structure of solvers and software is available.

### Multibody systems in automotive simulation

In 2013 also the solver modularization project for AVL-EXCITE has started. As for the AVL-CRUISE platform, within this project different types of AVL-simulation tools should cooperate in a common environment. In particular, an interface between AVL-EXCITE, which is a multibody dynamics simulation platform, and AVL-CRUISE, which is an over-all vehicle simulation tool, has been developed. The different time scales of the two environments require an efficient coupling strategy of the two platforms which is currently in development.

Additionally the work on the Kinetostatic project has been continued: for a time dependent flexible multi-body dynamic simulation it is necessary to have an appropriate initial state, which represents the preloaded conditions at the starting time point. To this end, we devel-

oped a model for the initial preloaded condition. Within this *kinetostatic model* the time dependent equations of momentum and angular momentum of a multi-body system were reformulated to a steady state system of equations with predetermined loads, velocities and accelerations. The model also was updated for valve train configurations. Further on, an adaption for time dependent joint forces was necessary (e.g. hydrodynamic forces in a lubricated bearing contact).

Also, the work on the development of methods for a modal analysis of multi-body systems was continued. The goal is to compute eigenmodes and eigenfrequencies for an assembly of bodies. Currently, a modal analysis is only possible for separate bodies, which does not take into account the influences due to connections to other bodies. To obtain a modal analysis for multi body systems, the equations of motions of the system were linearized and the according "modal matrices" were generated. From these matrices, the modal information can be extracted. In 2013, the modal analysis was also extended to flexible bodies resulting in a quadratic eigenvalue problem of sizes up to several thousands of degrees of freedom. The method was applied to a complex multi-body system representing a simplified driveline in which both flexible and rigid components are coupled. The obtained numerical results have been verified.

The project on an efficient approach for the dynamic simulation of valve springs within a multi-body system framework was finished. The method was validated on a single valve train system and the results were presented at two conferences.

### Computational Fluid Dynamics - Algebraic Multigrid Methods and Adaptivity

In the simulation of three-dimensional flows using the finite volume method, one must discretize the spacial domain. For this spacial discretization it is necessary that, on the one hand, the discretization allows for the computation of the solution with sufficient accuracy and, on the other hand, it has as few lattice cells as possible, since the number of operations to compute the solution of a given problem increases with the number of lattice cells. In many practically relevant cases, it is not known a priori in which areas a particularly fine resolution is needed; moreover the required resolution in an area can change during runtime, in the case of non-stationary flows.

In the field of industrially deployed software for fluid flow simulation, it is therefore exceedingly desirable to have a mechanism available that reliably handles the computation of a sufficiently accurate solution through the refinement of the finite volume discretization. In this

field, an added requirement is that the user of the software must be able to control the finite volume refinement, i.e., the user should have different options for defining the refinement criteria.

In the FIRE software package, established methods for adaptive lattice refinement were equipped with a user interface so that they can be used by a typical user without large programming costs. These established methods were also compared with current techniques from the literature. Since it showed promise, one of the residual estimators for a similar finite element method (from Jasak) was implemented. A quantitative comparison has shown that these techniques, for simple two-dimensional model problems, were indeed slightly better than established techniques, with respect to the achieved error reduction in dependence to the number of lattice points of the generated lattice.

The results in the working area "Automotive" have been published in [8-12].

**Simulation of a Sinter Plant** (Industrial partner: Siemens VAI)

For the efficient operation of a blast furnace in steel making, the burden material is usually prepared by sintering. In this process, iron-bearing materials of fine particle size are converted into coarse agglomerates through partial fusion. Siemens VAI currently operates a simulation of the sintering process to predict temperature, structure and chemical composition of the sinter material and the off-gas, given the chemical composition and grain size of the raw material and the operating conditions of the sinter plant. This simulation has been developed in an earlier project.

The primary focus of the present project is to reduce the calculation time for the simulation. Our project partners at Siemens VAI look for a speedup at least of a factor of four to fit the calculations into their workflow. After having achieved a speedup by a factor of about 1.8 with general code optimizations in 2012, we now concentrated on optimizing the most time-consuming part of the simulation, namely the evaluation of chemical reaction equations. In total, there are about 40 such reaction equations, composed from about 100 C++ classes in the code. Using the automatically generated reaction graphs developed in 2012, we analyzed the reaction equations and their interdependencies to identify bottlenecks, race conditions, inefficiencies in data handling and clusters of calculations that can be reused in different reactions. A Mathematica package was implemented to automate some of these tasks (of code analysis), and to generate an efficient C code for the reaction equations and the

partial derivatives of the reaction rates. The C code generation package was presented at the European Wolfram Technology Conference [13].

Based on this information and the C-code generated by Mathematica, most of the chemical reactions have been reformulated and implemented in a more efficient way. Another source of improvement comes from the Mathematica-generated derivatives: we were able to fix a number of errors in the calculation of derivatives in the legacy code, which results in a slightly faster convergence of the Newton iterations. As per December 2013, these optimizations result in a total speedup by a factor of about 4.25 compared to the original code. We believe that a moderate additional speedup is still possible by optimizing a number of remaining re-action equations as well as support classes.

In addition to the above code optimizations, a study of the temperature of the sinter material at the end of the sinter strand as a function of the speed of the strand and the height of the sinter bed was conducted at the request of Siemens VAI.

### Dipolar Bose Gas

We studied correlation effects and excitations in a dipolar Bose gas bilayer which is modeled by a one-dimensional double-well trap. We observe instabilities both for wide, well-separated layers dominated by intralayer attraction of the dipoles, and for narrow layers that are close to each other dominated by interlayer attraction. The behavior of the pair distribution function leads to the interpretation that the monomer phase becomes unstable when pairing of two dipoles becomes energetically favorable between or within layers, respectively. The results were published in [14-15].

### Computational Finance

Together with the cooperation partners at MathConsult, we have been working on computational challenges arising from changed market environments. Thus, the research of the computational finance group has been focused on the analysis and improvement of models for the valuation of financial instruments as well as their implementation.

The following topics were covered:

### Analysis of the Libor Market Model

In "Volatility and Correlation: The Perfect Hedger and the Fox", R. Rebonato proposes a two parameter correlation matrix for the forward Libor rates, which is not positive definite for long

time periods and certain values of these parameters. This intrinsic instability leads to unrealistic values for the coupons of long-lived (typically 30 years) financial instruments with variable compounding. A modification of the correlation functional as well as the inclusion of caplet data into the calibration function leads to parameters that are both stable and robust and result in a correlation matrix that is positive definite. The modified calibration process has been implemented and evaluated for different market situations. Several long lived financial instruments have been analyzed and the results have been compared to those of short rate models.

## Normal volatilities vs. lognormal volatilities

Due to the current state of the financial market, interest rates are very low or even negative. Therefore the Black76 model, which was the industry standard so far, can no longer be applied for the valuation of financial instruments. The Bachelier model is an alternative to the Black76 model and assumes normally distributed underlyings instead of lognormally distributed ones. Functions for the valuation of Vanilla caps and floors under the Bachelier model were implemented as well as formulas for the calculation of the Greeks (Delta, Gamma, Vega, Theta). Additionally a function to transform between normal and lognormal volatilities was derived and analyzed and the implementation of the calibration was extended such that stochastic interest rate models can be calibrated using Bachelier volatilities. Furthermore the model risk under both models was analyzed and the value at risk was compared.

## Multi Curve modeling

The development of financial markets after the credit crunch requires new methods for the valuation and modeling of financial instruments, since the basis spreads have increased and can no longer be neglected as it was done in the standard approach before. In this standard approach, the forward values of interest rates could be calculated from no-arbitrage arguments in the risk-neutral measure. This no-arbitrage arguments do not hold any more in actually traded fixed-income positions.

These market environments require a multi curve modeling approach, where different curves for the calculation of discount and forward rates are used. We analyzed and implemented several functions in the multi curve framework: a bootstrapping function was used for the calculation of the forward curve, valuation functions were used for basis instruments as well as a function for the calculation of the model drift (multi curve fitting). The results were collected in [16]. Additional a book on computational finance has been published [17].

**Thermomechanical modeling and simulation of heavy plates** (Cooperation partner: voestalpine Grobblech)

Heavy plates are used, e.g., for pipes in reservoir power stations or in pipelines. The mechanical requirements for these heavy plates are very high and can be positively influenced by adhering to a given temperature history during the production process of hot rolling.

We have been developing a surrogate model for the thermomechanical behaviour of heavy plates which allows the calculation of temperature profiles at arbitrary slices of the plate in real-time and which should, in a later stage, be the basis for the online control of plate temperatures.

Compared to an offline simulation (using ABAQUS, computing times are minutes), the calculated temperature results are of equivalent accuracy (also compared to measurements) but obtained within milliseconds. The results of the project have been published in [18].

**Monitoring of Wind Power Plants**

After finishing the FFG project 818098/16630 "Model based imbalance determination in wind turbines" ("Modellbasierte Unwuchtbestimmung in Windenergieanlagen") in November 2012, the focus in the first half of 2013 was in particular on the dissemination of the developments within the framework of the project. To this end, a paper summarizing the results of the project has been finished and submitted for publication [19]. The results were also presented at the annual conference of EWEA (European Wind Energy Association) in Vienna and during an invited talk at the Onshore O&M Forum in Hamburg, Germany. Additionally, a proposal for a follow-up project was prepared and submitted to the FFG. In June, the follow-up project "Frequency-dependant imbalance determination in wind turbines" ("Frequenzabhängige Unwuchtbestimmung für Windenergieanlagen-FaUb, project number 3733475) was accepted. Project start was January 1, 2014.

Additionally, performed a 3-month cooperation project with the Linz Center of Mechatronics (LCM), financed by LCM. The aim was the analysis of vibrational data and the identification of underlying parameters.

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## 6.8. Research Project "Applied Discrete Mathematics and Cryptography"

Researcher funded via ÖAW/Upper Austrian government funds:

Univ. Doz. Dr. A. Winterhof

Researcher externally funded:

Prof. Dr. H. Niederreiter (retired)

Dr. V. Ziegler (FWF, self-project, since 2013 for three years)

Dr. O. Yayla (TÜBITAK, since October 2013 for one year)

The research project DM focused on sequences for cryptography and quasi-Monte Carlo integration as well as Diophantine equations.

A highlight was the organisation of a special semester (D. Panario, A. Winterhof co-chairs, J. Schicho, H. Niederreiter co-organizers) on applications of algebra and number theory with 180 workshop participants. Its main part consisted of four workshops on

- uniform distribution and quasi-Monte Carlo methods
- algebraic curves over finite fields
- computer algebra and polynomials
- emergent applications of finite fields.

Moreover, it included two minor workshops

- Linz algebra research day
- Research days on the construction of combinatorial structures over finite fields

and the following tutorials:

- Gunther Leobacher: Quasi-Monte Carlo methods in finance
- Arne Winterhof: Applications of number theory
- Peter Mayr: Algorithmic abstract algebra
- Günter Pilz: Some Applications of Algebra
- Erich Kaltofen: Polynomial Factorization

The research project started an FWF project (Ziegler, 3 years) on Diophantine equations and applications and a TÜBITAK grant (Yayla, 1 year) on Hadamard-matrices and applications. Moreover, the research project participates with a subproject of the newly funded SFB "Quasi-Monte Carlo methods: Theory and Applications" (Winterhof, "Hierarchy of measures of pseudorandomness", first period 2014-2017).

Among DM's publications we emphasize the book [26] on finite fields and the eight survey articles [18-25] (five of them in the Handbook of Finite Fields). V. Ziegler focused on Diophantine equations [2,14,15], uniformly distributed sequences [1,10] and linear combinations of units in algebraic number fields [3,8,9] in view of possible cryptographic applications. H. Niederreiter suggested a new inversion method for non-uniform pseudorandom numbers [4] and analyzed hybrid sequences [5] which seem to be suitable, for example, for computer graphics, as well as other low-discrepancy sequences [7,12]. A. Winterhof analyzed several pseudorandom sequences and measures of pseudorandomness [6,11] as well as functions for cryptography [13,17] and coding theory [16].

## Publications:

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## 6.9. START Project "Sparse Approximation and Optimization in High Dimensions"

Project leader:

Prof. Dr. Massimo Fornasier

Researchers externally funded:

Dr. Dante Kalise (employed since 01.05.2013)

BA Martin Eller (employed until 05.04.2013)

In the year 2013 the START Project hosted one student of the Technical University of Munich, Mr. Martin Eller, and – in 2012 - Mrs. Juliane Sigl, who performed the experimental part of their thesis at RICAM. Both these theses have been developed far beyond the traditional scope of a Master thesis, having a strong research component. Indeed both led to very new results which have been published in corresponding papers. The Master thesis of Mr. Eller has been also awarded one of the Main Prizes at the Student Conferences of the OEMG-DMV in Innsbruck in September 2013. The thesis of Mr. Eller was on exemplar based image inpainting, following the variational approach proposed by Caselles et al. Differently from the approach currently followed in the literature, where patches from other parts of the image are rigidly matched with the part of the image to be inpainted, we introduced the additional freedom of considering matching independent of mutual rotation. The motivation for this additional degree of freedom is the fact that in several real-life and man-made images, many geometrical symmetries are present and, especially in presence of curved details, matching of these parts independent of rotations is certainly beneficial for a faster and smoother reconstruction of regular edges. The task of Mr. Eller was to adapt the algorithm proposed in in the paper [*Fast, robust, and efficient 2D pattern recognition for re-assembling fragmented images* (M. Fornasier and D. Toniolo), Pattern Recognition, Vol. 38, 2005, pp. 2074-2087] for image pattern matching independently of mutual rotation, in order to make a proper ranking

of best matching patches in the variational exemplar based image inpainting. Mr. Eller succeeded in performing the tasks assigned to him and produced exceptionally good results.

Mrs. Sigl has been working on applications of compressed sensing techniques for refining the data analysis of pulsating stars in cooperation with Prof. Michel Breger (Astronomy, University of Vienna) and Dr. Patrick Lenz (Copernicus Astronomical Center in Warsaw). She studied the behavior of several sparse recovery algorithms and she tested them on the real satellite data provided by our colleagues from Astronomy. Moreover, we formulated a mathematical model of the light spectra measurements which lead to a nonlinear compressed sensing problem. We proved that this problem is well-posed in the sense of establishing that the amount of information provided by such nonlinear measurements uniquely identifies the shape of a pulsating star, characterized by few modes of oscillation. We investigated iterative algorithms for solving the corresponding nonlinear inverse problem.

Additionally, the START Project hosted a new PostDoc, Dr. Dante Kalise, with whom we have been undertaking the following research directions:

- Optimal control of large-scale consensus models: we consider large scale dynamics describing the interaction of multi-agent systems and their stabilization around consensus by means of sparse, optimal controllers. One of the main difficulties of such a problem relates to the dimensionality of the system, and therefore, the development of an efficient and accurate solver is required. We are currently working on a numerical implementation based on the OCPIDDAE library for optimal control, in collaboration with Prof. Matthias Gerdts (Universität der Bundeswehr, Munich).

- Feedback stabilization of partial differential equations via model reduction: we develop a consistent numerical framework for the computation of feedback controllers for large-scale dynamical systems arising from discretization of partial differential equations. We bridge the existing gap between high-dimensional dynamics and feedback controls by means of model reduction techniques such as Balanced Truncation and Proper Orthogonal Decomposition. Furthermore, we consider the inclusion of observers and the design of robust controllers. This is work in collaboration with Dr. Axel Kroener (RICAM).

- Efficient numerical schemes for Hamilton-Jacobi-Bellman equations: the main drawback of HJB-based techniques in optimal control is the so-called curse of the dimensionality, which prevents them to be applied in (moderately) large-scale dynamical systems. Therefore, the development of efficient numerical schemes allowing higher dimensional resolution turns out to be a difficult and relevant task. In this direction, we are currently working on high-order based formulations, together with the development of efficient multigrid

solvers. This is work in collaboration with Dr. A. Alla (University of Hamburg) and Prof. M. Falcone (La Sapienza, Rome).

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