# **AUSTRIAN ACADEMY OF SCIENCES**

# **Annual Report 2006**

Johann Radon Institute for Computational and Applied Mathematics

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DIRECTOR: Prof. Heinz W. Engl

ADDRESS: Altenbergerstr. 69

A-4040 Linz

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This report has been compiled by the Institute Director Heinz W. Engl based on input by all group leaders and all members of the Institute. Because of the international composition of the Board, it is written in English. Although the report follows the general structure prescribed by the ÖAW, the section about scientific achievements and plans is grouped by working groups and Institute members in order to enable the Board and the ÖAW to get to know the scientific groups and employees individually.

# 1. THE DEVELOPMENT OF THE INSTITUTE IN GENERAL

### Personnel

As announced in the last annual report, the year 2006 was again a year of expansion of personnel towards the final size of the institute of about 60 scientists. On December 31, 2006, RICAM employed 35 scientists with a doctorate and 20 doctoral students; of those, 6 PostDocs and 18 doctoral students were employed by via external funds. The two doctoral students employed via the basic funds were mainly concerned with scientific issues of the two special semesters, so that this does not constitute a deviation from our policy to use the basic funds only for PostDocs.

Thus, at the end of 2006, RICAM had 55 scientific employees, 24 of them being externally funded. For 2007, our aim is to reach the planned state of 30 PostDocs funded via basis funds (Academy of Sciences and Upper Austrian Government).

In 2006, a new group (currently with two internally funded PostDocs) on "Mathematical Imaging" has been added; this group is led by Prof. Otmar Scherzer (University of Innsbruck) and has a scientific overlap with most of the other groups at RICAM (especially with Inverse Problems, Analysis of Partial Differential Equations and Symbolic Computation). A self-organized (by the PostDocs) working group on Imaging Techniques with internal seminars and external speakers has been organized.

In 2005, Prof. Hansjörg Albrecher from the University of Technology in Graz took over the leadership (joint with Prof. Walter Schachermayer) of the "Financial Mathematics" group. In 2006, the two parts of the group (Stochastic Finance and Number-Theoretic Methods) have been brought together more closely, and the group has already grown. Cooperations with other groups (especially with the Inverse Problems group) have been started.

If a current proposal will be granted, RICAM will be the scientific partner of the Industrial Mathematics Competence Center (IMCC) from 2008 (within the COMET program of the Austrian Government). Funds (mainly for personnel) in the range of three additional PostDocs will be dedicated to this purpose; we do not apply for new funds, but plan to shift these funds partly from money so far allocated to special semesters (which turn out to be cheaper than originally expected). Also, the new funding obtained from the Upper Austrian Government is partially dedicated to that purpose.

The following scientist left in 2006:

Name	Employed until	Left to	Position
Joachim Schöberl	15.03.2006	University of Aachen	Full Professor
Martin Burger (scientific advisor Inverse Problems group)	30.09.2006	University of Münster	Full Professor
Oliver Labs	31.03.2006	University of Saarbrücken	University Assistant
Herbert Egger	31.03.2006	University of Aachen	University Assistant

Pavel Chalmoviansky	31.03.2006	Comenius University,	Assistant Professor
		Bratislava	
Benjamin Hackl	31.05.2006	Industrial Mathematics	
		Competence Center	
Jürgen Hartinger	31.05.2006	Kärtner Landesversicherung	Actuary
Gergana Bencheva	30.06.2006	Bulgarian Academy	Research Scientist
		of Sciences	
Stefan Kindermann	31.08.2006	University of Linz	University Assistant
Andreas Hofinger	30.09.2006	Private Company Ecolog	Informatics development
Michael Barton	30.09.2006	Charles University,	Research Scientist
		Czech Republic	
Marie-Therese	31.10.2006	University of Münster	University Assistant
Wolfram			
Janka Pilnikova	31.12.2006	Comenius University,	University Assistant
		Bratislava	

In 2006, the following additional PostDocs and doctoral students were hired via RICAM basic funds:

PostDoc	At RICAM	Doctorate:	Came to RICAM from
Name	since	year, institution	
Keith Anguige	01.03.2006	1997, University of Oxford	University of Nottingham
Massimo Fonte	01.04.2006	2005, SISSA/ISAS of Trieste	PennState University, State
			College
Dylan Copeland	01.06.2006	2006, Texas A&M University	Texas A&M University
Massimo Fornasier	01.06.2006	2003, University of Padua	University of Vienna
Bastian Gebauer	01.10.2006	2006, University of Mainz	University of Mainz
Peter Elbau	01.10.2006	2006, ETH Zurich	ETH Zurich

The following PostDocs and doctoral students were hired and are externally funded:

PostDoc	At RICAM	Doctorate:	Came to RICAM from
Name	since	year, institution	
Lin He	01.07.2006	2006, UCLA	UCLA
Mourad Sini	01.09.2006	2002, University of	Yonsei University, Korea and
		Provence	Impedance Imaging Research
			Center
Esther Klann	01.10.2006	2006, University of Bremen	University of Bremen

Doctoral Student	At RICAM	Diploma:	Project: agency/number/leader
Name	since	year, institution	
Mario Kapl	01.01.2006	2005, University of Linz	FWF. SFB F1315, Schicho
Stefan Thonhauser	01.01.2006	2005, Graz University of	FWF, P18392, Albrecher
		Technology	
Dominik Kortschak	01.01.2006	2005, Graz University of	FWF, P18392, Albrecher
		Technology	
Astrid Sinwel	01.04.2006	2006, University of Linz	FWF, START Project, Schöberl
Nina Brandstätter	01.07.2006	2004, University of Vienna	FWF, P19004, Winterhof
Martin Huber	01.07.2006	2006, University of Linz	FWF, START Project, Schöberl
Niels Lubbes	01.07.2006	2004, University of Amster-	FWF, P18992, Schicho
		dam	

Brian Moore	01.07.2006	2000, Universite du Quebec a Trois-Rivieres	FWF. SFB F1303, Schicho
Kattrin Arning	15.07.2006	2006, University of Bremen	FWF, W1201, Engl
Olaf Benedix	01.09.2006	2006, TU Chemnitz	FWF, 18971, Rösch, Vexler

External funds in 2006 thus came from the following sources:

- Austrian Science Foundation FWF in the framework of a special research area (SFB F13 "Numerical and Symbolic Scientific Computing"), a START project (led Prof. Schöberl, who will be connected to the institute until the end of his START project in 2008), and the doctoral college "Molecular Bioanalystics".
- RICAM is also part of a new application of a doctoral college "Computational Mathematics"
- WWTF (Viennese Fund for Science and Technology) with the project "Modelling the Dynamics of Cellular Networks Using Inverse Methods"
- European Union in the framework of a Marie Curie Fellowship obtained by Dr. Massimo Fornasier

Our current policy still is to hire scientists only on non-permanent positions: usually for three years, extendable for another three years. Within the Austrian Academy of Sciences, an employment of six years in total is the maximum which is possible for non-permanent positions. In order to obtain a more stable personnel structure, we will slowly relax this policy and offer a few (very few!) permanent positions. This will be done only for people of exceptional high quality on the level of professors (e.g., for group leader positions). In that case, the current group leaders might withdraw from leading their groups on a daily basis to the position of a scientific advisor. We are negotiating with the University of Linz some kind of joint appointments, where, in addition to a permanent position with a salary on professorial level funded by the Austrian Academy of Sciences, the University will appoint the respective people as professors (without or with a very low teaching obligation, but with the possibility to teach, thus enabling them to advise doctoral and diploma students). In this way, RICAM will be more closely linked to the University, thus, on the one hand, having easier access to local students and, on the other hand, influencing the development of mathematics at the University of Linz. After initial talks between the rector, the president of the Austrian Academy of Sciences and the Institute Director in late 2006, a formal agreement is in preparation.

# Office Space

As indicated in the last report, four large apartments adjacent to the campus of the University have been rented in 2005. Due to the rapid expansion of the personnel (especially due to the increase in Third Party Funds), this office space was more than full already in mid 2006. With the help of the University we could rent another apartment (close to the existing ones) with a size of 257 square meters, so that at the beginning of 2007, RICAM has now 987 square meters of office space. This new larger apartment will be occupied by the group led by Prof. Langer "Computational Methods for Direct Field Problems"; the other apartments will remain to be occupied by "Financial Mathematics", "Symbolic Computation" and "Analysis of Partial Differential Equations". In the original offices at the campus (Hochschulfondsgebäude) there will be the groups "Inverse Problems", "Optimization and Optimal Control" and "Mathematical Imaging", between which close cooperations exist.

Of course, it would be better if all RICAM scientists could be housed in the same building. Although the two locations are at most ten minutes by foot apart, this distance is disadvantageous for spontaneous cooperations. In order to counteract this, we introduce a new policy for seminars and colloquia:

• RICAM Colloquia (once a week, usually every Wednesday): prominent external scientists, whose work is of interest to more than one of the groups and who will be asked to present their talks in such a way that they are accessible for a broad audience

- RICAM Seminars: by external and internal scientists, whose attendance is compulsory for all and which should be truly understandable to all!
- Group Seminars: can be more specialized and need not be attended by members of other groups, although this is encouraged in cases where the abstract indicates that this makes sense.

The plans to build a Science Park close to the University have been finalized; the construction of the first stage (which is to house the Mechatronics Department of the University) will be started soon. The University has reserved space for RICAM in the second phase and expects to complete this by 2009. It is expected that all Mathematical Institutes of the University will also move to that new space, and that also the Industrial Mathematics Competence Center will obtain offices there. Thus, from 2010, there will be ideal office conditions for a large mathematical cluster consisting of University institutes, RI-CAM and industry-related institutions.

### IT Infrastructure 2006

# **Network at Altenberger Strasse premises**

The premises are connected to the main RICAM building by a 10Mbit uplink. It has turned out that the capacity of the 10Mbit uplink is too small; but with some reorganization of the local network to avoid unnecessary access through the uplink it was possible to cope with it temporarily. An upgrade to 20Mbit is planned for 2007. The computers at the premises are connected together with 100Mbit switches to allow fast access between the workstations for fast cluster operation. The same network subsegment is used in both locations to provide access between all RICAM computers and servers. For security reasons the network at the Altenbergerstraße premises mainly used by Special Semester guests is separated from the RICAM internal network by the central firewall at RICAM. The premises are all fitted with wireless LAN access points. The wireless LAN access points are integrated into the WLAN infrastructure of University of Linz to allow the wireless network usage on the whole university campus without reconfiguration of the clients.

### Central Firewall:

The PC-server which was bought in 2005 for our Linux-based Phion firewall was replaced completely on warranty because of persistent hardware troubles and ongoing crashes of the firewall system caused by them. The firewall configuration was backed up and the firewall system was completely reinstalled before the firewall rules where loaded again. The firewall is running stably without any reboot since the replacement.

### Uninterruptible power supply:

An uninterruptible power supply was bought to protect our firewall and servers from damages caused by voltage spikes, over- or undervoltage and power line noise. The attached computers are kept running on battery power for some time; at longer power disorganization the computers are shut down to prevent filesystem damages and data loss due to unclean shutdown.

# **Special Semester Computer Access:**

For the Special Semester on Gröbner Bases and Related Methods 7 standard PC's where installed at a university lecture room. The PC's where used for tutorials with mathematical software and for email access during work breaks. The PC's where running Linux and mathematical software was installed as requested by the lecturers. The Linux Desktops where especially secured to avoid problems with public access.

#### Servers

# Computing Server:

The dedicated dual Processor Computing Server with 8GB of main memory available to all RICAM employees for large calculations was working well as expected; additional software was added if requested. As operating system Linux is installed. As scientific mathematics software Matlab, Mathematica and Maple is installed. For calculations, the Computing Server can be reserved for exclusive access if needed. It has turned out that the available computing power is not enough for all RICAM employees and that it is, mostly because of the limited main memory, not possible to calculate very large scale problems. Therefore the purchase of an even larger computing server was planned but due the budgetary situation in end of 2006 the purchase was delayed.

The larger computer will be bought in 2007.

### Communication server:

The server provides the RICAM web page including database access, email access through POP3 and IMAP, Spam and virus filter for email services, web mail access, groupware scheduler, mailing list manager and CVS repository. The operating System is Linux with extra access control kernel patches to add an extra security layer. All used software (except the virus scanner) is open source and free for use. In 2006 the CVS revision control system was replaced by its successor subversion. Many installed programs like the apache web server where updated to a recent version. For the Special Semester on Gröbner Bases and Related Methods, extra web pages and database based scripts for information, registration, program and time schedule were written.

### File Server:

The file server allows centralized user management and data storage for Windows and Linux Clients. Each user can access his or her data from any client in the network with both Linux and Windows clients. Data are backed up during every night to the central backup server owned by the Johannes Kepler University. The operating system is Linux with extra access control kernel patches to add an extra security layer. All used software is open source and free for use. In 2006 many installed programs where updated to a recent version. The LDAP server responsible for our network-wide user authentication was configured redundantly together with the administrator's workstation to provide failover if the file server is down. The DHCP server providing IP-addresses to mobile clients was moved from the administrator's PC to the fileserver. Redundant DHCP service is planned for 2007.

# Terminal server:

The terminal server allows access to Windows applications on Linux through the rdesktop client. The operating system is Windows2003 Server with Terminal Services licensed. In 2006, no changes to the configuration where made as everything is working well. Many installed programs were updated to a recent version.

#### **Clients**

# <u>Laptops:</u>

Fujitsu Siemens E Laptops were bought for the best compromise between mobility and power. Each laptop is equipped with 1 - 2 GB memory extension to reach better performance for calculations and a DVD burner + USB flash memory for data exchange. As operating systems both Linux and Windows are installed. MS Office is also usable under Linux with the help of the CrossOver Office Windows emulator. As scientific mathematics software Matlab, Mathematica and Maple for both Windows and Linux as needed is installed.

# Workstations:

PC architecture based dual processor workstations with Intel Dualcore CPU and 4 - 8 GB main memory where bought for scientific employees with need for large computing power. As operating system only Linux is installed.

Microsoft applications (mainly Microsoft Word and Powerpoint) can be used through the Windows 2003 Terminal Server which was bought in 2004.

The workstations are able to work in a cluster mode with parallel programmed applications or with the application transparent cluster software Mosix. As scientific mathematics software Matlab, Mathematica and Maple are installed as needed.

### **Standard PCs**:

Standard PCs where bought for scientific employees with no need for large computing power. As operating system only Linux is installed. Microsoft applications (mainly Microsoft Word and Powerpoint) can be used through the Windows 2003 Terminal Server which was bought in 2004. As scientific mathematics software Matlab, Mathematica and Maple are installed as needed.

### 2. THE SCIENTIFIC ACHIEVEMENTS AND PLANS OF THE INSTITUTE

# 2.1. GROUP "COMPUTATIONAL METHODS FOR DIRECT FIELD PROBLEMS"

# **Group Leader:**

O.Univ.-Prof. Dipl.-Ing. Dr. Ulrich Langer

# Researchers funded via ÖAW/Upper Austrian government funds:

Dr Gergana Bencheva (employed until June 30, 2006)

Dr. Dylan Copeland

Dr. Marco Discacciati

Dr. Johannes Kraus

Dipl.-Ing. David Pusch

Univ.-Prof. Dr. Joachim Schöberl (fully employed until March 15, 2006)

Dr. Satyendra Tomar

# Researchers externally funded by the FWF START project Y192 led by Prof. Joachim Schöberl:

Dipl.-Ing. Almedin Becirovic

Dipl.-Ing. Martin Huber

Dipl.-Ing. Astrid Sinwel

Dr. Sabine Zaglmayr

# Introduction by Group Leader Prof. Ulrich Langer

The "Computational Mathematics Group" (CMG) has focused on the development, analysis and implementation of novel fast computational methods for direct field problems arising in different fields of applications such as solid and fluid mechanics, electromagnetics, and magnetohydrodynamics.

The first group of methods, developed by J. Schöberl and S. Tomar, belong to Domain Decomposition (DD) solvers for large scale algebraic equations arising from the so-called hp finite element discretization of second-order elliptic Partial Differential Equations (PDEs) or systems of such equations. It is worth to mention that these DD solvers are highly parallel. J. Schöberl supervises the **FWF START project Y192** "hp-FEM" that is also devoted to fast solvers for hp finite element equations. In 2005, the START project was prolonged for further three years (until July 2008). M. Discacciati has also contributed to domain decomposition methods.

The second group of solvers, developed by J. Kraus, S. Tomar and D. Pusch, belong to geometric and algebraic multigrid methods. Algebraic multigrid methods are very important as black-box solvers for practical applications because they do not require any hierarchical discretization structure. J. Kraus and S. Margenov plan to write a monograph on robust algebraic multilevel methods and algorithms. J. Kraus submitted a research proposal on "Algebraic Multigrid and Multilevel Methods for Vector Field Problems" to the FWF in 2006. The project was granted by the FWF under the No. P19170-N18 for 3 years and will be started in February 2007.

Recent publications of the group leader have also contributed to these two main research fields in 2006. The publications [2, 4] are devoted to Boundary and Finite Element Tearing and Interconnecting techniques, whereas the papers [3,5] deals with geometric and algebraic multigrid methods for large scale data-sparse boundary element equations. The paper [1] is devoted to the construction and analysis of fast solvers for the systems arising from the multiharmonic finite element discretization of non-linear eddy current problems with harmonic excitations. The results on multiharmonic techniques and other results obtained in Computational Electromagnetics were presented in an invited talk at the CosComp 2006, Vienna, Austria, February 2006 [6]. The results on geometrical and algebraic multigrid preconditioners for data-sparse boundary element matrices were presented at a MAFELAP

minisymposium [8]. The new results on inexact, data-sparse Boundary Element Tearing and Interconnecting (BETI) methods and coupled BETI-FETI methods were presented in a plenary talk at the *MAFELAP* 2006, London, UK, June 2006 [7] and in an invited minisymposium talk at the *ICMP* 2006, Stuttgart, Germany, October 2006 [9].

- 1. F. Bachinger, U. Langer, J. Schöberl: Efficient Solvers for Nonlinear Time-Periodic Eddy Current Problems. *Computing and Visualization in Science*, Vol. 9, No. 4, 197-207, 2006.
- 2. U. Langer, C. Pechstein: Coupled Finite and Boundary Element Tearing and Interconnecting Methods Applied to Nonlinear Potential Problem. *Z. Angew. Math. Mech.* Vol. 86, No. 12, 915-931, 2006.
- 3. U. Langer, D. Pusch: Comparison of Geometrical and Algebraic Multigrid Precondition ers for Data-sparse Boundary Element Matrices. *Proceedings of the 5<sup>th</sup> International Conference on Large-Scale Scientific Computations LSSC 2005*, Sozopol, Bulgaria. Lecture Notes in Computer Science, Vol. 3743, pp. 130 137, Springer-Verlag, Heidelberg, Berlin, 2006.
- 4. U. Langer, G. Of, O. Steinbach, W. Zulehner: Inexact Fast Multipole Boundary Element Tearing and Interconnecting Methods. In "*Domain Decomposition Methods in Sciences and Engineering*" (ed. by D. Keyes and O. Widlund), Proceedings of the 16th Domain Decomposition Conference, held in New York, USA, January 2005, Lect. Notes Comput. Sci. Eng., Vol. 55, pp. 405 412, Springer-Verlag, Heidelberg, Berlin, 2006.
- 5. U. Langer, D. Pusch: Convergence Analysis of Geometrical Multigrid Methods for Solving Data-Sparse Boundary Element Equations. Submitted to *Computing and Visualization in Science*.
- 6. U. Langer: Computational Electromagnetics: From the Simulation to the Optimization, Invited lecture at the *CosComp 2006*, Vienna, Austria, February 2006.
- 7. U. Langer: Data-sparse Boundary and Finite Element Domain Decomposition Methods, Plenary lecture at the *MAFELAP 2006*, London, UK, June 2006.
- 8. U. Langer: Comparison of geometrical and algebraic multigrid preconditioners for datasparse boundary element matrices, Invited Mini-Symposium talk at the *MAFELAP 2006*, London, June 2006.
- 9. U. Langer: Coupled Finite and Boundary Element Tearing and Interconnecting Solvers for Nonlinear Potential Problems, Invited Mini-Symposium talk at the *International Conference on Multifield Problems, ICMP 2006*, Stuttgart, October 2006.

The CMG primarily has internal cooperation with the Inverse Problem Group (IPG), the Group "Optimization and Optimal Control" (OOC), the Symbolic Computation Group (SCG), and, of course, with the SFB and the Institute of Computational Mathematics at the Johannes Kepler University Linz. This internal cooperation as well as the international cooperation is presented in the individual reports by the researchers. In addition to this, the group leader especially cooperates with G. Haase (Graz), O. Steinbach (Graz) and G. Of (Stuttgart / Graz) on AMG and DD methods (see publications [3, 6]) as well as with V.G. Korneev (St. Petersburg) and C. Douglas (Lexington). The group leader was one of the co-organizers of the workshop "Fast Boundary Element Methods in Industrial Applications" held at Hirschegg, September 29 — October 2, 2006. See home page <a href="http://www.numerik.math.tu-graz.ac.at/tagungen/FastBEM2006.htm">http://www.numerik.math.tu-graz.ac.at/tagungen/FastBEM2006.htm</a> for more information. The 17<sup>th</sup> International Conference on Domain Decomposition Methods, held at St. Wolfgang / Strobl, Austria, July 3 — 7, 2006, was chaired by the group leader. Together with M. Discacciati, D. Pusch and W. Zulehner the group leader is preparing the DD17 proceedings which will be published by the Springer Verlag in the series Lecture Notes in Computational Science and Engineering (LNCSE). See DD17 home page <a href="http://www.ricam.oeaw.ac.at/dd17">http://www.ricam.oeaw.ac.at/dd17</a> for more information.

The group leader was the main organizer of the **Special RICAM Semester** on "Computational Mechanics" held at RICAM in Linz, October 3 – December 16, 2005. The main and most valuable results of the special semester are the joint scientific research activities of the participants which were initiated during the special semester and which have resulted in joint publications, in improved or new

software packages, in joint presentations at conferences, in joint organizations of conferences, workshops, minisymposia etc. Some of the lectures and survey talks will be published in the new Radon Series as a kind of proceedings. At least two monographs were initiated during the Special Semester. Both monographs will appear in the new Radon Series for Computational and Applied Mathematics which is published by Walter de Gruyter GmbH & KG. The first monograph written by S. Repin is devoted to his lectures on a posteriori estimates for differential equations which were given during the special semester. The second monograph on "Robust Algebraic Multilevel Methods and Algorithms" is prepared by J. Kraus and S. Margenov. Therefore, this follow-up phase has already indicated the long-term impact of this special semester on the scientific community. The homepage of the special semester on "Computational Mechanics" <a href="http://www.ricam.oeaw.ac.at/sscm/">http://www.ricam.oeaw.ac.at/sscm/</a> will be continuously updated with respect to the follow-up phase.

The CMG is a member of the **Austrian Grid Project** supported by the BMBWK under the grant GZ 4003/2-VI/4c/2004. In particular, the work package WP A-3b on "*Distributed Scientific Computing*" that is led by U. Langer, J. Schöberl and W. Zulehner deals with the development and the grid implementation of distributed mesh generators and distributed finite element solvers. See the Austrian Grid homepage <a href="http://www.austriangrid.at/">http://www.austriangrid.at/</a> for more information.

Joint **US-American - Austrian Research Project** "Fast Solvers for Computational Pharmacy, Life Sciences, Mathematics, Physics, and Environmental Modeling" supported by the NSF under the grant OISE-0405349 (2005-2006). This project is an interdisciplinary project led by Craig Douglas. Cache aware versions of the AMG methods developed in our FWF project are especially investigated in this joint US-American – Austrian research project. G. Bencheva has investigated a non-linear system of coupled diffusion-reaction problems describing the diffusion of ointments through the skin. See the project homepage <a href="http://www.mgnet.org/~douglas/ml-dddas-austria.html">http://www.mgnet.org/~douglas/ml-dddas-austria.html</a> for more information.

In December 2003 we made an agreement on a **Collaborative Research Project** titled "*Robust Scientific Computing Methods and High Performance Algorithms*" between the Johann Radon Institute for Computational and Applied Mathematics (RICAM) of the Austrian Academy of Sciences and the Institute for Parallel Processing (IPP) of the Bulgarian Academy of Sciences. In August 2006, J. Kraus and S. Margenov organized a minisymposium on "Robust Algebraic Multilevel". There are 3 joint publications (2 accepted, 1 submitted); see report by J. Kraus below. In addition to this, one monograph by J. Kraus and S. Margenov is in preparation.

Last but not least, J. Schöberl accepted an offer of a professorship position in "Scientific Computing" at the RWTH Aachen that is one of the best technical universities in Germany. He moved to Aachen in March 2006. However, he is still supervising his START project Y192 "hp-FEM" and he has many cooperations with different people working at RICAM, SFB, or University Institutes (e.g. IndMath, NuMa, RISC) in Linz.

# Almedin Becirovic advised by Prof. Joachim Schöberl

Degeneration Method for Plates and Shells: For the implementation of plate and shell models it is possible by the reduction of dimension to make the calculation on a 2D model. There are two different ways to obtain 2D model. The first way is the "mathematical" way.

In this case we start directly with a physical 2D domain (in 3D space) of a thin structure and then search one map, which maps the 2D reference domain (2D space) into the physical domain. For simple domains (for example cylinder) is this not difficult, but with more complicated domains we have big problems arise when defining the mapping function. The second way is the "degeneration" principle, which I prefer. In this method, we start with 3D do mains and with help of standard and differential geometry make the reduction to 2D domain.

Therefore there are several ways for the ansatz of the displacement, e.g. 5,6,7-parameter formulation. 6-parameter is standard and is implemented for the plates. Compare to the plates, the shells give us some troubles. This is mainly because the director (normal on the middlesurface) is for shells not constant as in the plate case. Hence the derivation of the director is not any more zero. 7-parameter formu-

lation is equivalent to EAS formulation. In this year I studied these shell models and started the implementation of the 6-parameter formulation where are still some details to include.

Starting to write my PhD-thesis "Primal-Dual Error Estimator for High Order Finite Elements": The main point of the thesis is a new error estimator for the laplace and linear elasticity equation. The idea is in the first step to compute finite element approximation  $u_-hp$  from the primal problem. In the second step we compute the flux  $p_-hp$  in high order H(div) finite element space. The computation runs local and it is possible to do it in two different ways. Thus we implemented two types of error estimator. In what follows I will briefly describe one of them. Firstly we make the L2 best approximation of the primal flux  $a\partial u_-hp$  in H(div) finite element space, such that the new flux is equivalent to the jumps of the primal flux on the interface  $(p_-hp \cdot n = [a\partial u_-hp \cdot n])$ . After that we update the inner degrees of freedom in order to fulfill the constraints  $(div \ p_-hp + f, s) = 0$ , for all s in polynomial space Pk orthogonal to the space of constants Po.

The difference between the two obtained fluxes (first from the primal solution and second from post-processing steps) in the L2 norm is taken as error estimator. In contrast to the ZZ-error estimator is, we project in H(div) space, which is a natural choice for this problem. In case of varying coefficients over the domains ZZ error estimator is not efficient whereas our estimator gives sharper bounds.

# **Scientific Cooperations**

#### Internal

Institute for Symbolic Computation, Combinatorics group: Prof. Peter Paule and his collaborators Veronika Pillwein (SFB013)

# External

A. Prof. H. Böhm: Institut für Leichtbau und Struktur Biomechanik, TU Wien Dr.-Ing. habil. Manfred Bischoff: Lehrstuhl für Statik, TU München

Prof. Rolf Stenberg: Institute of Mathematics, Helsinki University of Technology

### Scientific Visits and Talk

# Scientific Visits

- 1. September 2<sup>nd</sup>-30<sup>th</sup>, 2006 visit of the Institute of Mathematics (Prof. R. Stenberg), University of Technology, Helsinki.
- 2. October 2006 December 2007 visit of the Center for Computational Engineering (Prof. J. Schöberl), RWTH Aachen.

# Scientific Talks

A. Becirovic: *Primal-Dual Error Estimator for High Order Finite Elements*, Helsinki, September 8, 2006.

### **Publications 2006**

### Appeared

A. Becirovic. P. Paule, V. Pillwein, A. Riese, C. Schneider and J. Schöberl: Hypergeometric Summation Algorithms for High-order Finite Elements. November 24, 2006. Springer-Verlag 2006, Computing 78, pp. 235-249.

# Dr. Gergana Bencheva

#### Scientific Achievements 2006

Dr. Gergana Bencheva was working for RICAM until June 30, 2006 and has left back to Institute for Parallel Processing, Bulgarian Academy of Sciences.

Her research was mainly focussed on time dependent reaction diffusion equations coupled through nonlinear reaction terms as they arise in biochemistry. The problem is posed in an anisotropic multi-layered domain and has to be solved with respect to the concentrations of a given number of species. The practical question hidden behind this mathematical model is "How the prodrug concentrations in transdermal drug delivery systems change as a function of time and dermal layer?"

A solution approach based on operator splitting techniques is proposed and analyzed in [S1]. Special attention is focused on the possibilities for implementation in the framework of parallel computing and GRID infrastructure.

During 2006, Dr. G. Bencheva was nominated for the award after the name of John Vincent Atanasoff and distinguished with diploma (second place). J.V. Atanasoff has been called the father of the computer and his machine, the Atanasoff-Berry Computer, is known as the first electronic digital computer. The award is given annually since 2003 by the Bulgarian president to young researchers for their contribution in the area of information and communication technologies. In relation to this nomination, Dr. Bencheva was invited to participate in the Young researchers session of the IEEE 2006 International Symposium on Modern Computing. The paper [A3] presents part of her achievements in the area of parallel algorithms.

Research papers [A1] and [A2] are also devoted to analysis of parallel preconditioners and were already discussed in the previous RICAM annual report.

### **Scientific Cooperations**

#### Internal

- 1. Dr. Marco Discacciati (RICAM)
- 2. Dr. Johannes Kraus (RICAM)

### External

- 1. Prof. Svetozar Margenov, Ivan Georgiev: Institute for Parallel Processing, Bulgarian Academy of Sciences, Sofia, Bulgaria
- 2. Prof. Maya Neytcheva: Department of Information Technology, Uppsala University, Uppsala, Sweden
- 3. Dr. Jirří Starý: Institute of Geonics, Academy of Sciences of Czech Republic, Ostrava, Czech Republic
- 4. Justin Clay Harris: Department of Chemistry, Kentucky University, USA
- 5. Prof. Istvan Farago: Department of Applied Analysis and Computational Mathematics, Eotvos Lorand University, Budapest, Hungary

### Participation at Conferences, Scientific Visits and Talks

### Conferences

1. IEEE 2006 John Vincent Atanasoff International Symposium on Modern Computing, Young researchers session, October 3-6, 2006, Sofia, Bulgaria.

### Scientific Visits

Short term visit at the Department of Applied Analysis and Computational Mathematics, Eotvos Lorand University, Budapest Hungary, Nov. 16<sup>th</sup>-29<sup>th</sup>, 2006

#### **Publications 2006**

# Appeared[A]

- 1. G. Bencheva, S. Margenov, J. Starý, *Parallel PCG Solver for nonconforming FE problems: overlapping of communications and computations*, Large-Scale Scientific Computing, Springer LNCS, 3743 (2006), 646-654.
- 2. G. Bencheva, S. Margenov, J. Starý, *MPI Implementation of a PCG Solver for Nonconforming FEM Problems: Overlapping of Communications and Computations*, Technical Report 2006-023, Uppsala University, May 2006 (http://www.it.uu.se/research/publications/reports/2006-023/).
- 3. G. Bencheva, *Parallel Incomplete Factorization Algorithms*, G. Angelova, K. Boyanov, K. Fillyov, V. Getov eds, Proceedings of Young Researchers Session, 2006 John Vincent Atanasoff Information Days, Sofia, Bulgaria, October 2006, 7-13. ISBN: 954-91743-5-2.

# Submitted[S]

4. G. Bencheva, *Towards simulation of chemicals' concentration through the layers of the human skin*, To be submitted and to be available as RICAM Report.

# Dr. Dylan Copeland

# Work before joining RICAM

I joined RICAM in June 2006, after finishing my doctoral studies at Texas A&M University, USA, under the supervision of Prof. J.E. Pasciak.

My research interests are in numerical methods for applications in computational electromagnetics. Prior to joining RICAM, my research focused on finite element methods for dimension-reduced axisymmetric Maxwell equations. The topic of my doctoral research was analysis of negative-norm least-squares methods for axisymmetric static and time-harmonic Maxwell equations.

Further, I have worked in collaboration with Prof. J.E. Pasciak and Prof. J. Gopalakrishnan (University of Florida, USA) on a mixed method for the axisymmetric static Maxwell equations. Both the theoretical and computational work for this method have been continued at RICAM, and a paper reporting the results will be finished soon.

### Scientific Achievements of 2006

Study of negative-norm least-squares methods for nonlinear Maxwell equations: In the interest of continuing prior research on negative-norm least-squares methods, I investigated the possibility of applying such methods to nonlinear problems in electromagnetics. The conclusion was negative. Evidently, such a method would be both theoretically dubious and computational inefficient. The resulting linear system may be unsolvable, and in any case may be very ill-conditioned even if nonsingular. Therefore, we decided that negative-norm least-squares methods should not be applied to nonlinear Maxwell equations.

A mixed method for axisymmetric div-curl systems: This work is in collaboration with Prof. J.E. Pasciak and Prof. J. Gopalakrishnan. Div-curl systems generalize static Maxwell equations, and we consider the dimension-reduced systems in the case of symmetry with respect to an axis. In this setting with the necessary weighted spaces, we analyzed finite element discretizations. Also, I have implemented the method in Netgen/NGSolve, a finite element software package developed by Prof. Prof. J. Schöberl and colleagues in RICAM. We expect to submit a research paper on this method soon.

Boundary element based finite element method for Maxwell equations on polyhedral meshes: I began a research project on the utilization of local boundary element spaces in obtaining finite element spaces and discrete operators for three-dimensional electromagnetic scattering problems on general unstructured polyhedral meshes, with elements of arbitrary geometry. A theoretical foundation for such a method has been established, and current work is focused on implementation and performing computations.

# **Scientific Cooperations**

#### Internal

- 1. Dr. Sabine Zaglmayr (RICAM)
- 2. Dipl. Ing. C. Pechstein: Institute of Computational Mathematics, Johannes Kepler University Linz, Austria
- 3. Dipl.-Ing. David Pusch (RICAM)
- 4. Dipl.-Ing. Astrid Sinwel (RICAM)

### External

- 5. Prof. Jay Gopalakrishnan, Department of Mathematics, University of Florida (USA)
- 6. Prof. Joseph E. Pasciak, Department of Mathematics, Texas A&M University (USA)

Participation at Conferences, Scientific Visits and Talks

### Conferences

- 1. 2006 MAA-SIAM Joint Meeting, Auburn, Alabama (USA), March 31<sup>st</sup> to April 1<sup>st</sup>, 2006.
- 2. 17<sup>th</sup> International Conference on Domain Decomposition Methods, St. Wolfgang, Strobl, Austria, July 3rd to 7th, 2006.
- 3. Fast Boundary Element Methods in Industrial Applications, Kleinwalsertal, Austria, September 29<sup>th</sup> to October 2<sup>nd</sup>, 2006.

### **Scientific Talks**

- 1. *Least-squares Methods for Axisymmetric Maxwell Equations*. Public defense of Ph.D. thesis, Texas A&M University, March 1<sup>st</sup>, 2006.
- 2. *Least-squares Methods for Axisymmetric Maxwell Equations*. 2006 MAA-SIAM Joint Meeting, Auburn, Alabama (USA), April 1<sup>st</sup>, 2006.

### **Publications 2006**

D.M. Copeland and J.E. Pasciak: *A least-squares method for axisymmetric div-curl systems*. Numerical Linear Algebra with Applications, vol. 13, Issue 9, 733-752, 2006.

### Dr. Marco Discacciati

### **Scientific Achievements 2006**

# Numerical analysis of magneto-hydrodynamic (MHD) problems.

This work is part of a collaboration with the group of "Optimization and Optimal Control" led by Prof. K. Kunisch (RICAM and University of Graz), in particular with Dr. R. Griesse (RICAM). The aim of this research project is to apply optimal control methods for designing the magnetic fields used in industrial processes such as, e.g., aluminium production, to impose a desired behavior to liquid metals. We have studied a nonlinear system formed by the Maxwell and Navier-Stokes equations coupled by Ohm's law and Lorentz's force. In particular, we have proved that this coupled system is well-posed under suitable assumptions on the smallness of the data. We have proposed a discrete approximation based conforming finite elements, which uses the classical Lagrangian, Raviart-Thomas and Nédélec elements. Moreover, we have analyzed an iterative method to compute the numerical solution of the coupled problem, based on an operator-splitting approach. This algorithm allows us to compute the global solution by independently solving the Maxwell's equations and the (Navier-)Stokes problem. The finite element approximation and the iterative scheme have been implemented within the 3D Finite Element Solver NGSolve and several numerical experiments have been carried out.

# **Scientific Cooperations**

#### Internal

- 1. Dr. Roland Griesse (RICAM)
- 2. Prof. Joachim Schöberl (RICAM)

### External

- 3. Prof. Alfio Quarteroni, Ecole Polytechnique Fédérale de Lausanne (Switzerland) and MOX-Politecnico di Milano (Italy)
- 4. Prof. Alberto Valli, Department of Mathematics, University of Trento (Italy)
- 5. Dr. Simone Deparis, Department of Mechanical Engineering, MIT Massachussets Institute of Technology, Boston (USA)

# Participation at Conferences, Scientific Visits and Talk

# Conferences

MAFELAP 2006, Brunel University, London, 13-16 June, 2006

17<sup>th</sup> International Conference on Domain Decomposition Methods, Strobl (Austria), 3-7 July 2006

#### Scientific Talks

- 1. M. Discacciati: *Multiphysic problems and domain decomposition methods*. RICAM seminar, Linz, 31 May 2006.
- 2. M. Discacciati: *Numerical approximation of a steady magnetohydrodynamic problem*. MAFE LAP 2006, Brunel University, London, 13-16 June 2006 (minisymposium ,,Hyrbid Decomposition Methods" organized by Profs. A. Klawonn, U. Langer and B. Wohlmuth)
- 3. M. Discacciati: *Mathematical and numerical analysis of a steady magnetohydrodynamic problem.* 17<sup>th</sup> International Conference on Domain Decomposition Methods, Strobl (Austria), 3-7 July 2006 (minisymposium "Multiphysics Problems" organized by Profs. R. Hoppe and R. Kornhuber).

### **Publications 2006**

# Appeared [A]

- 1. S. Deparis, M. Discacciati, G. Fourestey and A. Quarteroni: Fluid-structure algorithms based on Steklov-Poincaré operators. Comput. Methods Appl. Mech. Eng. 195, p. 5797-5812, 2006
- 2. S. Deparis, M. Discacciati, G. Fourestey and A. Quarteroni: Heterogeneous domain decomposition methods for fluid-structure interaction problems. In *Domain Decomposition Methods in Science and Engineering*, Lecture Notes in Computational Science and Engineering, O. Widlund and D. Keyes, eds., v. 55, pp. 41-52, Springer, New York, 2006.

### Submitted [S]

- 3. M. Discacciati: Mathematical and numerical analysis of a steady magnetohydrodynamic problem. (RICAM Report, Nr. 2006-38).
- 4. M. Discacciati, A. Quarteroni and A. Valli: Robin-Robin methods for the Stokes-Darcy coupling. (RICAM Report, Nr. 2006-04).

# Martin Huber advised by Prof. Joachim Schöberl

# Work before joining RICAM

I joined RICAM (Start Project: "High Order Finite Elements", by Prof. J. Schöberl) in July 2006 after having finished my diploma thesis in Physics under the supervision of Univ. Doz. Dr. Kurt Hingerl at the Institute of Semiconductor and Solid State Physics (Johannes Kepler University Linz).

One of my research interests was the modeling of Photonic Crystals, especially the influence of such crystals on thermal radiation. In my diploma thesis, I was able to show that one-dimensional Photonic Crystals, which can be yet produced with high accuracy, can suppress thermal emission of a light bulb and simultaneously rise the emission in the visible spectral range. This work was done in cooperation with Siemens.

Further I investigated the solution of Maxwell equations for media with a refractive index varied periodically in space like gratings. With the help of Fourier expansion one is able to calculate the far field pattern as well as the intensities of reflection and transmission for the different orders of diffraction. At RICAM I have continued working on this topic.

#### Scientific Achievements of 2006

Modeling of 1D-periodic gratings with FEM: In the interest of continuing my prior researches on periodic structures, I investigated the usage of Finite Elements in order to describe the optical behavior of a one-dimensional grating in a two-dimensional space and the implementation of such problems in Netgen/NGSolve.

If light incidents onto a grating it is diffracted and transmitted into certain directions. While these directions are easy to calculate and depend only on the periodicity, the computation of the corresponding intensities which depend on the shape of the grating turns out to be much more complicated.

Modeling such gratings with FEM, the computational domain can be reduced to one single unit cell, where we have to formulate periodic boundary conditions in order to describe the behavior of the grating. A critical point is the treatment of the far-field. The polynomial basis functions of the FEM domain have to be coupled with the plane wave basis functions describing the far field pattern. The innovation of my approach is to perform this coupling by the method of Nitsche.

By using a plane wave expansion in the far field, the simulation can be easily compared with optical experiments, where similar quantities are measured.

# **Scientific Cooperations**

#### Internal

- 1. Prof. Dr. Joachim Schöberl (RICAM + RWTH Aachen University)
- 2. Dr. Sabine Zaglmayr (RICAM)
- 3. Dipl.-Ing. Astrid Sinwel (RICAM)
- 4. Dipl.-Ing. Almedin Becirovic (RICAM)

#### External

- 6. A.Univ.Prof. Dr. W. Heiß, Institute of Semiconductor and Solid State Physics (JKU Linz)
- 7. Univ.Doz.Dr. K. Hingerl, Institute of Semiconductor and Solid State Physics (JKU Linz)

### **Publications 2006**

M.Bergmair, M.Huber and K.Hingerl: *Band Structure, Wiener bounds and Coupled Surface Plasmons in 1D Photonic Crystals.* Applied Physics Letters, 89 p.081907, 23.8.2006

Maksym V. Kovalenko, Erich Kaufmann, Dietmar Pachinger, Jürgen Roither, Martin Huber, Julian Stangl, Günter Hesser, Friedrich Schäffler, and Wolfgang Heiss: *Colloidal HgTe Nanocrystals with Widely Tunable Narrow Band Gap Energies: From Telecommunications to Molecular Vibrations*, J. Am. Chem. Soc.; 2006; 128(11) pp 3516 - 3517; (Communication)

#### Dr. Johannes Kraus

### **Scientific Achievements 2006**

Multilevel preconditioning of non-conforming finite element problems: We investigated and studied algebraic two- and multilevel preconditioning algorithms for second-order elliptic boundary-value problems, where the discretization is done using Crouzeix-Raviart and Rannacher-Turek non-conforming finite elements. We presented a general setting of hierarchical splittings of the related finite element spaces and derived new estimates for the constant in the strengthened CBS inequality, which plays an important role in the convergence analysis of algebraic multilevel iteration methods [A4,A5,S2].

Multilevel methods for discontinuous Galerkin approximations of two- and three-dimensional isotropic and anisotropic elliptic problems: We constructed optimal order multilevel methods for the solution of linear systems aring from interior-penalty discontinuous Galerkin (DG) finite element discretizations. We proposed a specific assembling process, which allows for a local characterization of the hierarchical splitting. Applying the corresponding two-level basis transformation recursively, a sequence of algebraic problems is generated that can be associated with a hierarchy of coarse versions of DG approximations of the original problem. The presented framework applies to two- and three-dimensional isotropic and anisotropic elliptic boundary-value problems [S1,S3].

# **Scientific Cooperations**

### Internal

- 1. Prof. Dr. Josef Schicho (RICAM)
- 2. Dr. Marco Discacciati (RICAM)
- 3. Dr. Satyendra Tomar (RICAM)
- 4. Dr. Josef Synka (Institute for Industrial Mathematics, Johannes Kepler University Linz)

#### External

- 1. Prof. Dr. R. Falgout, Prof. Dr. V. E. Henson, Prof. Dr. P. Vassilevski: CASC, Lawrence Livermore National Laboratory, CA, USA
- 2. Prof. Dr. L. Zikatanov: Department of Mathematics, Pennsylvania State University, PA, USA
- 3. Prof. Dr. S. Margenov, Ivan Georgiev: Institute for Parallel Processing, BAS, Sofia, Bulgaria
- 4. Prof. Dr. R. Hiptmair: Department of Mathematics, Swiss Fed. Inst. of Technology, ETH Zürich, Switzerland
- 5. Prof. Dr. G. Haase: Institute for Mathematics, University of Graz, Austria
- 6. Dr. Dalibor Lucas: University of Ostrava, Czech Republic

# Participation at Conferences, Scientific Visits and Talks

### Conferences

- 1. Second Austrian Numerical Analysis Day, Graz, Austria, April 27 28, 2006.
- 2. 17th International Conference on Domain Decomposition Methods, St. Wolfgang/Strobl, Austria, July 3 7, 2006.
- 3. Sixth International Conference on Numerical Methods and Applications, Borovets, Bulgaria, August 20 24, 2006.
- 4. International Conference on Multifield Problems, Stuttgart, Germany, October 4 6, 2006.

# Scientific Visits

Guest Scientist at the Bulgarian Academy of Sciences, Institute for Parallel Processing (IPP), Sofia, August 18<sup>th</sup>-September 15<sup>th</sup>, 2006

### Scientific Talks [T]

- 1. J.K. Kraus: *Multilevel Preconditioning of 2D Rannacher-Turek Finite Element Problems*. Second Austrian Numerical Analysis Day, Graz, Austria, April 28, 2006.
- 2. J.K. Kraus: *On the Construction of a Hierarchical Topology with Application to Algebraic Multilevel Preconditioning*. 17th International Conference on Domain Decomposition Methods, St. Wolfgang/Strobl, Austria, July 4, 2006.
- 3. J.K. Kraus: *Multilevel Preconditioning of 2D Rannacher-Turek FE Problems; Multiplicative and Additive Methods*. Sixth International Conference on Numerical Methods and Applications, Borovets, Bulgaria, August 21, 2006.
- 4. J.K. Kraus: Algebraic Subproblems in Multilevel Preconditioning Methods. International Conference on Multifield Problems. Stuttgart, Germany, October 6, 2006.
- 5. J.K. Kraus: *An Edge-Based Algebraic Multigrid Method for Finite Element Elasticity Problems*. Institute for Parallel Processing, Bulgarian Academy of Sciences, Sofia, Bulgaria, September 12, 2006.

#### **Publications 2006**

# Appeared [A]

- 1. J.K. Kraus: Algebraic multilevel preconditioning of finite element matrices using local Schur complements. Num. Lin. Alg. Appl., 13 (2006) 49-70.
- 2. J.K. Kraus: On the utilization of edge matrices in algebraic multigrid. Springer LNCS 3743 (2006), 121-129.
- 3. J.K. Kraus and J. Schicho: Algebraic multigrid based on computational molecules, I: Scalar elliptic problems. Computing, 77 (2006), 57-75.
- 4. I. Georgiev, J.K. Kraus, and S. Margenov: Multilevel preconditioning of 2D Rannacher-Turek FE problems; additive and multiplicative methods. Lecture Notes in Computer Science, to appear.
- 5. I. Georgiev, J.K. Kraus, and S. Margenov: Multilevel preconditioning of rotated bilinear non-conforming FEM problems. Computers & Mathematics with Applications, to appear. (Also available as RICAM-Report No. 2006-3.)

# Submitted [S]

- 1. J.K. Kraus and S. Tomar: *Multilevel preconditioning of elliptic problems discretized by a class of discontinuous Galerkin methods*. Submitted to SIAM J. Sci. Comput. and also available as RICAM-Report No. 2006-36.
- 2. J.K. Kraus, S. Margenov, and J. Synka: *On the multilevel preconditioning of Crouzeix-Raviart elliptic problems*. Submitted to Num. Lin. Alg. Appl., December 2006.
- 3. J.K. Kraus and S. Tomar: *A multilevel method for discontinuous Galerkin approximation of three-dimensional anisotropic elliptic problems.* Submitted to Num. Lin. Alg. Appl., December 2006 and to be available as RICAM-Report No. 2006-39.

### David Pusch advised by Prof. Ulrich Langer

# **Scientific Achievements 2006**

Hierarchical Matrices: In order to increase the performance of constructing and using the H-matrices in the multigrid software code, we implemented the software package HLib (www.hlib.org). We compared the efficiency of constructing a matrix hierarchy level by level with H-matrices and constructing the hierarchy with the Galerkin method. It turned out that the latter is considerably faster. Moreover, since HLib provides a low-rank decomposition sorted by the singular values, one can speed-up the construction by reducing the rank on the coarser levels.

Convergence Results: We finished the convergence result for the multigrid V-cycle applied on system matrices of H-matrix type. Based on the result of Bramble, Leyk and Pasciak combined with perturbation arguments we can formulate a complete convergence analysis.

Boundary Element based Finite Element Method: This topic was motivated by F. Brezzi and Y. Kuznetsov, who investigated finite difference methods for polygonal and polyhedral meshes. Typical examples including this sort of meshes arise by treating geological layers consisting of porous media. Our new approach is now to treat a polygonal or polyhedral finite element mesh as domain decomposition of the whole computational domain, where the size of the subdomains are of the same order as the meshsize of the boundary discretization. Applying boundary element methods on each (polygonal or polyhedral) subdomain yields an element matrix which is the approximated Steklov-Poincarè operator. Assembling all the element matrices leads to a sparse symmetric and positive definite system matrix. In order to solve our Dirichlet boundary value problem for the Laplace equation efficiently, we are using multigrid methods. More precisely, we are applying algebraic multigrid (PEBBLES), since for general polygonal (or polyhedral) meshes no mesh hierarchy is available. The error estimation in

2D for the discretization error is mainly determined by the discretization error for standard linear finite elements on triangles. Finally, applying Strang's Lemma yields the result.

### **Scientific Cooperation's**

### Internal

Prof. Dr. U. Langer: RICAM & Institute of Computational Mathematics, Johannes Kepler University Linz, Austria

Dr. D. Copeland, RICAM, Austrian Academy of Science, Linz

#### External

Dr. G. Of: Institut für numerische Mathematik, TU Graz

# Participation at Conferences, Scientific Visits and Talk

### Conferences

- 17<sup>th</sup> International Conference on Domain Decomposition Methods, Strobl/St.Wolfgang, Austria, July 3 7, 2006.
- IABEM 2006, International Association for Boundary Element Methods, Graz, Austria, July 10 12, 2006.
- 4<sup>th</sup> Workshop: Boundary Element Methods in Inudstrial Applications, Kleinwalsertal, Austria, September 29 October 2, 2006.

# Scientific Visits

### Scientific Talks

- D. Pusch: *Multigrid Methods for Boundary Element Equations*, IABEM 2006, International Association for Boundary Element Methods, Graz, Austria, July 10 12, 2006.
- D. Pusch: *Sparse Approximations on Polygonal Meshes based on BEM Domain Decomposition Techniques*, 4<sup>th</sup> Workshop: Boundary Element Methods in Industrial Applications. Kleinwalsertal, Austria, September 29 October 2, 2006.
- D. Pusch: Sparse Approximations on Polygonal Meshes based on BEM Domain Decomposition Techniques, Research Seminar, JKU Linz, October 24, 2006.

### **Publications 2006**

### **Appeared**

1. U. Langer, D. Pusch. *Comparison of Geometrical and Algebraic Multigrid Preconditioners for Data-sparse Boundary Element Matrices*. Proceedings of the 5<sup>th</sup> International Conference on Large-Scale Scientific Computations LSSC 2005, Sozopol, Bulgaria. Lecture Notes in Computer Science, Vol. 3743, p. 130 – 137, 2006.

### Submitted

- 2. U. Langer, D. Pusch. Convergence Analysis of Geometrical Multigrid Methods for Solving Data-sparse Boundary Element Equations. Computing and Visualization in Science, submitted, 2006.
- 3. U. Langer, D. Pusch. Convergence Analysis of Geometrical Multigrid Methods for Solving Data-sparse Boundary Element Equations. Proceedings of 5<sup>th</sup> European Multigrid Conference EMG2005, Scheveningen, The Hague, submitted, 2006.

#### Prof. Joachim Schöberl

### **Scientific Achievements 2006**

J. Schöberl started a Professorship at the RWTH Aachen University on March 15. He stayed affiliated with RICAM. In particular, he continued to supervise the Start project "hp-Finite Elements" hosted at RICAM. Here, J. Schöberl works together with

- DI. Dr. S. Zaglmayr (high order FEM for Maxwell equations)
- DI. A. Becirovic (a posteriori error estimators)
- DI. M. Huber (scattering on periodic gratings)
- DI. A. Sinwel (mixed methods for elasticity)

Together with Prof. D. Braess, J. Schöberl worked on a posteriori error estimators of equilibrated residual type. Here, an upper bound for the error can be given without the appearance of a generic constant. Existing error estimators of these type could be simplified, and thus extended to the three dimensional case and to Maxwell equations (paper is submitted). Furthermore, a high order version was tested. Numerical experiments show robustness in the polynomial order. Proving that is work in progess.

Together with Prof. L. Demkowicz and Prof. J. Gopalakrishnan, J. Schöberl works on polynomial preserving extension operators for the function spaces H(curl) and H(div). Such operators are the last missing part of the hp-error analysis for Maxwell equations. The results are proven, the paper is in preparation.

In 2006, J. Schöberl started with discontinuous Galerkin methods for the convection diffusion problem. A hybrid formulation allows to reduce the unknowns to the element interfaces. The motivation is the simulation of transport of charged particles such as in semiconductor devices. This is work together with Prof. R. Stenberg (UT Helsinki), and Dr. H. Egger at RWTH Aachen.

### **Scientific Cooperations**

### Internal

- SFB 1301/19 "A special function toolbox for high order finite elements", Prof. P. Paule and DI V. Pillwein
- SFB 1306 "Adaptive Multilevel Methods for Nonlinear 3D Mechanical Problems", co-investigator with Prof. U. Langer
- JKU Comp Math: Prof. U. Langer, A.Prof W. Zulehner, Dr. S. Beuchler
- JKU Mechatronik: Prof. H. Irschik, Prof. R. Scheidl, Dr. J. Gerstmayr
- JKU Physik: A.-Prof. W. Heiss

# **External**

- Prof. D. Braess, Prof. C. Carstensen, Prof. L. Demkowicz, Prof. J. Goppalakrishnan, Jun.-Prof. T. Hohage, Prof. R. Lazarov, Prof. R. Stenberg, Prof. R. Winther,
- RWTH Aachen: Prof. M. Behr, Prof. D. Bothe, Prof. W. Dahmen, Prof. W. Marquardt, Prof. A. Reusken

# Participation at Conferences, Scientific Visits and Talk

### Conferences

- European Finite Element Fair, Zürich, 2-3 June, 2006
- MAFELAP 2006, Brunel University, London, 13-16 June, 2006

• 17<sup>th</sup> International Conference on Domain Decomposition Methods, Strobl (Austria), 3-7 July, 2006

# Scientific Visits

- University Stuttgart, 15-16 January, Prof. B. Wohlmuth
- University Göttingen, 27-29 March, Jun.-Prof. T. Hohage
- Helsinki University of Technology, 26 Aug 29 Sept, Prof. R. Stenberg
- TU Berlin, 14-15 Oct, Prof. D. Hömberg

### Scientific Talks

see above

### **Publications 2006**

# Appeared

- 1. Boffi, F. Kikuchi, and J. Schöberl: Edge element computation of Maxwell's eigenvalues on general quadrilateral meshes. Mathematical Models and Methods in Applied Sciences, 16, 265-273, 2006
- 2. C. Carstensen and J. Schöberl: Residual-based a posteriori error estimate for a mixed Reissner-Mindlin plate finite element method. Numerische Mathematik, 103, 225-250, 2006
- 3. S. Beuchler and J. Schöberl: New shape functions for triangular p-FEM using integrated Jacobi polynomials, Numerische Mathematik, 103, 339-366, 2006
- 4. J. Gerstmayr and J. Schöberl: A 3D finite element method for flexible multibody systems, Multibody System Dynamics, 15, 309-324, 2006
- 5. F. Bachinger, U. Langer, and J. Schöberl: Efficient Solvers for Nonlinear Time-Periodic Eddy Current Problems. Computing and Visualization in Science, 9, 197-207, 2006
- 6. Becirovic, P. Paule, V. Pillwein, A. Riese, C. Schneider, and J. Schöberl: Hypergeometric Summation Algorithms for High-order Finite Elements. Computing, 78, 235-249, 2006
- 7. S. Hein, T. Hohage, W. Koch, and J. Schöberl: Acoustic Resonacnes in a High Lift Configuration. Journal of Fluid Mechanics, accepted
- 8. J. Schöberl, J. Melenk, C. Pechstein, S. Zaglmayr: Additive Schwarz preconditioning for p-Version Triangular and Tetrahedral Finite Elements. IMA Journal of Numerical Analysis, accepted
- 9. M. Schinnerl, M. Kaltenacher, U. Langer, R. Lerch, J. Schöberl: Numeical Simulation of Magneto-Mechanical Sensors and Actuators, Surveys on Mathematics for Industry, accepted

### Submitted

- 1. J. Schöberl and W. Zulehner: Symmetric Indefinite Preconditioners for Saddle Point Problems with Applications to PDE-Constrained Optimization Problems, submitted
- 2. D. Braess and J. Schöberl: Equilibrated Residual Error Estimators for Maxwell Equations, submitted
- 3. J. Schöberl and R. Stenberg: Multigrid Methods for Stabilized Reissner Mindlin Plate Formulations, submitted

### Astrid Sinwel advised by Prof. Joachim Schöberl

### Work before joining RICAM

I joined RICAM as a member of Joachim Schoeberl's start project "High Order Finite Elements" in April 2006. Before this I was studying Technical Mathematics at Linz University. I finished my di-

ploma studies in March 2006, supervised by Prof. Walter Zulehner, Institute for Computational Mathematics, JKU Linz.

My Diploma thesis on "Numerical Methods for Contact Problems with Coulomb Friction" was concerned with the analysis and simulation of elastic two-body contact problems. The problem was described as a mixed variational inequality, which was then discretized by the finite element method.

#### **Scientific Achievements 2006**

## Mixed methods for elasticity:

The Hellinger Reissner formulation of elasticity involves the displacements as well as the stress fields as unknowns. We choose the displacement space to be H(curl). In order to obtain a stable mixed system, the stress space has to be chosen such that the divergence of the stress tensor lies in H<sup>-1</sup>(div). We call this space H(divdiv).

Finite elements for the space H(curl) require a continuous tangential component to be conforming. To get a conforming subspace of H(divdiv), the normal-normal component of the stress tensor needs to be continuous across element interfaces. For the displacement space, we use hierarchical finite elements of variable polynomial order, which were developed within the start project by J. Schoeberl and S. Zaglmayr. For the stresses, we construct hierarchical, symmetric, tensor-valued elements satisfying the required normal-normal continuity. Therefore we use a two-step exact sequence for elasticity.

We hybridize the method to obtain a symmetric, positive definite system matrix. Then a simple block-precondtioner can be used for nearly incompressible materials. The method is locking-free for both anisotropic elements and nearly incompressible materials.

### **Scientific Cooperations**

#### Internal

Prof. Dr. DI Joachim Schöberl, RICAM Linz / RWTH Aachen Dr. DI Sabine Zaglmayr, RICAM Linz DI Martin Huber, RICAM Linz DI Marie-Therese Wolfram, RICAM Linz

# **External**

Dr. DI Herbert Egger, Department for Mathematics CCES, RWTH Aachen, Germany Prof. Rolf Stenberg, Institute of Mathematics, Helsinki University of Technology, Finland

### Participation at Conferences, Scientific Visits and Talk

### Conferences

- 2<sup>nd</sup> Austrian Numerical Analysis Day, Graz, 27.-28. 04. 2006
- MAFELAP, Brunel University, Uxbridge, London, 13.-16. 06. 2006

### Scientific Visits

1. Prof. Rolf Stenberg, Institute of Mathematics, Helsinki University of Technology, Finland, 02. 09. - 02. 10. 2006

# Scientific Talks

- 2. J. Schoeberl and A. Sinwel: *Tangential-Displacement and Normal-Normal-Stress Continuous Mixed Finite Elements for Elasticity*, 2<sup>nd</sup> Austrian Numerical Analysis Day, Graz, 28. 04. 2006
- 3. J. Schoeberl and A. Sinwel: *Mixed Finite Elements for Contact Problems with Friction*, Minisymposium "Contact Problems and Biomechanics", MAFELAP, Brunel University, Uxbridge, London, 15. 06. 2006
- 4. J. Schoeberl and A. Sinwel: *Tangential-Displacement and Normal-Normal-Stress Continuous Mixed Finite Elements for Elasticity*, Institute of Mathematics, Helsinki University of Technology, Finland, 08. 09. 2006

#### **Publications 2006**

### Submitted

B. Juettler, M. Oberneder, A. Sinwel: On the existence of biharmonic tensor-product Bezier surface patches (submitted to CAGD)

### Dr. Satyendra Tomar

#### **Scientific Achievements 2006**

We (with Prof. J.J.W. van der Vegt) developed a higher order accurate discontinuous Galerkin finite element method for the simulation of linear free-surface gravity waves. The method uses the classical Runge–Kutta method for the time-discretization of the free-surface equations and the discontinuous Galerkin method for the space-discretization. In order to circumvent numerical instabilities arising from an asymmetric mesh a stabilization term is added to the free-surface equations. In combination with a higher order velocity recovery technique this stabilizes the numerical discretization with minimal effect on the accuracy of the wave computations. Stability analysis of the semi and fully-discrete scheme has been conducted, which suggested that for a suitable choice of the stabilization constant a relatively large time step can be chosen for accurate simulations over a long period of time. Theoretical study is supported with numerical examples of a number of problems.

We (Dr. J. Kraus) developed optimal order multilevel preconditioners for interior-penalty discontinuous Galerkin (DG) finite element discretizations of elliptic boundary-value problems. The problems varied from 2D isotropy to 3D anisotropy. A specific assembling process was proposed which allowed to characterize the hierarchical splitting locally. This is also the key for a local analysis of the angle between the resulting subspaces. Applying the corresponding two-level basis transformation recursively, a sequence of algebraic problems is generated. These discrete problems can be associated with coarse versions of DG approximations (of the solution to the original variational problem) on a hierarchy of geometrically nested meshes. A new bound for the constant in the strengthened Cauchy-Bunyakowski-Schwarz inequality is derived. To support the theoretical analysis and demonstrate the potential of the approach a number of numerical test cases were considered.

We (with Prof. S. Repin and R. Lazarov) developed functional a posteriori error estimates for DG approximations of elliptic boundary-value problems. These estimates are based on a certain projection of DG approximations to the respective energy space and functional a posteriori estimates for conforming approximations developed by Prof. S. Repin. On these grounds we derived two-sided guaranteed and computable bounds for the errors in "broken" energy norms. A number of numerical examples were considered to confirm the efficiency of the estimates.

# **Scientific Cooperations**

### <u>Internal</u>

Dr. Johannes Kraus (RICAM)

#### External

Prof. J.J.W. van der Vegt (University of Twente, Netherlands)

Prof. R. Lazarov (Texas A&M, College Station, Texas, USA)

Prof. S. Repin (St. Petersburg, Russia)

Prof. R. Stenberg (Helsinki University of Technology, Finland)

# Participation in Conferences and Scientific Visits

12<sup>th</sup> Conference on The Mathematics of Finite Elements and Applications, Brunel University, London, UK, June 13-16, 2006.

17<sup>th</sup> International Conference on Domain Decomposition Methods, St. Wolfgang/Strobl, Austria, July 3-7, 2006.

Seminar on Numerical Analysis and Computational Science, Institute of Mathematics, Helsinki University of Technology, Finland, Oct. 29 to Nov. 5, 2006.

### Scientific Talks/Lectures

- S.K. Tomar (with R. Lazarov and S. Repin): A posteriori error estimates for discontinuous Galerkin method, RICAM Group Seminar, 1<sup>st</sup> June 2006.
- S.K. Tomar (with R. Lazarov and S. Repin): A posteriori error estimates for discontinuous Galerkin method, MAFELAP, 15<sup>th</sup> June 2006.
- S.K. Tomar (with J. Kraus): Multilevel preconditioning of elliptic problems discretized by a class of discontinuous Galerkin methods, Minisymposia on advanced multigrid methods for system of PDEs , DD 17,  $4^{th}$  July 2006.
- S.K. Tomar (with S. Repin): Functional a posteriori error estimates for discontinuous Galerkin approximations of elliptic problems, Helsinki University of Technology, 30<sup>th</sup> October 2006.

### **Publications 2006**

### Appeared

- 1. S.K. Tomar: h-p spectral element method for elliptic problems on non-smooth domains using parallel computers, *Computing*, 78, 117-143, 2006.
- 2. S.K. Tomar and J.J.W. van der Vegt: A Runge-Kutta discontinuous Galerkin method for linear free-surface gravity waves using high order velocity recovery. Computer Methods in Applied Mechanics and Engineering (2006), doi:10.1016/j.cma.2006.11.007.

### Submitted

- 3. J.K. Kraus and S.K. Tomar: Multilevel preconditioning of elliptic problems discretized by a class of discontinuous Galerkin methods.
- 4. J.K. Kraus and S.K. Tomar: A multilevel method for discontinuous Galerkin approximation of three-dimensional anisotropic elliptic problems.
- 5. R. Lazarov, S. Repin and S.K. Tomar: Functional a posteriori error estimates for discontinuous Galerkin approximations of elliptic problems.

# Sabine Zaglmayr advised by Prof. Joachim Schöberl

### **Scientific Achievements 2006**

The main achievement of S. Zaglmayr in 2006 was finishing her PhD-thesis "High Order Finite Elements Methods for Electromagnetic Field Computation" under the supervision of Prof. Dr. J. Schöberl (RICAM and RWTH Aachen).

The main contribution was to introduce new tensor-product based shape functions for the whole sequence of H<sup>1</sup>-, H(curl)- and H(div)-conforming high-order FE-discretizations.

In order to allow for hybrid mehes and geometric h-refinement all common element geometries (triangles, quadrilaterals, tetrahedra, prisms and hexahedra) have to be provided.

The innovation is to formulate the discrete version of the de Rham diagram also in a local sense corresponding to each single edge, face and cell of the mesh - the local exact sequence property. Practically, this is achieved by including an explicit basis for the kernel of the natural differential operator in the construction of the basis function, e.g. in case of the H(curl)-space the gradient fields of the basis functions corresponding H^1-conforming FE-space are explicitly used. This allows arbitrary and variable choice of the polynomial degree on each edge, face and cell.

In the second part S. Zaglmayr focuses on the numerical solution of a challenging class of Maxwell problems in three space dimensions including equations of the type: curl curl u + k u = j, with small values of the parameter k, as well as the Maxwell eigenvalue problem. Here, the logic of the separating the H(curl)-conforming shape functions into gradients and non-gradients is crucial for building cheap, but still efficient ASM-preconditioners for the curl-curl problem with resulting condition numbers independent of the small parameter k.

# Perfectly Matched Layers (PML) for Piezoelectric Equations:

This work states an extension of the mathematical model used for periodic piezoelectric surface acoustic wave filters. Up to now the absorption of the acoustic waves into the material were modelled by first order absorbing boundary conditions, where a crucial point was stated by the indefiniteness of the piezoelectric problem. The method of perfectly matched layers got recently popular and established for truncating open domain problems in acoustics, as well as for electromagnetic problems. The open domain is truncated by an artificial boundary layer where the solution is extended into the complex-plain. S. Zaglmayr formulated and implemented the PML-method for the piezoelectric equations by its interpretation as complex-coordinate stretching. She successfully applied the PML-approach on source and eigenvalue problems modelling periodic piezoelectric SAW-filters.

# **Scientific Cooperations**

### Internal

Prof. Joachim Schöberl (RICAM and RWTH Aachen)

DI Astrid Sinwel (RICAM)

DI Martin Huber (RICAM)

DI Clemens Pechstein (Institut für Numerische Mathematik, JKU Linz)

Dr. Marco Discacciati (RICAM)

# Dr. Dylan Copeland (RICAM)

#### External

Prof. Dr. Leszek Demkowicz, Institute for Computational Engineering and Sciences (ICES), University of Texas at Austin, USA.

Dr. H. Egger, Center for Computational Engineering Sciences (CCES), RWTH Aachen, Germany.

Prof. Dr. C. Wieners, Institute for Scientific Computing and Mathematical Modelling, University Karlsruhe, Germany.

Dr. K. Wagner, Epcos AG, Munich, Germany.

Participation at Conferences, Scientific Visits and Talk

### Conferences

- 2<sup>nd</sup> Austrian Numerical Analysis Day, TU Graz, Austria, 27.-28. April 2006.
- MAFELAP 2006, BICOM Brunel University, Uxbridge, UK, 13-16.06.2006.
- 8<sup>th</sup> IMACS International Symposion on Iterative Methods in Scientific Computation: 14.-17. Novermber, College Station, Texas, USA.

# Scientific Visits

- 1. Prof. Dr. J. Schöberl, CCESS, RWTH Aachen, 8.-18.05, 3.-11.11., 10.-15.12. 2006.
- 2. Prof. Dr. R. Stenberg, Institute of Mathematics, Helsinki University of Technology, 1.09.-1.10.2006.
- 3. Prof. Dr. L. Demkowicz, Intitute of Computational Engineering and Sciences (ICES), University of Texas at Austin, USA.

#### Scientific Talks

- 1. S. Zaglmayr (with J.Schöberl): *High Order Nedelec Elements for Electromagnetic Field Computation*, 2<sup>nd</sup> Austrian Numerical Analysis Day, TU Graz, Austria, 27.-28. April 2006.
- 2. S. Zaglmayr (with J.Schöberl, U.Langer, M.Hofer): *Eigenvalue Problems in Piezoelectric Surface Acoustic Wave Filter Simulations*, Seminar-Talk, RWTH Aachen, Germany, 11.05.2006.
- 3. S. Zaglmayr (with J. Schöberl): *On high order Nedelec Elements and the Maxwell Eigenvalue Problem*, MAFELAP 2006, BICOM Brunel University, Uxbridge, UK, 14. 06.2006.
- 4. S. Zaglmayr: *High Order Finite Element Methods for Electromagnetic Field Computation*, Rigorosum, J.Kepler University, Linz, 24.08.2006.
- 5. S. Zaglmayr (with J.Schöberl): *On high order Nedelec Elements and Maxwell Eigenvaluesolvers using inexact projection*. 8<sup>th</sup> IMACS International Symposion on Iterative Methods in Scientific Computation, College Station, USA, 16.11.2006.
- 6. S. Zaglmayr: Computer Exercises for Mini-Course Finite Element Methods for Maxwell's Equations (held by J. Schöberl) at TKK Helsinki University of Technology, September 2006.

### **Publications 2006**

# <u>Appeared</u>

S. Zaglmayr: "High Order Finite Elements Methods for Electromagnetic Field Computation", PhD-thesis, Insitute for Computational Mathematics, Johannes Kepler University, Linz, Austria, 2006.

# Submitted

J. Schöberl, J. Melenk, C. Pechstein, S. Zaglmayr: Additive Schwarz Preconditioning for p-Version Triangular and Tetrahedral Finite Elements (submitted to IMAJNA).

# 2.2. GROUP "INVERSE PROBLEMS"

### **Group Leader:**

o.Univ.-Prof. Dipl.-Ing. Dr. Heinz W. Engl

# Researchers funded via ÖAW/Upper Austrian government funds:

Dr. Stefan Müller

PD Dr. Ronny Ramlau

Dr. Elena Resmerita

PD Dr. Arnd Rösch

Prof. Dr. Sergei Pereverzyev

### Researchers externally funded:

Dipl.-Tech. Kattrin Arning

MSc Hui Cao

MSc Svetlana Cherednichenko

Dr. Herbert Egger

Dr. Benjamin Hackl

Dr. Lin He

Dr. Andreas Hofinger

Dr. Stefan Kindermann

Dr. Esther Klann

DI Klaus Krumbiegel

Dr. James Lu

MSc Shuai Lu

Mag. Svetlana Metla

Dr. Hanna Katriina Pikkarainen

Dr. Mourad Sini

DI Marie-Therese Wolfram

In addition, Prof. Martin Burger and Dr. Philipp Kügler (Industrial Mathematics Institute, Univ. of Linz) cooperate with the group in and advisory/supervisory role for specific projects.

# Introduction by Group Leader Prof. Heinz W. Engl

In addition to the group leader, the group consists of 12 (senior) PostDocs and 7 doctoral students. Also, two members of the Industrial Mathematics Institute of JKU (Martin Burger, Philipp Kügler) contributed to the scientific work of the institute in an advisory role within externally funded projects.

Out of these 19 positions, 5 are funded by the ÖAW. External funds come from the FWF in the framework of single projects (led not only by the group leader, but also by the PostDocs Pereverzyev, Ramlau and Rösch), the SFB "Numerical and Symbolic Scientific Computing" and the Doctoral College "Molecular Biophysics" the Viennese fund WWTF for a project in systems biology jointly led by Peter Schuster (University of Vienna) and the group leader.

The composition of the group is quite international; during 2006, new PostDocs coming from Germany, Korea and the U.S. joined, while other collaborators left: Martin Burger accepted a call to a Full Professorship at the University of Münster (as the successor of Frank Natterer), Andreas Hofinger went to industry after having obtained his PhD, and Marie-Therese Wolfram left to Münster to continue her PhD work with Martin Burger.

The group was (and will continue to be) dealing with a wide variety of topics in inverse problems and related fields, especially control and imaging, as can be seen in more detail from the individual reports below. These can be grouped into methodological and applications-oriented topics, of course with close relations between both.

On the methodological side, the work concerned, e.g., regularization methods for nonlinear inverse problems with an emphasis on implementable parameter choice strategies with optimal convergence properties (like the "balancing principle") theory of and use of sparsity in regularization methods regularization methods in a non-Hilbert space setting like Bregman iteration, level set methods, BV and inverse scale space regularization, with close connections to imaging, maximum entropy and EM methods a convergence theory (in distribution) for stochastic inverse problems including the first quantitative convergence results for Bayesian inversion, measured in the Prokhorov and Ky Fan metrics.

Major application fields addressed were

- inverse problems in finance
- inverse scattering
- parameter identification and inverse bifurcation problems in systems biology (where sparsity plays a major role)
- inverse problems for semiconductors and ion channels.

The closest internal cooperations in 2006 were with the Control Group (the PostDocs Griesse and Rösch even having a joint FWF project), Finance, and Imaging (a topic which is not only represented in this group and the Imaging Group, but also in the Analysis Group).

In addition to Martin Burger, also Arnd Rösch received a call to a Full Professorship from the University of Duisburg-Essen; he has accepted this offer.

### Prof. Dr. Sergei Pereverzyev

# **Scientific Achievements 2006**

In accordance with the Scientific Plans for the year 2006 one of the research directions followed is an application of the Rregularization methodology in Learning Theory. More precisely, the problem of an adaptive parameter choice for regularized learning algorithms has been studied. Although in the theory of ill-posed problems there is a long history of choosing regularization parameters in an optimal way without a priori knowledge of a smoothness of the element of interest, known parameter choice rules cannot be applied directly in Learning Theory. The point is that these rules are based on estimations of the stability of regularization algorithms measured in the norm of the space where an unknown element of interest should be recovered. But in the context of Learning Theory this norm is determined by an unknown probability measure, and is not accessible. This situation has been analyzed in cooperation with the Group of Statistical Learning & Image Processing of Genova University (Italy) It is interesting to note that this cooperation was started within the framework of the Radon Special Semester-2005, when the member of this group, Lorenzo Rosasco, visited RICAM for one month. As a result, a new parameter choice strategy adjusted to learning from examples has been developed. It consists in adaptive regularization performed simultaneously in a Hypothesis space and in a space equipped with an *empirical norm*. Both these spaces are accessible and known parameter choice rules such as a balancing principle can be used there. Then a parameter for the regularization in the inaccessible space is chosen as the minimal among the parameters selected for the above mentioned accessible spaces. It has been proven that under rather mild assumptions such a strategy guarantees an optimal order of the risk.

In the course of FWF-Project P17251-N12 "Fixed point regularization schemes for nonlinear ill-posed problems and their discretization" the scientific supervision for project team members Mag. Shuai Lu and Mag. Cao Hui has been provided. As a result, the *natural linearization* approach has been extended to parameter identification problems for non-linear elliptic and parabolic systems with the solution dependent coefficients. Moreover, the natural linearization technique has been adjusted to regularization of ill-posed Cauchy problem for non-linear elliptic equations. Another Project direction scheduled for year 2006 was connected with an analysis of Tikhonov regularization for non-linear ill-posed problems under general smoothness assumptions. Here an adaptive parameter choice strategy for Tikhonov regularization realized in the form of the TIGRA – algorithm has been developed in cooperation with Dr. Ronny Ramlau.

### **Scientific Cooperations**

#### Internal

Joint research in progress with PD. Dr. Ronny Ramlau and Mag. Shuai Lu (RICAM Inverse Problems Group) with the aim to develop an adaptive parameter choice strategy for the reconstruction of the sparse structure.

### External

Dr. Lorenzo Rosasco and Dr. Ernesto De Vito (Genova University) Joint research on Regularization Algorithms in Learning Theory.

PD. Dr. Peter Mathé (Weierstrass-Institute, Berlin) and Dr. Frank Bauer (University of Göttingen) Joint research on the impact of the noise covariance structure upon the accuracy of estimation. As a result, an invited paper for the Special Issue of the Journal of Geodesy devoted to Inverse Problems has been prepared.

Prof. Dr. Bernd Hofmann (Technische Universität Chemnitz)

Research in progress on the use of Distance functions in non-linear regularization methods.

Prof. Dr. Ullrich Tautenhahn (University of Applied Sciences Zittau/Görlitz) Research in progress on Regularized Total Least Squares.

Prof. Dr. Thamban Nair (Indian Institute of Technology, Madras).

Joint research on Regularized Collocation Method. As a result, joint article has been submitted to Journal of Complexity.

### Participation at Conferences, Scientific Visits and Talk

# Conferences

Workshop on Statistical Inverse Problems, University of Goettingen, Germany, March 23 - 25, 2006. Invited key-note lecture "Regularization Algorithms in Learning Theory".

International Symposium on Approximation Theory and Remote Sensing Applications, Kunming, China, April 22 - 27, 2006. Invited key-note lecture "Regularization Algorithms in Learning Theory".

Dagstuhl Seminar "Algorithms and Complexity for Continuous Problems", Internationales Begegnungs- und Forschungszentrum für Informatik (IBFI) Schloss Dagstuhl, Germany, September 24 – 29, 2006. Invited talk "Adaptive regularization in Learning Theory".

Oberwolfach Workshop "Statistical Methods for Inverse Problems", Mathematisches Forschungsinstitut Oberwolfach, Germany November 26 – December 2, 2006. Invited talk "Adaptive Regularization Algorithms in Learning Theory".

### Scientific Visits

April, 18 – 22, 2006 – Mathematical Department of Beijing Normal University, Beijing, China. Colloquium talk "Balancing principle in Regularization Theory".

September, 14.-15, 2006 - Fraunhofer-Zentrum Kaiserslautern, Germany Colloquium "There is nothing more practical than a good theory"

October 29 – November 11, 2006 – Research Unit "Statistical Learning and Image Processing", University of Genova, Italy. Joint research project on Learning Theory. Seminar talk "Adaptive regularization strategy for Learning from Examples".

November 20 - 25, 2006 - Technische Universität Chemnitz, Germany. Joint research project "Distance functions in the non-linear regularization theory".

Talk in Chemnitzer Mathematisches Colloquium with the title "Balancing principle for solving illposed and well-posed problems".

### **Publications 2006**

# Appeared

- 1. S. Lu, S. V. Pereverzyev, Numerical differentiation from a viewpoint of regularization theory, Mathematics of Computations, v. 75 (2006), pp. 1853 1870.
- 2. P. Mathe, S. V. Pereverzyev, Regularization of some linear ill-posed problems with discretized random noisy data, Mathematics of Computations, v. 75 (2006), pp.1913 1929.
- 3. H. Cao, S. V. Pereverzyev, Natural linearization for the identification of a diffusion coefficient in a quasi-linear parabolic system from short-time observations, Inverse Problems v. 22 (2006), pp. 2311 -2330.
- 4. F. Bauer, P. Mathe, S. V. Pereverzyev, Local Solutions to Inverse Problems in Geodesy. The Impact of the Noise Covariance Structure upon the Accuracy of Estimation, Journal of Geodesy, 81 (2006).
- 5. P. Mathe, S. V. Pereverzyev, The discretized discrepancy principle under general source conditions, Journal of Complexity J. Complexity, v. 22 (2006), 371 381
- 6. F. Bauer, S. V. Pereverzyev, An utilization of a rough approximation of a noise covariance within the framework of multi-parameter regularization, International Journal of Tomography and Statistics, v. 4 (2006), 1 12.

#### Submitted

- 1. F. Bauer, S. V. Pereverzyev, L. Rosasco, On Regularization Algorithms in Learning Theory.
- 2. M.T. Nair, S. V. Pereverzyev, Regularized Collocation Method for Fredholm Integral Equations of the First Kind.

# Shuai Lu advised by Prof. Sergei Pereverzyev

Member of the Inverse Problems Group of RICAM, under the FWF-Project P17251-N12 "Fixed point regularization schemes for nonlinear ill-posed problems and their discretization"

# **Scientific Achievements 2006**

An analysis of Tikhonov regularization for nonlinear ill-posed problems under general smoothness assumptions.

We discuss an adaptive regularization scheme based on algorithms for minimization of the Tikhonov functional to reconstruct the solution of a nonlinear ill-posed problem. Under the assumption that Frechet derivative F' is Lipschitz-continuous, a choice of the regularization parameter and the stopping

criteria for minimization algorithms are presented. We prove that under general source condition given in terms of a nonlinear operator F the error between the regularized approximation and the solution is order optimal.

Sparse reconstruction using the standard Tikhonov method

It is a common belief that the Tikhonov scheme with L2-penalty fails in sparse reconstruction. We show, however, that for some operators this standard regularization can help if the stability measured in the L1-norm will be properly taken into account in the choice of the regularization parameter.

# **Scientific Cooperations**

### Internal

Prof. Dr. Pereverzyev

PD Dr. Ramlau

# Participation at Conferences, Scientific Visits and Talk

# Scientific Visits

- MFO Seminar Interferometric Imaging (2006 June), Oberwolfach Germany.
- 7th World Congress on Computational Mechanics (2006 July), Los Angeles USA.
- Minisymposium presentation on "An analysis of Tikhonov regularization for nonlinear ill-posed problems under general smoothness assumption".
- Algorithms and complexity for continuous problems (2006 Sep.), Dagstuhl Germany.
- 25 Minutes presentation on "Sparsity reconstruction using standard Tikhonov method".
- Chemnitz Symposium on Inverse Problems (2006 Sep.), Chemnitz Germany.
- 25 Minutes presentation on "An analysis of Tikhonov regularization for nonlinear ill-posed problems under general smoothness assumption".

#### **Publications 2006**

# **Appeared**

- 1. S Lu, S Pereverzyev, Numerical differentiation from a view point of Regularization Theory, Mathematics of Computations, 75:1913-1929, 2006.
- 2. Z J Cai, D Q Chen, S Lu, Reconstruction of a fractal rough surface, Physica D: Nonlinear Phenomena, 213:25-30, 2006.
- 3. S Lu, Y Wang, First and Second Order Numerical Differentiation with Tikhonov Regularization, Frontiers of Mathematics in China, 1:354-367, 2006.

# Submitted

- 4. S Lu, S Pereverzyev, R Ramlau, An analysis of Tikhonov regularization for nonlinear ill-posed problems under general smoothness assumption, to appear in Inverse Problems.
- 5. R Lazarov, S Lu, S Pereverzyev, On the balancing principle for some problems of Numerical Analysis, submitted.

# Cao Hui advised by Prof. Sergei Pereverzyev

I am a team member of FWF-ProjectP17271-N12 "Fixed point regularization schemes for nonlinear ill-posed problems and their discretization". The main topic of my research is natural linearization for parameter identification problems.

### Scientific achievements 2006

In this year the paper "Natural linearization for the identification of a diffusion coefficient in a quasilinear parabolic system from short-time observations" was published in the journal "Inverse problems". In this work the idea of natural linearization is extended to the identification of solutiondependent diffusion coefficients. The natural linearization technique allows us to avoid the difficulty arising in solving nonlinear inverse problem. However, when we apply this method, we have to solve a linear ill-posed problem with incomplete information about the noise level. Therefore, in order to choose a suitable regularization parameter, a balancing principle is suggested, because it can select an appropriate regularization parameter and specify the noise level simultaneously. Moreover, we prove that the regularization parameter selected by the balancing principle gives the accuracy of optimal order.

### Scientific activities

- International Symposium on Approximation Theory and Remote Sensing Applications, 22-26 April, 2006, Kunming, China. Presentation with the title "Balancing principle for Cauchy problem".
- Oberwolfach-Seminar: Mathematical and Computational Problems in Interferometric Imaging, 4-6 June, 2006, Oberwolfach mathematics institute, Germany.
- 7th World Congress on Computational Mechanics, 16-22 July, 2006, Los Angeles, United States. Talk in the minisymposium "Inverse problem" with the title "<u>Discretized Tikhonov-Phillips regularization for a naturally linearized parameter identification problem</u>".
- Workshop "Algorithms and Complexity for Continuous Problems", 24-29 September, Dagstuhl, Germany. Talk with the title "Balancing principle for solving naturally linearized elliptic Cauchy problem".

### **Publications in 2006**

# <u>Appeared</u>

Natural linearization for the identification of a diffusion coefficient in a quasi-linear parabolic system from short-time observations, *Inverse problem* **22** (2006), 2311-2330 (together with Prof. Dr. Sergei Pereverzyev).

### Submitted

Balancing principle for solving naturally linearized elliptic Cauchy problems.

# PhD program

As a registered PhD student at JKU, I took the following courses:

- Adaptive finite element methods (by Dr. Boris Vexler)
- Image processing (by Dr. Arjan Kuijper)

### Plan for 2007

**FWF-ProjectP17271-N12** "Fixed point regularization schemes for nonlinear ill-posed problems and their discretization" and PhD program will be continued in 2007.

It is planned to present the PhD dissertation in April 2007 and defend the thesis before August 2007.

### Dr. Ronny Ramlau

### **Scientific Achievements 2006**

*Regularization of nonlinear ill – posed problems with sparsity constraints:* 

In [2] we have introduced Tikhonov regularization with one – homogeneous sparsity constraints, and have presented an iterative optimization strategy for the minimization of the functional. The method is based on so called Surrogate Functionals, where the original functional is replaced by a sequence of approximating functionals with better properties. Besides the investigation of the convergence properties of the optimization method, we also investigated an a – priori parameter choice rule for a special penalty term. In [11], the developed regularization approach was generalized to sparsity terms that can be expressed as a weighted p – norm of sequences, which includes scales of Besov – spaces.

### Shape Optimization problems:

In [7], we have considered the reconstruction of a piecewise constant object from its tomography data. The focus was on the reconstruction of the function and its shape, which was done by using a Mumford – Shah type functional. The minimization of the functional was obtained by means of shape optimization. Recently, we have investigated the dependence of the method on the regularization parameter, and have proposed a parameter choice rule that ensures convergence of the function as well as the shapes. A first presentation of the results is given in [8].

In a different approach we have investigated the reconstruction of the shape of an object from measurements of its data Af, where A is a linear operator. The reconstruction of the shape is obtained via the minimization of a Tikhonov functional with BV penalty, its minimization is again computed by Surrogate functionals [10].

### Inverse Imbalance Reconstruction

After developing regularization methods for the reconstruction of imbalance distributions in rotating systems [5], the focus was this year mainly on the application of the developed methods to wind power plants. In particular, we have used filtering methods for the preprocessing of the measured data, and the developed models of the plants were optimized with respect to eigenfrequencies [4,9]. Recently, we were working on the implementation of the methods to Condition Monitoring Systems.

### **Grants**

# FWF – Project P19029-N18

Title: Mumford – Shah – Models in Tomography

Project Leader: PD. Dr. R. Ramlau and Prof. Dr. W. Ring (Graz)

Project members: Dr. Esther Klann (RICAM) and Mag. Rer. Nat. E. Hötzl (Graz)

Project start: July 2006

# FWF – Project P19496-N18

Title: Sparse Reconstructions in Inverse Problems

Project Leader: PD. Dr. R. Ramlau Project members: 1 open PhD position

Project start: March 2007

Cooperation: PD Dr. G. Teschke, Zuse Institute for applied mathematics and computer science, Berlin,

Project co-funded by DFG

# **Scientific Cooperations**

# <u>Internal</u>

Dr. Esther Klann

Dr. Stefan Kindermann

Prof. Dr. Andreas Neubauer

Prof. Sergei Pereverzyev

Mag. Shuai Lu

# Dr. Massimo Fornassier (RICAM/Princeton)

# External

Prof. Dr. Wolfgang Ring, University of Graz, Austria

Mag. rer. nat. Elena Hötzl, University of Graz, Austria

PD Dr. Gerd Teschke, Konrad – Zuse Institute, Berlin, Germany

Dipl. Math. Mariya Zharyi, Konrad – Zuse Institute, Berlin, Germany

Dr. Jenny Niebsch, Konrad – Zuse Institute, Berlin, Germany

Prof. Dr. Peter Maass, University of Bremen, Germany

Dr. Lutz Justen, University of Bremen, Germany

Prof. Dr. E. Brinksmeier, Laboratory for Precision Machining, University of Bremen, Germany

Prof. Dr. Martin Burger, University of Münster, Germany

Dipl.-Math. Marie Therese Wolfram, University of Münster, Germany

Prof. Dr. F. Noo, Utah Center for Advanced Imaging Research, University of Utah, Salt Lake City, USA

Prof. Dr. Rolf Clackdoyle, Laboratoire Traitement du Signal et Instruments (CNRS UMR 5516), St. Etienne, France

# **Industrial Cooperations**

Dr. - Ing. M. Lang, Siemens GmbH, Automation and Drives, Berlin, Germany

Dr. R. Usbeck, Fielax GmbH, Bremerhaven, Germany

Ing. M. Melzheimer Deutsche Windguard Dynamix GmbH, Berlin, Germany

Ing. H. Fritsch, MySen GmbH, Rudolstadt, Germany

Dr. G. Stüber, Oerlikon Leybold Vacuum GmbH, Cologne, Germany

# Participation at Conferences, Scientific Visits and Talk

### Conferences

- The Third International Conference "Inverse Problems: Modeling and Simulation", Fethiye, Turkey, May 29 June 2, 2006.
- Inverse Problems Reunion Conference, Lake Arrowhead, California, USA, June 11-16, 2006
- Mathematical Methods in Tomography, Oberwolfach, Germany, July 30 August 5, 2006
- 7th International Conference on Rotor Dynamics, Vienna, September 26 29, 2006
- DEWEK 2006, 8th German Wind Energy Conference, Bremen, November 23 24, 2006

### Scientific Visits

- Centre for Industrial Mathematics, University of Bremen, Germany, January 10-12, 2006 (Prof. P. Maass)
- University of Graz, Austria, March 30 31 (Prof. Ring)
- Konrad Zuse Institute, Berlin, Germany, April 12 -14, 2006 (Dr. Gerd Teschke)
- Centre for Industrial Mathematics, University of Bremen, Germany, September 7-9, 2006 (Prof. P. Maass)
- Centre for Industrial Mathematics, University of Bremen, Germany, October 26-28, 2006 (Prof. P. Maass)
- Centre for Industrial Mathematics, University of Bremen, Germany, November 23-25, 2006 (Prof. P. Maass)
- Institute for Medical Psychology, November 28-29, 2006 (Dr. H. Preissl)

# Scientific Talks / Posters

- Inverse Problems in Rotordynamics, Radon Seminar, Linz, Austria, March 1, 2006
- Tikhonov regularization for nonlinear operator equations with sparsity constraints convergence results and numerical aspects, The Third International Conference "Inverse Problems: Modeling and Simulation", Fethiye, Turkey, June 1, 2006

- *Tikhonov regularization with sparsity constraints*, Inverse Problems Reunion Conference, Lake Arrowhead, California, USA, June 15, 2006
- *Tikhonov regularization with non standard constraints for Tomography*, Mathematical Methods in Tomography, Oberwolfach, Germany, August 4, 2006
- Effiziente Methoden zur Regularisierung von schlecht gestellten Problemen: Analysis und Anwendungen, University of Bonn, Germany, September 20, 2006
- *Inverse Imbalance Reconstructions in Applications*, 7th International Conference on Rotor Dynamics, Vienna, September 27, 2006
- *Model based Imbalance Monitoring*, DEWEK 2006, 8th German Wind Energy Conference, Bremen, November 23, 2006

## **Publications 2006**

# Appeared / Accepted

- [1] L. Justen, R. Ramlau, *A non-iterative regularization approach to blind deconvolution*, Inverse Problems, 22, 771-800, 2006,
- [2] R. Ramlau, G. Teschke, A Tikhonov-based projection iteration for nonlinear Ill posed problems with sparsity constraints, Numerische Mathematik, 104, 177 203, 2006,
- [3] E. Klann, P. Maass, R. Ramlau, *Two-step regularization methods for linear inverse problems*, Journal of Inverse and Ill Posed Problems, 14, 6, 583-607, 2006,
- [4] R. Ramlau, J. Niebsch, *Automatische Unwuchterkennung am Rotor*, Erneuerbare Energien, 5, Mai 2006,
- [5] R. Ramlau, V. Dicken, P. Maass, A. Rienäcker, C. Streller, *Inverse Imbalance Reconstruction in Rotordynamics*, ZAMM, 86, 5, 385-399, 2006,
- [6] S. Lu, S. Pereverzyev, R. Ramlau, *An analysis of Tikhonov regularization for nonlinear ill-posed problems under general smoothness assumptions*, to appear in Inverse Problems, 2006
- [7] R. Ramlau, R. Ring, A Mumford-Shah approach for contour tomography, J. Comp. Physics, in press, 2006
- [8] R. Ramlau, *Tikhonov regularization with non standard constraints for Tomography*, A. K. Louis, F. Natterer, E. T. Quinto, Mathematical Methods in Tomography, 34/2006, Oberwolfach Report, 62-64, 2006,

# **Submitted**

- [9] J. Niebsch, R. Ramlau, *Inverse Imbalance Reconstruction in Applications*, submitted for publication, 2006.
- [10] S. Kindermann, R. Ramlau, Surrogate Functional and Tresholding for Invers Interface problems, submitted for publication, 2006,
- [11] R. Ramlau, Regularization Properties of Tikhonov Regularization with sparsity constraints, submitted for publication, 2006,
- [12] E. Klann, R. Ramlau, *Regularization by fractional filter methods and data smoothing*, submitted for publication.

## Dr. Esther Klann advised by Dr. Ronny Ramlau

# Work before joining RICAM (joined RICAM 10/01/2006)

Dr. Esther Klann joined the Radon Institute for Computational Mathematics in October 2006. Before that she has been a PhD-student (and since January 2006 a Postdoc) at the Centre for Industrial Mathematics at the University of Bremen, Germany. Her main research topics are the construction and the analysis of regularization methods as well as ill-posed problems in medical imaging. At the RI-CAM, Dr. Klann is working in the FWF-Project P19029-N18 "Mumford-Shah Models for the Inversion of Tomography Data" of PD Dr. Ronny Ramlau.

#### **Scientific Achievements 2006**

# Two-step methods for linear ill-posed problems

In [1,2] we have studied two-step methods for linear ill-posed problems. In [1] the general concept of two-step methods as combination of a data smoothing and a reconstruction operation was introduced. We suggested to choose the data preprocessing step to be adapted to the smoothness properties of the data whereas the reconstruction step should be adapted to the properties of the operator under consideration. In [1,2] we linked these different requirements using the unifying concept of Hilbert scales. In [2] we studied in detail the combination of wavelet shrinkage and classical regularization methods (Tikhonov, Landweber) . For this two-step method we proved quasi-optimal convergence rates. Test calculations for the linear SPECT operator were done which confirm the theoretical results.

# Fractional filter methods

In [3] we introduced and analyzed fractional filter methods. It is well-known that classical regularization methods like the Tikhonov and Landweber method oversmooth the solution and hence sharp or fine features of the solution are lost. In [3] we explained this effect and introduced fractional filter method as a modification of the classical Tikhonov (Landweber) method. This method involves fractional powers of operators and allows to control the amount of damping and hence to avoid oversmoothing. We proved that the fractional methods are order optimal as long as the additional parameter varies within a certain range. For the application of the modified methods we considered as a first approach a series expansion and performed test calculations for the integration operator.

### **Scientific Cooperations**

#### Internal

PD Dr. Ronny Ramlau

### External

Mag. rer. nat. Elena Hötzl, University of Graz, Austria Prof. Dr. Wolfgang Ring, University of Graz, Austria

Dr. Dirk Lorenz, University of Bremen, Germany

Prof. Dr. Peter Maass, University of Bremen, Germany

# Participation at Conferences, Scientific Visits and Talk

## Scientific Visits

- 1. RICAM, University of Linz, Austria, March 15-19, 2006, (PD Dr. Ronny Ramlau)
- 2. University of Graz, December 5-8, 2006, (Prof. Dr. Wolfgang Ring)

### **Scientific Talks**

- 3. Regularization of Linear Ill-posed Problems in Two Steps: Combination of Data Smoothing and Reconstruction Methods, PhD-Kolloquium, University of Bremen, Germany, January 11, 2006.
- 4. Combination of Data Smoothing and Reconstruction Methods for Ill-posed Problems, Industrial Mathematics Seminar, Johannes Kepler Universität Linz, Austria, October 17, 2006

### **Publications 2006**

#### Appeared

- [1] E.Klann. Regularization of Linear Ill-posed Problems in Two Steps: Combination of Data Smoothing and Reconstruction Methods. PhD-Thesis, University of Bremen, 2006.
- [2] E.Klann, P.Maass and R.Ramlau. *Two-Step regularization methods for linear inverse problems*, J. Inv. Ill-Posed Problems, Vol. 14, No. 6, 583-607, 2006.

### Submitted

[3] E.Klann and R.Ramlau. Regularization by Fractional Filter Methods and Data Smoothing.

#### Dr. Arnd Rösch

#### Scientific Achievements 2006

The research in 2006 was focused on several mathematical fields:

1. Regularity of adjoint variables - Regularization of state constrained optimal control problems

Adjoint equations and the regularity of their solutions play an important role in the theories of inverse problems and optimal control. A new general result on existence of regular Lagrange multipliers is shown in a joint paper with F. Tröltzsch (TU Berlin). Moreover, higher regularity for the optimal control was shown. Mixed constrained optimal control problems occur as regularized state constrained problems. In a joint work with Klaus Krumbiegel we established a new virtual control approach.

## 2. Numerical analysis

We studied the discretization error for distributed and boundary control problems with point wise inequality constraints on control and state. Our goal is to find optimal discretization strategies for such problems. A qualitative new result was found in a joint work with D. Wachsmuth. We were able to prove error estimates for a nonlinear problem based on the numerical solution.

### 3. Nonlinear problems

Here, we studied optimal control problems with point wise mixed control-state constraints and control constraints. Based on the regularity results sketched above we proved the Lipschitz stability of the optimal solution with respect to perturbations. This is a joint work of our FWF-project P18056 and W. Alt (Jena). This result is important for the convergence analysis of Newton type methods.

# **Scientific Cooperation**

## Internal Cooperation with

- 1. Roland Griesse (Group Optimization and Control)
- 2. Boris Vexler (Group Optimization and Control)

# External Cooperation with

- 1. Prof. F. Tröltzsch (TU Berlin)
- 2. Prof. W. Alt (FSU Jena)
- 3. Prof. M. Mateos (Oviedo)
- 4. Dipl.-Math. D. Wachsmuth (TU Berlin)
- 5. Dipl.-Ing. C. Meyer (TU Berlin)
- 6. Dipl.-Math. R. Simon (SFB 013 Linz)
- 7. Prof. T. Apel (Universität der Bundeswehr München)
- 8. Dipl.-Math. G. Winkler (Universität der Bundeswehr München)
- 9. Prof. M. Hinze (Universität Hamburg)

### Participation at conferences

- 1. Application Workshop of the DFG-SPP 1253, Bad Honnef, February 6-7, 2006.
- 2. Numerical Techniques for Optimization Problems with PDE Constraints, Oberwolfach, February 27-March 3, 2006.

- 3. International Congress on the Applications of Mathematics, Santiago de Chile, March 13-17, 2006.
- 4. Numerical Analysis Day, Graz, April 27-28, 2006.
- 5. MAFELAP London, June 13-16, 2006.
- 6. MMAR 2006, Miedzyzdroje, August 28-31, 2006.
- 7. FEM-Symposium, Chemnitz, September 25-27, 2006.
- 8. Workshop on Inverse Problems, September 28-29, 2006.
- 9. Kick-Off-Meeting of the SPP 1253, Thurnau, November 20-21, 2006.

#### **Publications**

# Appeared

- 1. A. Rösch, Error estimates for linear-quadratic control problems with control constraints., Optimization Methods and Software, 21, 1, 121-134, February, 2006,
- 2. C. Meyer, A. Rösch, F. Tröltzsch, Optimal Control of PDEs with regularized pointwise state constraints., Computational Optimization and Applications, 33, 2-3, 209-228, March, 2006,
- 3. A. Rösch, F. Tröltzsch, Existence of regular Lagrange multipliers for elliptic optimal control problem with pointwise control-state constraints, SIAM Journal Control and Optimization, 45, 2, 548-564, 2006,
- 4. A. Rösch, B. Vexler, Optimal control of the Stokes equations: A priori error analysis for finite element discretization with postprocessing, SIAM Journal Numerical Analysis, 44, 5, 1903-1920, 2006,
- 5. A. Rösch, F. Tröltzsch, Sufficient second-order optimality conditions for an elliptic optimal control problem with pointwise control-state constraints, SIAM Journal Optimization, 17, 3, 776--794, 2006.
- 6. S. Cherednichenko, A. Rösch, Error estimates for the regularization of optimal control problems with pointwise control and state constraints, accepted for publication in ZAA, 2006,
- 7. A. Rösch, Finite Dimensional Approximation of Optimal Control Problems Governed by Partial Differential Equations, Proceedings of the 12th International Conference on Methods and Models in Automation and Robotics in Miedzyzdroje (Poland), 101--104, 2006,
- 8. A. Rösch, D. Wachsmuth, Regularity of solutions for an optimal control problem with mixed control-state constraints., TOP, 14, 2, 263-278, December, 2006,

## Submitted

- 1. A. Rösch, R. Simon, Superconvergence properties for optimal control problems discretized by piecewise linear and discontinuous functions, submitted, 2006,
- 2. W. Alt, R. Griesse, N. Metla, A. Rösch, Lipschitz Stability for Elliptic Optimal Control Problems with Mixed Control-State Constraints, submitted, 2006,
- 3. A. Rösch, D. Wachsmuth, Verification of optimality conditions, submitted, 2006,!
- 4. A. Rösch, F. Tröltzsch, On regularity of solutions and Lagrange multipliers of optimal control problems for semilinear equations with mixed pointwise control-state constraints, submitted, 2006.
- 5. K.Krumbiegel, A.Rösch, A virtual control concept for state constrained optimal control problems, submitted, 2006,

#### **Talks**

- 1. A. Rösch, Herausforderungen und Perspektiven bei der optimalen Steuerung partieller Differentialgleichungen, January 6, 2006, Kiel
- 2. A. Rösch, A virtual control concept for optimal control problems with pointwise state constraints, February 27-March 3, 2006, Oberwolfach,
- 3. A. Rösch, New superconvergence results in optimal control, March 13-17, 2006, ICAM, Santiago de Chile,
- 4. A. Rösch, Numerical analysis for optimal control problems in nonconvex domains, April 27-28, 2006, Numerical Analysis Day, Graz,

- 5. A. Rösch, Wie gut sind numerische Lösungen für Optimierungsprobleme bei partiellen Differentialgleichungen?, May 4, 2006, Duisburg,
- 6. A. Rösch, How accurate are numerical solutions of optimization problems governed by PDEs, June 1, 2006, Gijon, Spain,
- 7. A. Rösch, A posteriori error estimates for semilinear problems, June 13-16, 2006, MAFELAP, London.
- 8. A. Rösch, Finite dimensional approximations of optimal control problems governed by partial differential equations, August 28-31, 2006, MMAR 2006, Miedzyzdroje,
- 9. A. Rösch, On the finite element approximation of elliptic optimal control problems with Neumann boundary control, September 25-27, 2006, FEM-Symposium, Chemnitz,
- 10. A. Rösch, Lagrange multipliers measures or functions?, September 28-29, 2006, Workshop on Inverse Problems, Chemnitz,
- 11. A. Rösch, Wie gut sind numerische Lösungen für Optimierungsprobleme bei partiellen Differentialgleichungen?, November 3, 2006, Greifswald,

#### **Visits**

Gijon (University of Oviedo), Spain, May 21-June 2, 2006, cooperation with M. Mateos

### **Activities**

Organization of a minisymposium Finite Elements in Optimal Control at the MAFELAP in London, June 13-16, 2006 (together with B. Vexler).

### **Offers**

I got an offer for a full professorship (W3) for nonlinear optimization at the University Duisburg-Essen.

# **Projects**

- 1. FWF-Project P18056-N12 SSC and SQP for mixed constrained optimal control problems (joint project with Roland Griesse), positions: Nataliya Metla (1PhD)
- 2. FWF-Project P 18090-N12 Approximation of optimal control problems governed by PDEs, positions: Svetlana Cherednichenko, Klaus Krumbiegel (2PhDs)
- 3. FWF-Project P 18971-N18 Numerical analysis and discretization strategies for optimal control problems with singularities (joint project with B. Vexler and T. Apel (Munich), part of the DFG priority program 1253) positions: Olaf Benedix (1PhD)

### **Scientific Plans for 2007**

Dr. Rösch has accepted the call and will leave RICAM at the end of March 2007

# Klaus Krumbiegel advised by Dr. Arnd Rösch

# **Scientific Achievements 2006**

We developed error estimates for feasible solutions of optimal control problems with pointwise control constraints concerning the optimal solution of this problem. These feasible solutions can be related to iterative solvers of such optimal control problems. Furthermore, this estimate can be used as a stopping rule for iterative methods. In joint work with M. Hinze we applied this to the primal-dual active set strategy and to the projected gradient method.

Moreover, we considered optimal control problems with pointwise state in the domain constraints and pointwise control constraints on the boundary. We introduced a virtual control concept, which overcomes analytical and numerical difficulties. Moreover, we derived an estimate for the regularization error. The error estimate was confirmed in different numerical examples.

# **Scientific Cooperation**

## Internal

S. Cherednichenko, Group Inverse Problems

Dr. B. Vexler, Group Optimization and Optimal Control

Dr. R. Griesse, Group Optimization and Optimal Control

# **External**

Prof. Dr. M. Hinze, University of Hamburg, Department of Mathematics

Dr. C. Meyer, Weierstrass Institute for Applied Analysis and Stochastics (WIAS)

I. Yousept, TU Berlin, Department of Mathematics

# Participation at Conferences, Scientific Visits and Talk

## Conferences

06/04 Numerical Analysis Day Graz 06/10 FEM-symposium Chemnitz 06/10 Inverse Day Chemnitz

### **Invited Talks**

06/08/01 Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Feasible iterative methods - Error estimates and numerical treatment

### Scientific Talks

06/04/28 Numerical Analysis Day Graz, Linear quadratic optimal control problems- error estimates and numerical treatment

06/10/27 FEM-symposium Chemnitz, A new iterative concept for solving linear-quadratic optimal control problems

### **Publications 2006**

- 1. B. Hofmann, D. Düvelmeyer, K. Krumbiegel, Approximate source conditions Some new analytical and numerical studies, Mathematical Modelling and Analysis, 41-56, 3, 2006
- 2. K.Krumbiegel, A.Rösch, A virtual control concept for state constrained optimal control problems, submitted, 2006

# Svetlana Cherednichenko advised by Dr. Arnd Rösch

## **Scientific Achievements 2006**

I studied linear-quadratic optimal control problems with pointwise control and state constraints. Moreover we discussed regularity properties of solutions for discrete problems in a joint work with Dr. Christian Meyer. In a joint work with Dr. Arnd Rösch we discussed the regularization error for a Lavrentiev type regularization of the pointwise control and state constraints. We considered discrete regularized and unregularized problems and analyzed the order of convergence analytically and numerically. Numerical tests confirm our theoretical findings and show even better convergence rates for regularized problem.

# **Scientific Cooperation**

#### Internal

DI. K. Krumbiegel (Group Inverse Problems)

MSc. N. Metla (Group Inverse Problems)

Dr. Arnd Rösch (Group Inverse Problems)

### External

Dr. C. Meyer, Weierstrass Institute for Applied Analysis and Stochastics (WIAS)

# Participation at Conferences, Scientific Visits and Talk

## Conferences

- 19th Chemnitz FEM Symposium 2006, Chemnitz, 25-27/09/06.
- Chemnitz Symposium on Inverse Problems, Chemnitz, 28-29/09/06.

## Scientific Talks

- "Elliptic equations. Single boundary measurements", on industrial mathematics seminar, Linz, 24/04/2006.
- "Lavrentiev regularization of state constrained optimal control problems", Chemnitz Symposium on Inverse Problems, Chemnitz, 29/09/06.
- "The discretization of constrained optimal control problems", on industrial mathematics seminar, Linz, 12/12/06.

#### **Publications 2006**

## **Appeared**

"Error estimates for the regularization of optimal control problems with pointwise control and state constraints", Journal for Analysis and its Applications, accepted for publication.

# Nataliya Metla advised by Dr. Arnd Rösch and Dr. Roland Griesse

#### Scientific Achievements 2006

In my research I investigate nonlinear optimal control problems with pointwise mixed control-state constraints and additional control constrains.

The Lipschitz stability and sensitivity of the optimal solution with respect to perturbations for the linear elliptic problem was investigated and these results were extended to nonlinear elliptic problems. First results for convergence analysis of the SQP method in case of linear mixed constrains for elliptic problem was obtained and verified by numerical tests.

## **Scientific Cooperation**

#### Internal

MSc. Cherednichenko (Group "Inverse Problems")

DI. Krumbiegel (Group "Inverse Problems")

Dr. Rösch (Group "Inverse Problems")

Dr. Griesse (Group "Optimization and Control")

#### External

Prof. Dr. Walter Alt, Friedrich-Schiller-Universität Jena, Germany

# Participation at Conferences, Scientific Visits and Talk

#### Conferences

- Euro Summer Institute 2006 (August 18th September 2nd 2006, Lutherstadt-Wittenberg, Germany)
- 19th Chemnitz FEM Symposium 2006 (September 25-27th 2006, Chemnitz, Germany)
- Chemnitz Symposium on Inverse Problems (September 28-29th 2006, Chemnitz, Germany)

# Scientific Talks

- "Elliptic Equations. Single Boundary Measurements." (April 26th 2006, RICAM, Industrial Mathematics Seminar, Linz)
- "Lipschitz Stability for linear-quadratic elliptic problems with mixed constraints" (September 1st 2006, ESI, Lutherstadt-Wittenberg)
- "Lipschitz stability for linear-quadratic elliptic problems with mixed constraints" (September 29th 2006, Chemnitz Simposium on Inverse Problems, Chemnitz)
- "Convergence of SQP method for nonlinear elliptic problems with mixed constraints" (December 12th 2006, RICAM, Industrial Mathematics Seminar, Linz)

#### **Publications 2006**

### Submitted

W. Alt, R. Griesse, N. Metla and A. Rösch, "Lipschitz stability for elliptic optimal control problems with mixed control-state constraints" (submitted)

#### Dr. Elena Resmerita

## **Scientific Achievements 2006**

Elena Resmerita's work in 2006 has focused mainly on regularization of ill-posed operator equations in Banach spaces.

The research on joint Kullback-Leibler regularization for positive linear inverse problems (i.e., positive kernel and right-hand side, positive solutions), carried out with R.S. Anderssen, has been finalized and submitted for publication [4].

Convergence rates for Bregman iterations and inverse scale space for image restoration have been obtained in cooperation with M. Burger. It is remarkable that the techniques employed for proving the results do not follow patterns of previous works in the literature. Dr. Lin He has recently joined in this research. The corresponding manuscript [5] will be submitted in January 2007.

A numerical implementation of the expectation-maximization (EM) algorithm for a Poisson model has been pursued to support the analysis that has been made so far in an infinite dimensional setting [6].

The collaboration with O. Scherzer on variational regularization with non-quadratic penalty has been continued. A draft presentation of preliminary results is being currently developed.

The long-term research initiated with D. Butnariu has focused this year on the stability of proximal operators (used in methods for approaching variational inequalities) when Mosco type perturbations are taken into account. As a result, the paper [3] was submitted and is going to be published in 2007.

Note: E. Resmerita has worked in 2006 for about six months, due to a maternal leave and a part-time period of work.

# **Scientific Cooperations**

#### Internal

Prof. Heinz Engl - J. Kepler University of Linz and RICAM

Dr. Lin He – J. Kepler University of Linz and RICAM

Prof. Otmar Scherzer - University of Innsbruck and RICAM

## External

Dr. Robert S. Anderssen - CSIRO Mathematical and Information Sciences, Canberra, Australia

Prof. Martin Burger – University of Münster, Germany

Prof. Dan Butnariu - University of Haifa, Israel

Prof. Alfredo Iusem - Instituto de Matematica Pura e Aplicada, Rio de Janeiro, Brasil

# Participation at Conferences, Scientific Visits and Talks

- November 2006: Talk at the Workshop "The 5<sup>th</sup> Ballarat Workshop on Global and Nonsmooth Optimization: Theory, Methods and Applications", Ballarat, Australia: Error estimates for non-quadratic regularization of ill posed inverse problems.
- December 2006: Invited colloquium talk at the Mathematical Sciences Institute, Australian National University, Canberra, Australia: Joint Kullback-Leibler residual minimization and regularization for linear inverse problems.
- December 4-8, 2006: Visiting fellow at the CSIRO Mathematical and Information Sciences and at the Mathematical Sciences Institute, Australian National University, both in Canberra, Australia.

### **Publications 2006**

# **Appeared**

- [1] E. Resmerita and O. Scherzer: Error estimates for non-quadratic regularization and the relation to enhancing, Inverse Problems, 22:801-814, 2006.
- [2] D. Butnariu and E. Resmerita: Bregman distances, totally convex functions and a method for solving operator equations, Abstract and Applied Analysis, Article ID 84919, 1-39, 2006.

### Accepted

[3] D. Butnariu and E. Resmerita: Mosco stability of proximal mappings in reflexive Banach spaces, Journal of Nonlinear and Convex Analysis, 8(1), 2007.

# Submitted/in progress

- [4] E. Resmerita and R.S. Anderssen: Joint additive Kullback-Leibler residual minimization and regularization for linear inverse problems submitted, 2006.
- [5] Error estimation for Bregman iterations and inverse scale space methods in image restoration (with M. Burger and L. He) to be submitted in January 2007.
- [6] A perturbed expectation-maximization algorithm in infinite dimensional spaces (with H. Engl and A. Iusem) in preparation, 2006.

# Dr. Herbert Egger

### Introduction

Dr. Herbert Egger has been working in the Subproject F1308, "Computational Inverse Problems and Applications" of the SFB013, "Numerical and Symbolic Scientific Computing" until April 1, 2006, when he moved to RWTH Aachen. Dr. Egger's main topics of research are the design and analysis of preconditioning techniques for iterative regularization methods and inverse problems in finance.

### **Scientific Achievements 2006**

During spring 2006 Dr. Egger has carried out research in the following directions:

# 1.) Acceleration of iterative regularization methods:

The numerical treatment of inverse problems, in particular in connection with PDEs, typically leads to large-scale linear or non-linear systems of equations, which in many cases can be tackled only via iterative (regularization) methods. The ill-posedness of inverse problems gives rise to ill-conditioning of the the equations to be solved, and hence the convergence of iterative methods applied to the solution of inverse problems is usually very slow. In order to speed up convergence, preconditioning techniques have to be used.

It turns out that — in contrast to well-posed problems — appropriate preconditioners for inverse problems have to be unbounded operators, or at least have to approximate an unbounded operator, and therefore the analysis of preconditioned iterations is delicate. In [1], Dr. Egger continued work started in his PhD thesis, and showed that a large class of so-called semi-iterative regularization methods can be accelerated drastically by preconditioning in Hilbert scales, while optimal convergence rates with respect to data noise can be maintained. In [2] it was shown that Hilbert scale preconditioning can even be used to accelerate CGNE. This was surprising, since the fast convergence of CGNE relies on the fast decay of singular values of the underlying operator, which is somehow disturbed by preconditioning. In [3], Dr. Egger analyzed preconditioning of fully iterative Newton-type methods for non-linear inverse problems, and showed that the overall number of inner iterations can be reduced to about the square-root by appropriate preconditioning.

In recent research, so called Y-scale regularization methods have been considered: In this class of methods, the preconditioner is applied in the image space (Y) of the operator. This allows to apply preconditioning in Hilbert scales to a new class of problems, and further seems to have some advantages from a numerical point of view. However, the analysis of such methods is more involved, e.g., the discrepancy principle, which can be seen as the standard stopping rule for iterative regularization methods, cannot be applied. In [4] it was shown that still optimal convergence rates can be derived and the number of iterations can be reduced drastically, when a Lepskij-type criterion is used as a stopping rule.

# 2.) Parameter identification in inverse finance:

In cooperation with Prof. B. Hofmann and Dr. T. Hein from TU Chemnitz, earlier research on volatility identification in extended Black-Scholes models has been continued. In [5] the authors could show that under assumption of a special (non-parametric) structure of the local volatility surface, the parameter identification problem can be decomposed into two separate subproblems, whose solution is computationally much faster and more stable.

# **Scientific Cooperations**

#### <u>Internal</u>

on "stabilized mixed and hybrid finite element methods for convection dominated elliptic problems", with Prof. J. Schöberl (START, RWTH Aachen)

### External

on "Decoupling of smile a term structure of volatility in inverse option pricing", with Prof. B. Hofmann (TU Chemnitz).

# Participation at Conferences, Scientific Visits and Talks

Dr. Egger was invited to present recent results of his research on the following conferences and seminars:

#### Conferences

International conference on "Inverse Problems: Modelling and Simulation", Fethiye, 2006. Invited talk on "Preconditioning Iterative Regularization Methods in Hilbert Scales"

GAMM-SIAM conference on "Applied Linear Algebra", Düsseldorf, 2006. Invited talk on "Acceleration of Iterative Methods for Inverse Problems"

# Scientific Talks

- "Preconditioning Iterative Regularization Methods in Hilbert Scales", IGPM, RWTH Aachen, 2006.
- "Iterative Regularization in Hilbert Scales", NAM, Universität Göttingen, 2006.
- "Stabilized mixed FEM for EHD", TKK Helsinki, 2006.
- "Iterative Solution of Inverse Problems", CCES, RWTH Aachen, 2006.

## **Publications 2005**

## Articles in Journals:

- 1. H. Egger, Semiiterative regularization in Hilbert scales, SIAM J. Numer. Anal. 44, 66-81, 2006.
- 2. H. Egger, T. Hein and B. Hofmann, "On decoupling of the volatility smile and term structure in inverse option pricing", Inverse Problems, 22, 1247-1259, 2006.
- 3. H. Egger, Preconditioning CGNE Iterations for Inverse Problems, Numerical Linear Algebra with Applications, 2006, accepted.

### Submitted

- 4. H. Egger, Y-Scale Regularization, 2006, submitted to SINUM.
- 5. H. Egger, Fast Fully Iterative Newton-type Methods for Inverse Problems, 2006, submitted to J. Inverse and Ill-posed Problems.

# Dr. Benjamin Hackl

## **Scientific Achievements 2006**

In 2006 Mr. Hackl finalized his Phd Thesis [4] on geometric inverse problems governed by partial differential equations. In the focus of this thesis was the perimeter regularization method and its numerical realization allowing and forcing topology changes. While level set methods are supposed to allow topological changes, theory and practice show that these topological changes might not happen. To force topological changes whenever appropriate three approaches were developed: The first one incorporates the concept of topological gradients into the level set methods (Burger, Hackl & Ring) with the drawback that it is not applicable to perimeter regularized geometric inverse problems, because the perimeter is not topologically differentiable. The second method incorporates the more reliable topological expansion into level set methods [4, 5], allowing to construct even Newton type methods to force topology changes for perimeter regularized geometric inverse problems. Finally, the third method is based solely on the phase field method which seems to provide an attractive alternative to level set methods for perimeter regularized geometric inverse problems [5].

Although phase field methods are widely used, they are rarely applied to perimeter regularized geometric inverse problems. In [5] the applicability of the phase field method to perimeter regularized geometric inverse problems was studied. The numerical results were very promising. [5] Also investigates G-convergence of the phase field method applied to the perimeter regularized geometric inverse problem.

## **Scientific Cooperations**

#### Internal

Dr. Martin Burger, Industrial Mathematics Institute, JK University Linz, Austria and Scientific Adviser at RICAM, Group "Inverse Problems". Level set methods for geometric inverse problems [3].

# External

Dr. Hend Ben Ameur, Laboratoire de Modelisation Mathematique et Numerique, Ecole Nationale d'Ingenieurs de Tunis. Level set methods for geometric inverse problems [3].

# Participation at Conferences, Scientific Visits and Talk

### Conferences

### Scientific Visits

### Scientific Talks

- [1] Geometry Variations, Level sets and Phase field for Perimeter Regularized Geometric Inverse Problems Graz, March 2006
- [2] Geometry Variations, Level sets and Phase Field for Perimeter Regularized Geometric Inverse Problems DCAMM Seminar, Lyngby, Mai 2006

#### **Publications 2006**

# **Appeared**

- [3] Hend Ben Ameur, Martin Burger, Benjamin Hackl, "Cavity identification in linear elasticity and thermoelasticity", Mathematical Methods in the Applied Sciences, 2006 accepted
- [4] Benjamin Hackl, "Shape Variations, Level Set and Phase-field Methods for Perimeter Regularized Geometric Inverse Problems", PhD Thesis, JK University Linz, September 2006

## Submitted

[5] Benjamin Hackl, "Methods for reliable topology changes for perimeter regularized geometric inverse problems", submitted

After having finished his thesis, Dr.Hackl left RICAM and now works in the Industrial Mathematics Competence Center.

# Dr. Andreas Hofinger

## **Scientific Achievements 2006**

In the period January - April 2006, Andreas Hofinger was mostly involved in the final preparation of his PhD thesis, which was successfully defended on April 25th.

The title of the thesis is "Ill-posed problems: Extendending the deterministic theory to a stochastic setup"; it was supervised by Prof. H. W. Engl.

From May to September 2006, he prepared several corresponding publications.

Dr. Hofinger left RICAM in September 2006.

The research of Dr. Hofinger during 2006 can be divided into the following topics:

### (i). Stochastic Inverse Problems:

Here, one goal is to extend the existing deterministic theory of inverse problems to a stochastic setup. A second goal is to transfer stochastic approaches (in particular the Bayesian approach) to the same common framework. The first was accomplished in the PhD-thesis of Andreas Hofinger, the second goal has partly been resolved successfully together with Dr. Pikkarainen (see below).

# (ii). Sampling and Learning Theory:

In the past years regularization methods for neural networks have been studied. In the chosen approaches it was always assumed that full measurements are given, nonetheless in practice only discrete, noisy observations are available. Using Koksma-Hlawka-type inequalities it could now be shown that the previously derived approaches also work in the discrete setup.

(iii). Acceleration of Algorithms in Multiyield-Plasticity:

In multi-surface elastoplasticity a system of nonlinear equations must be solved in each timestep, for every grid-point of the finite element grid, the solution of this problem is therefore a time-critical step. An extrapolation technique was successfully applied to this problem and could reduce the computation time by approximately a factor of 10.

# **Scientific Cooperations**

### Internal

On topic (i) there are cooperations with Heinz W. Engl, Stefan Kindermann and Hanna Pikkarainen.

#### External

The sampling problem (ii) was studied together with Friedrich Pillichshammer, Financial Mathematics Institute, Linz.

The acceleration problem (iii) was posed by Jan Valdman, SFB F013, Linz.

## Participation at Conferences, Scientific Visits and Talks

### Conferences

On March 23-25, Dr. Hofinger attended the workshop "Statistical Inverse Problems" in Göttingen, where he gave a poster-presentation (topic (i)).

### **Publications 2006**

### Appeared

Hofinger, A.: Ill-posed Problems: Extending the Deterministic Theory to a Stochastic Setup, vol. 51 of Schriften der Johannes-Kepler-Universität Linz. Reihe C: Technik und Naturwissenschaften, Trauner Verlag, Linz, 2006. ISBN: 3854990197.

Hofinger, A.: Nonlinear Function Approximation: Computing Smooth Solutions with an Adaptive Greedy Algorithm, Journal of Approximation Theory, 2006.

Hofinger, A.: The Metrics of Prokhorov and Ky Fan for Assessing Uncertainty in Inverse Problems, to appear in "Sitzungsberichte und Anzeiger, Math.-nat. Klasse, Austrian academy of sciences"

### Submitted

Hofinger, A.: Assessing Uncertainty in Linear Inverse Problems with the Metrics of Ky Fan and Prokhorov (SFB-Report, 2006-23).

Hofinger, A., Valdman, J.: Numerical solution of the two-yield elastoplastic minimization problem (SFB-Report, 2006-18).

Hofinger, A., Pillichshammer, F.: Learning a Function from Noisy Samples at a Finite Sparse Set of Points (SFB-Report, 2005-18).

Hofinger, A., Kindermann, S.: Assessing Uncertainty in Nonlinear Inverse Problems with the Metric of Ky Fan (SFB-Report, 2006-31).

Hofinger, A., Pikkarainen, H. K.: Convergence rates for the Bayesian approach to linear inverse problems (SFB-Report, 2006-32).

#### Dr. Hanna Katriina Pikkarainen

#### Scientific Achievements 2006

# Dynamical inverse problems:

In paper [1], a certain class of nonstationary linear inverse problems were studied as state estimation problems. The novel contribution of the paper was the analysis of the space discretization of the corresponding state estimation system. The distributions of the discretization errors in the discretized state evolution and observation equations were introduced. A finite-dimensional filtering method taking into account discretization errors was presented.

Numerical implementation of the method introduced in paper [1] was done in collaboration with Ph. Lic. Janne Huttunen (University of Kuopio, Finland) in a one-dimensional model case. The results and the effectiveness of the method were presented in article [2].

## Convergence results for the Bayesian inversion theory:

Recently, the metrics of Ky Fan and Prokhorov were introduced as a tool for studying convergence in stochastic ill-posed problems. In paper [3], it was shown that the Bayesian approach to linear inverse problems can be examined in the new framework as well. In paper [3], the finite-dimensional case where the measurements are disturbed by an additive normal noise and the prior distribution is normal was considered. Convergence and convergence rate results were obtained when the covariance matrices are proportional to the identity matrix.

### **Scientific Cooperations**

#### Internal

Dr. Andreas Hofinger Prof. Dr. Josef Schicho

#### External

Ph. Lic. Janne Huttunen, Department of Applied Physics, University of Kuopio, Finland Dr. Jarmo Malinen, Institute of Mathematics, Helsinki University of Technology, Finland

# Participation at Conferences, Scientific Visits and Talk

### Conferences

- Workshop on Statistical Inverse Problems, Göttingen, Germany, March 23-25, 2006
- The Third International Conference "Inverse Problems: Modeling and Simulation", Fethiye, Turkey, May 29 June 2, 2006.
- Inverse Problems in Applied Sciences, Sapporo, Japan, July 3-7, 2006.
- Inverse Days 2006, Tampere, Finland, December 13-15, 2006

### Scientific Visits

- Department of Mathematical Sciences, University of Oulu, Finland, January 3-4, 2006 (Dr. Sari Lasanen)
- Institute of Mathematics, Helsinki University of Technology, Finland, January 5, 2006 (Prof. Dr. Erkki Somersalo)
- Institute of Mathematics, Helsinki University of Technology, Finland, August 21 September 1, 2006 (Dr. Jarmo Malinen)
- Institute of Mathematics, Helsinki University of Technology, Finland, December 18-21, 2006 (Prof. Dr. Erkki Somersalo, Prof. Dr. Matti Lassas, Dr. Jarmo Malinen)

### Scientific Talks

- Bayesian approach to inverse problems, SFB Status Seminar, Strobl, Austria, April 22, 2006
- *Integral Geometry and Tomography*, Industrial Mathematics Seminar, Johannes Kepler Universität Linz, Austria, May 15, 2006
- *Discretization error in dynamical inverse problems*, The Third International Conference "Inverse Problems: Modeling and Simulation", Fethiye, Turkey, June 1, 2006
- State estimation approach to nonstationary inverse problems: discretization error and filtering problem, Inverse Problems in Applied Sciences, Sapporo, Japan, July 4, 2006
- Convergence rates for the Bayesian approach to linear inverse problems, Inverse Days 2006, Tampere, Finland, December 14, 2006

#### **Publications 2006**

# **Appeared**

[1] H K Pikkarainen. State estimation approach to nonstationary inverse problems: discretization error and filtering problem. Inverse Problems 22(1), pp. 365-379, 2006.

# Submitted

- [2] J M J Huttunen and H K Pikkarainen. Discretization error in dynamical inverse problems: one-dimensional model case.
- [3] A Hofinger and H K Pikkarainen. Convergence rates for the Bayesian approach to linear inverse problems.

#### Dr. Mourad Sini

Member of the Inverse Problems Group of RICAM since September 2006.

### Works before joining Ricam

I received my Phd from University of Provence, France, in late 2002. In 2003, I moved to Japan for a post doc position with the Japan Society for Promotion of Sciences (JSPS) for two years. After that, I spent the academic year 2005-2006 at the University of Yonsei, South Korea, supported by the Korean science foundation KOSEF and the funding BK21 of Yonsei University.

I worked mainly on two (related) topics. The first one is the qualitative studies of operators arising from partial differential equations. Precisely,

- 1. Qualitative studies of topographical wave-guides.
- 2. Spectral study of acoustic and elastic operators with periodic coefficients.

The second one concerns inverse problems. In the recent 3 years, I considered the following aspects:

1. Inverse spectral problems for rough coefficients including Borg-Levinson type problems and nodal problems.

- 2. Inverse scattering problems for complex obstacles, as the problem of radar detection.
- 3. Inverse dynamical problems and control of pde systems of multiple velocities. This is motivated by the problem of connected beams in civil engineering.
- 4. Magnetic Resonance Electrical Impedance Tomography.
- 5. Inverse problems for wave-guides. Acoustic and elastic wave guides. Models related to the imaging of the seabed and marine ecology.

#### **Scientific Achievements 2006**

- 1. Reconstruction of complex obstacles from far field measurements. In collaboration with Prof. G. Nakamura and Prof. J. Liu, we gave a quite complete solution to the problem of reconstructing complex obstacles from far field measurements. This ended up with a paper with Prof. Nakamura explaining the analysis for the point-wise formulas for the detection and a second paper with Prof. Liu and Prof. Nakamura where we applied these ideas to the 2D electromagnetic version and gave numerical tests justifying these types of formulas.
- 2. **Detection of the shearing coefficients for a system of connected beams.** This work (jointly with Prof. A. Morassi, Prof. G. Nakamura, Dr. K. Shirota) concerns reconstruction of the shearing coefficients in a system of connected beams. These coefficients are responsible for the integrity of the mentioned systems. This is modelled by a coupling between second and fourth order operators which makes the analysis complicated. We wrote a first paper where we explained in detail the necessary analysis which enables us to set up an optimization method. This method is tested numerically in a second paper where we compared the results with real data.
- 3. Justification of the B\_z algorithm in Magnetic Resonance Electrical Impedance Tomography. In 2002, Prof. J.K. Seo and his group in Seoul proposed the B\_z algorithm to reconstruct the anomaly from few (two) MRI measurements. The idea is based on the remark that one can produce, from these measurements, the main component of the magnetic field inside the body. This algorithm has been tested very successfully for phantom experiments. During my stay with them, I concentrated on the mathematical justification of the fast convergence of this algorithm.

In collaboration with Prof. J. Liu, Prof. J.K Seo and Prof E. J. Woo, we wrote a paper where we explained with mathematical rigor the exponential convergence of this algorithm in case where we have relatively small contrast of the conductivity.

4. Continuation of the dynamical Dirichlet-to-Neumann map for transversally isotropic materials. This project concerns the continuation property for anisotropic media. We are interested in continuing the given dynamical Dirichlet-to-Neumann map, for sufficiently large time T, to any desired time T'>T. This can be useful to transform the difficult inverse dynamical problem to the one for an elliptic problem. The main difficulty is that we deal with an anisotropic elastic medium.

# **Scientific Cooperations**

# Internal

Dr. Stefen Kindermann

Dr. Lin He

Dr. Eva Sincich

### **External**

Prof. Gen Nakamura (Hokkaido University, Japan)

Prof. Roland Potthast (University of Reading, UK)

Prof. Antonino Morassi (University of Udine, Italy)

Prof. Jijun Liu (South east University, China)

Prof. J. K. Seo (Yonsei University, South Korea)

Prof. Fioralba Kakoni (University of Delaware, USA)

Prof. R. Kress (University of Gottingen, Germany)

Dr. Kenji Shirota (Ibaraki University, Japan)

# Participation at Conferences, Scientific Visits and Talk

## Scientific Visits

- 1. Two working visits to Hokkaido University. The first one in January 2006 for two weeks and the second one in July for two weeks also.
- 2. One week visit to Gottingen University on December 19<sup>th</sup>, 2006.
- 3. One day visit to the Impedance Imaging Research Center (IIRC) of Kyung Hee University (Korea) where the experiments for the MRIT are done and the real data are actually collected.

### Conferences

- 1. Inverse problem reunion conference, Lake Arrowhead, California, USA.
- 2. Conference at Hokkaido University (Sapporo, Japan) Inverse Problems in Applied Sciencestowards breakthrough.

#### Seminar Talks

- 1. Yonsei University, South Korea.
- 2. Ricam, Linz.
- 3. Gottingen, Germany.

### **Publications 2006**

### Appeared or accepted

- 1. G. Nakamura, R. Potthast and M. Sini, Unification of the probe and singular sources methods for the inverse boundary value problem by the no-response test. Communication in PDE, 2006, 31, No. 10: 1505--1528
- 2. N. Honda. G. Nakamura, R. Potthast and M. Sini, The no-response approach and its relation to other sampling methods. Annali di Matematica Pura ed Applicata, 2006. Appeared online.
- 3. C-L. Lin, G. Nakamura and M. Sini, Unique continuation for transversally isotropic dynamical systems and its applications. To appear in SIAM J. Math. Anal.
- 4. A. Morassi, G. Nakamura, K Shirota and M. Sini, A variational approach for the inverse dynamical problem for connected beams. To appear in European Journal of Applied Mathematics
- 5. J. Liu, G. Nakamura, M. Sini, Reconstruction of the shape and surface impedance from acoustic scattering data for arbitrary cylinder. Accepted by SIAM J. Applied. Math.

#### Submitted

- 1. J.J Liu, J. K. Seo, M. Sini and E. J. Woo, On the convergence of the harmonic \$B\_z\$ algorithm in MREIT.
- 2. G. Nakamura and M. Sini, Point-wise determination of the surface impedance for partially coated obstacles from scattering data. The acoustic case.

## Dr. Lin He

## Introduction

Dr. Lin he received her Ph.D. degree from the department of mathematics in University of California, Los Angeles in June 2006. And since July 2006 she is employed in the group of Inverse Problem of RICAM by project F1308. Her main topics of research are inverse problems with PDEs, image processing and computational tomography, and level set methods and its applications.

### **Scientific Achievements 2006**

Since July 2006 Dr. He has carried out research in several directions:

1) Inverse Problems related with Ion Transport

Ion channels are proteins with a hole down their middle that allow ions move across otherwise impermeable cell membranes, thereby controlling many important physiological functions, such as conducting electrical signals down nerves and initiating muscle contraction. Connecting two baths of fixed ionic concentrations, a single ion channel is immersed in hard-sphere fluid with charged ions. In a previous work by M. Burger, R. Eisenberg and H. Engl inverse problems related with ion channels are investigated. The movement of the ions is simplified to be onedimensional and the particle transport is described as friction-limited drift-diffusion with all excess chemical potentials given by the density functional theory of Rosenfeld. Furthermore, the applied local electrostatic potential is modeled through the Poisson-Nernst-Planck (PNP) equations, a system of nonlinear PDEs. They tried to determine one of the structural features of a channel, its permanent charge, from measurements of output currents depending on different input voltages. They also tried to design channels with desirable properties such as particular selectivity properties by using the methods of inverse problems. However, much work still needs to be done. With authors mentioned above and two other Ph.D. students K. Arning and Maria Therese Wolfram, I try to study the linearized PNP models to calibrate the conductance coefficient as a function of structural features of the ion channel, such as the total charges, constraining potentials, length of the channels and etc.

 Reconstruction of the Shape and Surface Impedance from Acoustic Scattering Data by Level Set Methods

The inverse scattering problem is to identify some properties of an obstacle from the information contained in the scattered wave for given incident waves. Introduced by Santosa to the inverse scattering field, the level set method has made a strong contribution to this field. With S. Kindermann, M. Sini, I have been working on to reconstruct the shape of the obstacle with an impedance boundary condition, where the impedance function is unknown. This is based on the work of M. Sini and his collaborators. Due to the non-convex property of this problem, we plan to use their results of the obstacle shape and the surface impedance from some indicator functions as an initial guess for the level set method. This result, directly linked to the far-field pattern by the indicator functions, is obtained by a global method and the computation is fast. Starting from this initial condition, we are expected to converge to the true global minimizer fast.

- 3) Topological Derivatives on Image Segmentation
  - To extend the success of the application of the topological derivative from [3], 7), we modified [2] the rigorous definition of the topological derivative to a discrete one and apply it specifically to solve the active contour Chan-Vese model. This model is a 2-phase piecewise-constant Mumford-Shah segmentation model. It is formulated by a level set method which depends on two constants c1 and c2, where c1 and c2 respectively represent the average intensity of outside and inside the zero level set curve. Therefore we can determine c1 and c2 solely by the level set function. By doing so, we reformulated [2] this model as a shape optimization problem and we applied the topological derivative to this modified Chan-Vese energy functional without the length term. In addition, we used a multiphase level set framework to segment complex images with triple junctions, multiple layers and etc. Our method converges extremely fast (within 3 iterations) and it is more robust than the standard multiphase level set method in terms of initial conditions. To reintroduce the length term we applied a preprocessing step on the given image, thus our algorithm is also insensitive to noise.
- 4) Image Inpainting using the *H\_1* norm of the TV Regularization Image inpainting is the filling in of damaged or missing regions of an image using information from surrounding areas. Relying on a principle that variational denoising, segmentation and in-

painting models all have an underlying notion of what constitutes an image, Chan and Shen have used the total variation based denoising model for inpainting. This model also includes a fidelity term that ensures the solutions close to the given image in non-inpainting regions. The new model can successfully propagate sharp edges into the damaged domain. However, since the use of the TV regularization also puts a penalty on the length of edges, this inpainting model cannot connect contours across very large distances. A different approach to inpainting, based on nonlinear PDE, was proposed by Bertalmio et al.. They propagate the information of an image smoothness estimator, simply defined as the Laplacian of the image, in the direction of isophotes given by the contour of constant grayscale image intensity. In a subsequent work with Bertozzi, they realized that the above nonlinear PDE has intimate connections with two dimensional fluid dynamics problems through the Naiver-Stokes equation. Recently Bertozzi et al. proposed a twostep Cahn-Hilliard model for inpainting of binary images, which is done by choosing two different values of the measure parameter epsilon according to different initial conditions. Based on this two-step Cahn-Hilliard model, M. Burger and C. Schoenlieb and I let the measure parameter epsilon goes to zero. As a direct result, the two-step procedure is not needed. Instead, we obtain a new equation, which is the summation of the gradient flow of the  $H_{-1}$  norm of the TV regularization and the gradient flow of the L 2 norm of the fidelity term. By using the H 1 norm of the TV regularization, there is no penalty on the length of the edges. Therefore, contours can be connected even across large distances. Existence of this new model can be proved and our numerical experiments show the robustness in terms of the initial condition. Most important of all, with the use of TV regularization, we have extended from inpainting of binary images by the Cahn-Hillard model to inpainting of non-texture images by our model.

5) Convergence rates of a Bregman iterative regularization method for image denoising Based on the success of the Bregman distance based iterative regularization method for image denoising, M. Burger, E. Resmerita and I estimate the error in terms of the Bregman distance between the given image f and the iterative minimizer  $u_k$  at the kth iteration. The theoretical results are obtained for the case of f is noise free and/or noisy. Numerical results are also presented to demonstrate the validity of our theorems.

# **Scientific Cooperation 2006**

# **Internal**

• on "Reconstruction of the Shape and Surface Impedance from Acoustic Scattering Data by Level Set Methods", with Dr. Mourad Sini (Inverse Problems group/RICAM) and Dr. Stefan Kindermann (Inverse Problems group/RICAM).

#### External

- on "Inverse Problems related with Ion Transport", with Kattarin Arning (Inverse Problems group/RICAM), Prof. Dr. Martin Burger (Westfaelische Wilhelms Universitaet Muenster, Germany), Prof. Robert Eisenberg (Rush University, USA), Prof. Dr. Heinz Engl (Inverse Problems group/RICAM), Maria Therese Wolfram (Westfaelische Wilhelms Universitaet Muenster, Germany).
- On "Image Inpainting using the *H\_1* norm of the TV Regularization" with Prof. Dr. Martin Burger (Westfaelische Wilhelms Universitaet Muenster, Germany) and Carola Schoenlieb (Vienna University).
- On "Convergence rates of a Bregman iterative regularization method for image denoising" with Prof. Dr. Martin Burger (Westfaelische Wilhelms Universitaet Muenster, Germany) and Dr. Elena Resmerita (Inverse Problems group/ RICAM)
- On "Topological Derivatives on Image Segmentation" with Prof. Stanely Osher (UCLA, USA)

## **Work Before Joining RICAM**

6) MR Image Reconstruction by Using the Iterative Refinement Method and Nonlinear Inverse Scale Space Methods

Many applications in magnetic resonance imaging (MRI) require very short scan time while the image reconstruction can be performed off line. To this end, during the scanning process it is necessary to sample the frequency plane (or k-space) very sparsely. This usually results in image artifacts and/or low signal to noise ratio (SNR). Recently, Candes et al. demonstrated the possibility of recovering the signal from incomplete frequency information for numerical phantoms. Based on these ideas, with my colleagues at Siemens Corporate Research (SCR), I proposed the following method. The method in [4] is based on minimizing a sparse representation of the target signal while maintaining the original sparse frequency samples by enforcing the constraint. However we encountered difficulties in applying the method to raw measurement data which is collected from a multi coils/channels scanner, and has more complicated data structure. The challenges in this problem are that (i) the raw data is not on uniform grids, thus the fast Fourier transform (FFT) is not a good operator to enforce the constraint, (ii) the target signal/image is sometimes not a piecewise constant image which means the total variation or the wavelet transform alone is not a good sparse representation of the target signal/image. To tackle these problems, we used [4] a non-uniform fast Fourier transform (NFFT/NUFFT) and we incorporated the wavelet transform with the total variation as an approximate sparse representation of a piecewise smooth image. In addition, we applied the Bregman iteration to this procedure. The numerical experiments show that the reconstructed MR image quality surpasses the conventional techniques and finer details are obtained after every Bregman iteration. To expedite this Bregman iteration, we further replace [4] the Bregman iteration by the nonlinear inverse scale space method, which can be considered a time-continuous formulation of the Bregman iteration. This inverse scale space method obtains similar results as the Bregman iteration and it is 2-5 times faster.

7) Cooperating Topological Derivatives with the standard level set method on Shape Reconstruction and Optimization Problems

In some applications to structure designs, the level set approach based on the shape sensitivity may get stuck at shapes with fewer holes than the optimal geometry. To address this issue, Burger et al. introduced a modified level set method that includes the topological derivative. This derivative measures the influence of creating a small hole in the interior domain. But in their work, they only applied this new approach to a rather simple example: the minimization of a least squares functional. Thus we generalized this approach to any objective functional by assuming some continuity conditions of the objective functional. Particularly, we applied the topological derivative to the shape derivative based level set methods to maximize the band gaps of photonic crystals and acoustic drum problems. The combination of these two derivatives yields an efficient algorithm which has more flexibility in shape changing and may escape from local optimals.

# Participation at Conferences, Scientific Visits and Talks 2006

### Conferences

- Lin He, MR Image Reconstruction by Using the Iterative Refinement Method and Nonlinear Inverse Scale Space Methods, Mathematics and Image Analysis, University Paris Dauphine, Paris, Sept 2006.
- Lin He, *MR Image Reconstruction by Using the Iterative Refinement Method and Nonlinear Inverse Scale Space Methods*, Variational and PDE Level Set Methods, University of Innsbruck, Obergurgl, Sept 2006.

### Scientific Talks

- Lin He, *Applications and Generalizations of the Iterative Refinement Method*, RICAM, Seminar talk, Oct 2006.
- Lin He, *MR Image Reconstruction by Using the Iterative Refinement Method and Nonlinear Inverse Scale Space Methods*, Laboratory of Mathematics and Applications of Mathematics, University of Bretagne Sud, Vannes, Sept 2006.

### **Publications 2006**

### Published

1. Lin He, Martin Burger, and Stanley Osher. *Iterative total variation regularization with non-quadratic fidelity*. J. of Mathematical Imaging and Vision, 2006.

#### Submitted

- 2. Lin He and Stanley Osher. *Solving the Chan-Vese model by a multiphase level set algorithm based on the topological derivative*. CAM Report 06-56, UCLA, 2006. Submitted.
- 3. Lin He, Chiu-Yen Kao, and Stanley Osher. *Incorporating topological derivatives into shape derivatives based level set methods*. CAM Report 06-44, UCLA, 2006. Accepted by J. Comp. Phys..
- 4. Lin He, Ti-Chiun Chung, Stanley Osher, Tong Fang, and Peter Speier. *MR image reconstruction* by using the iterative refinement method and nonlinear inverse scale space methods. CAM Report 06-35, UCLA, 2006.

# Marie-Therese Wolfram advised by Prof. Martin Burger

## **Scientific Achievements 2006**

During 2006, M.Wolfram worked on inverse problems which arise when identifying doping profiles in semiconductor devices from transient indirect measurements. In particular she considered a special linearization of the drift-diffusion equations, which was introduced by Martin Burger.

She worked on the numerical realization of this method and developed forward and inverse solvers for one and two dimensional problems considering semiconductor devices. In addition, she was able to show existence and uniqueness for such problems. Furthermore, she was working on special numerical methods for mixed systems, such as Uzawa type algorithms.

Additionally, M.Wlfram considered different regularization methods for bipolar semiconductor devices to avoid multiple regularized solutions. This was joint work with Ronny Ramlau, who provided the knowledge about Tikhonov type regularization methods and wavelet analysis.

Another point of interest was the mathematical modelling of ion channels, which can be described by models similar to semiconductor devices. During the last months of her employment, she worked on the development of a numerical solver for 2-D problems, which is still work in progress (and to be continued).

## **Scientific Cooperations**

## Internal

Ronny Ramlau

Martin Burger

### Participation at Conferences, Scientific Visits and Talk

# Conferences

February 7<sup>th</sup>-10<sup>th</sup>, MathMod, Vienna, Austria

June 11<sup>th</sup>-16<sup>th</sup>, IPAM Reunion Conference Inverse Problems, Lake Arrowhead, USA

August 7<sup>th</sup>-12<sup>th</sup>, Summer school on Multiscale Modeling and Applications, Cargese, France

### **Talks**

M.-T. Wolfram, Inverse Dopant Profiling For Highly Doped Semiconductor Devices, Vienna, February 2006

M.-T. Wolfram, Forward and Inverse Solvers for PNP Systems Lake Arrowhead, June 2006

M.-T. Wolfram, Inverse Problems for PNP Systems, Cargese, August 2006

## **Publications 2006**

SFB-report "Semiconductor Inverse Dopant Profiling from Transient Measurements", February 2006

Marie-Therese Wolfram left RICAM and works now with Martin Burger at the University of Münster; she continues to cooperate with RICAM (Lin He, Kattrin Arning, Heinz Engl) on inverse problems for ion channels

### Kattrin Arning advised by Prof. Heinz W. Engl

I started to work as a doctoral student at the Johann Radon Institute for Computational and Applied Mathematics (RICAM) in the middle of September this year.

# Work before joining RICAM

Before coming to the RICAM I finished my diploma in "Technomathematik" (industrial mathematics) at the University of Bremen, Germany, in September 2006. My diploma thesis dealt with the enhancement of rotor models using inverse problems techniques. It was a cooperation with the Siemens AG in Berlin for adjusting mathematical models of large rotor machines on the basis of measured oscillations.

## PhD Program

As a PhD student in the Inverse Problems group at RICAM I am also a member of the FWF doctoral college "Molecular Bioanalytics" (MoBA), an interdisciplinary graduate research program involving the Institutes of Biophysics, Analytical Chemistry, Applied Physics, Organic Chemistry and Theoretical Physics from the Johannes-Kepler-University Linz, RICAM and the Upper Austrian Research. The project I am currently working on deals with inverse problems related to ion channels. Ion channels are proteins that allow certain types of ions to pass through an otherwise impermeable membrane. Thereby they are of great importance to living organisms, as they control vital cell functions. The behavior of ions passing through the channels can be described by a system of nonlinear partial differential equations. Based on current measurements, the goal is to identify certain channel properties, which leads to an ill-posed problem to which regularization techniques have to be applied.

### Participation at Workshops and Scientific Talks

#### Workshops

EMS Summer School "Mathematics in Cell Biology" at the RICAM,11.-22.09.06 Molecular Bioanalytics Summer School, 08.09.06

### Scientific Talks

- "Improvement of Rotor Models" (RICAM, February) diploma colloquium "Improvement of Rotor Models" (University of Bremen, September)
- "Inverse Problems in Ion Channels" (Molecular Bioanalytics Summer School, November)
- "Inverse Problems related to Ion Channels" (group seminar RICAM, November)

# **Scientific Cooperations**

**Internal Cooperations** 

Dr. Lin He

DI Marie-Therese Wolfram

## **External Cooperations**

Prof. Martin Burger (University of Münster)

Prof. Robert S. Eisenberg (Rush University Medical Center, Chicago)

Dr. Martin Regener (Siemens, Germany)

#### Dr. James Lu

#### Scientific Achievements 2006

Work continued on applying inverse methods to molecular biology, consisting of two types: 1) reconstruction of biochemical parameters from time-series experimental data; 2) inference and design of biological systems for observed and desired qualitative dynamical behaviors.

- 1) Progress has been made towards developing methods for performing parameter identification. As analytical extensions to the SBML ODE Solver Library (Solid, developed in collaboration with the Theoretical Biochemistry Group in Vienna), API for solving forward and adjoint sensitivity equations have been developed, allowing for easy usage of SOSLib within general gradient-based optimization libraries. In particular, SOSLib has been used in conjunction with the interior point optimization library IPOPT and applied to a suite of benchmark problems. Parameter identification has been successfully performed using sparsely-promoting l\_p penalty as the regularization term. Currently in progress is the concatenation of scatter search (as a globalization strategy) with local, gradient-based method.
- 2) Inverse dynamical analysis has been proposed as a methodology that can be applied throughout the experiment-model-experiment loop, from the initial model-building to the proposal of new experiments. In addition, once a model has been developed that sufficiently captures the properties of the biological system of interest, the method can be used to design various bifurcation phenotypes that exhibit certain dynamical properties. The overall process consists of two main steps, namely inverse eigenvalue and inverse bifurcation analyses. The former step is used to probe the possibility of the system to exhibit desired qualitative behaviors and characterize the resulting parameter combinations. The latter is used to identify mechanisms in the model that can give rise to a set of bifurcation phenotypes, which can then be used in the iterative loop of the experiment-model-experiment process; if the model sufficiently captures the experimental observations, inverse bifurcation analysis can additionally be used to design the biological system to the desired dynamical characteristics. To infer 'influential' parameters and mechanisms, sparsity-promoting 1 p penalty term has been used. While a theory for the regularization properties of such a penalty term is so far lacking for the case p<1, numerical results are encouraging for models with dozens of parameters: in combination with hierarchical strategies, sparsity penalty has yielded useful insight into understanding the regulatory mechanisms of various biological systems.

## **Scientific Cooperations**

#### Internal

Prof. Heinz W. Engl, Stefan Mueller, Philipp Kügler

### External

Prof. Peter Schuster, Rainer Machne', Lukas Endler, Stefanie Widder, Christoph Flamm, Theoretical Biochemistry Group, University of Vienna.

# Participation at Conferences, Scientific Visits and Talk

### Conferences

SFB Status Semilar, April 2006, Strobl, Austria.

IPAM Workshop on Systems Biology and Molecular Modeling, May 2006, UCLA, California, USA. IPAM Inverse Problems Reunion Conference, June 2006, Lake Arrowhead, California, USA.

Applied Dynamical Systems Workshop, June 2006, Ghent, Belgium.

International Conference on Systems Biology, October 2006, Yokohama, Japan.

### **Publications 2006**

### Appeared

R. Machne', A. Finney, S. Mueller, J. Lu, C. Flamm: The SBML ODE Solver Library: a native API for symbolic and fast numerical analysis of reaction networks, Bioinformatics (3), 2006.

- J. Lu, H. W. Engl, P. Schuster: Inverse bifurcation analysis: applications to simple gene systems, Algorithms for Molecular Biology 1 (11), 2006.
- J. Lu, H. W. Engl, R. Machne', P. Schuster: Inverse bifurcation analysis of a model for the mammalian G1/S regulatory module. Proceedings for Bioinformatics in Research and Development '07, Lecture Notes in Bioinformatics, Springer-Verlag, 2007.

### Submitted

Studying evolution of the bifurcation phenotype: inverse dynamical analysis and phylogenic reconstruction of the GATA transcription factor networks, working paper.

# Dr. Stefan Müller

### **Scientific Achievements 2006**

Stefan Mueller continued his work on the dynamics of cellular networks using both forward and inverse methods. His studies included (i) parameter identification in biochemical reaction networks, (ii) bifurcation analysis in gene regulatory networks, (iii) minimal cell models, and (iv) chemical reaction kinetics

#### Parameter identification:

In cooperation with James Lu, Stefan Mueller extended the SBML ODE Solver Library (SOSlib) with the capability to solve adjoint equations. Gradient based parameter identification methods using adjoint equations are more efficient than those using finite differences or standard linearization. In addition to local optimization methods (calling the forward and adjoint solvers of SOSlib), global optimization methods have been implemented. In particular, Stefan Mueller implemented an evolutionary algorithm called scatter search. In contrast to other evolutionary methods like genetic algorithms, scatter search is founded on the premise that systematic designs and methods for creating new solutions show significant benefits beyond pure randomization. It uses strategies for search diversification and intensification that have proved effective in a variety of optimization problems.

# Bifurcation analysis:

Stefan Mueller continued with the bifurcation analysis of simple gene regulatory systems. In particular, he studied GATA-type transcription factor systems with a focus on the cascade of GATA factors in *C. elegans* endoderm specification. Starting from a well-established model of a single autoactivating gene with a hysteretic (bistable) bifurcation phenotype, he investigated some plausible

minimal evolutionary scenarios for creating more complex GATA factor networks by gene and genome duplication events. In cooperation with Rainer Machne, he showed that the *C. elegans* cascade could in principle arise through a minimal evolutionary scenario involving two different duplication events, as well as only two or three (point) mutations.

### Minimal cells:

In cooperation with Christoph Flamm and Lukas Endler, Stefan Mueller developed a self-consistent minimal cell model with a physically motivated scheme for molecular interaction. The genetic and metabolic reaction network of the cell is modeled by nonlinear ODEs, which are derived from biochemical kinetics. The strategy behind this modeling approach is to keep the model sufficiently simple in order to be able to perform studies on evolutionary optimization in populations of cells. At the same time the model should be complex enough to handle the basic features of genetic control of metabolism and coupling to environmental factors.

### Chemical Reactions:

Stefan Mueller improved the flow reactor model of the chlorine dioxide-iodide reaction system. Starting from an existing ODE model, he eliminated rapid equilibria using methods from singular perturbation theory.

## **Scientific Cooperations**

### Internal

Cooperation with Prof. Heinz Engl and Dr. Philipp Kuegler on parameter identification in biochemical systems, and with Dr. James Lu on bifurcation analysis in gene regulatory networks

### External

Cooperation with Prof. Josef Hofbauer (Department of Mathematics, University College London) on bifurcation analysis in gene regulatory networks

Cooperation with Mag. Rainer Machne (Institute for Theoretical Chemistry, University of Vienna) on evolutionary scenarios for gene regulatory networks

Cooperation with Dr. Christoph Flamm and Mag. Lukas Endler (Institute for Theoretical Chemistry, University of Vienna) on minimal cell models

Cooperation with Mag. Erwin Gaubitzer (Institute for Theoretical Chemistry, University of Vienna) on a mathematical model of the chlorine dioxide-iodide reaction

# Participation at Conferences, Scientific Visits and Talks

### Talks

Deterministic and Stochastic Models of (Bio-)chemical Reaction Networks, SFB Status Seminar, Strobl, April 22-24, 2006

Forward and inverse bifurcation analysis of a synthetic gene regulatory network (the repressilator), International Conference on Systems Biology, Yokohama, October 9-13, 2006

### **Publications**

### Appeared

S. Müller, J. Hofbauer, C. Flamm, L. Endler, S. Widder, P. Schuster, A Generalized Model of the Repressilator, Journal of Mathematical Biology, 53(6):905-937, 2006

R. Machne, A. Finney, S. Müller, J. Lu, C. Flamm, The SBML ODE Solver Library: a native API for symbolic and fast numerical analysis of reaction networks, Bioinformatics, 22(11):1406-7, 2006

# **Submitted**

C. Flamm, L. Endler, S. Müller, S. Widder, P. Schuster, A minimal and self-consistent in silico cell model based on macromolecular interactions, Phil. Trans. R. Soc. B, Towards the artificial cell

#### Dr. Stefan Kindermann

Stefan Kindermann was working as a Research Scientist for the Group "Inverse Problems" at RICAM from September 2005 until September, 31<sup>st</sup> 2006. His main research interest are in the fields of parameter identification problems, the level set method and PDE methods for image processing. He is now an Assistant Professor at the Industrial Mathematics Institute of JKU and still closely coopeating with RICAM.

## **Scientific Achievements 2006**

Several research projects have been started or continued in 2006:

# 1. Inverse Problems and Stochastics:

This collaboration with A. Hofinger (RICAM) was an extension of the research on regularization theory for stochastic problems. In [4] we extended some results for ill-posed problems with random parameter to nonlinear problems. This work is a continuation of previous research using probabilistic metrics for inverse stochastic problems by Hofinger and of the results of Engl, Hofinger and Kindermann.

## 2. Parameter identification in a random environment:

This is a cooperation together with V. Capasso (Univ. of Milan) and H. Engl. In this work we considered identification problems in random environments, for instance, for crystallization processes. In a random environment the crystallization procedure is governed by a random process, which itself depends on random parameters ("double stochasticity"). The aim of this collaboration was to find regularization procedures for identifying this random parameter. While the corresponding singly stochastic inverse problem can be considered a deterministic problem by a suitable averaging, the doubly stochastic case leads to a stochastic inverse problem. For this we could employ the regularization theory for stochastic inverse problem (see the previous paragraph) to show that nonlinear Tikhonov regularization is a convergent method for this identification problem. Also sufficient conditions for convergence rates can be formulated in this case. This work is still in progress, a preprint will be published soon.

# 3. Inverse problems in finance:

In a joint cooperation with the RICAM-finance group we continued previous research on identification problems in option pricing. Some expertise in this field has already been gained at the RICAM by work of H. Engl and H. Egger on the identification of the volatility in Black-Scholes model. In this cooperation we investigated the used of regularization theory to a more general asset-price model: the local Levy-model. There we used nonlinear Tikhonov regularization to identify the local speed function for option prices. The forward problem involves a parabolic partial integro-differential equation with the speed function as unknown parameter. We could prove well-posedness of the forward problem and convergence of nonlinear Tikhonov regularization for the inverse problem. Furthermore, a detailed analysis of the ill-posedness shows that the local Levy problem is more ill-posed than the corresponding Black-Scholes identification problem. This is a cooperation with P. Mayer, H. J. Albrecher (RICAM finance group leader) and H. Engl, still in progress. Also for this work a preprint will be published soon.

# 4. Regularization for interface problems

In an cooperation with R. Ramlau (RICAM) we were interested in developing new methods and algorithms for inverse interface problems [3]. This research combines two fields: the theory of surrogate functionals coming from regularization theory and the method of exact relaxation coming from image processing. As a result we developed an algorithm for interface problems, based on thresholding. This algorithm can be used as an alternative to level-set methods: it is faster and easier to implement.

# 5. Dynamic Programming and Regularization

We were continuing the cooperation with A. Leitao (F. Univ. Santa Catharina, Florianopolis) on regularization using dynamic programming. We extended the previous theory to time dependent operators [2].

# 6. Inverse scattering Problems:

Recently, an internal cooperation with M. Sini and L. He (both RICAM) has been started on using the level-set method for inverse scattering problems with general impedance boundary condition. This is work in progress.

# **Scientific Cooperations**

#### Internal

- with Ronny Ramlau on inverse interface problems (publ. submitted)
- with Andreas Hofinger on nonlinear stochastic inverse problems (publ. submitted)
- with Phillipp Mayer, Hansjörg Albrecher and Heinz Engl on inverse problems in finance (in progress)
- with Lin He and Mourad Sini (in progress)

#### <u>External</u>

- with Vincenzo Capasso and Heinz Engl on identification in random environments (in progress)
- with Antonio Leitao on regularization with dynamic programming (publ. submitted)

### Participation at Conferences, Scientific Visits and Talk

### Conferences

May 2006, SIAM Conference on Imaging Science, Minneapolis, MN, US; contributed talk on "Saddle point formulation for a cartoon-texture decomposition"

May/June 2006, Inverse Problems: Modeling and Simulation, Fethiye Turkey; 2 contributed talks on "Regularization by dynamic programming" "Surrogate functionals and thresholding for inverse problems"

# Scientific Visits and Talks

March, 2006, Visit to Michael Hintermüller, Karl-Franzens-University Graz, talk on "On a cartoon-texture decomposition for image processing"

#### **Publications 2006**

# **Appeared**

[1] S. Kindermann, S. Osher, J. Xu, "Denoising by BV-Duality", J. Sci. Comp. 28, Nr 2/3, 411-444, 2006

### Submitted

- [2] S. Kindermann, A. Leitao, "Regularization by dynamic programming", submitted to J. Inv and Illposed Probl.
- [3] S. Kindermann, R. Ramlau, "Surrogate functionals and thresholding for inverse interface problems" submitted to J. Inv. and Ill-posed Probl.
- [4] A. Hofinger, S. Kindermann, "Assessing Uncertainty in Nonlinear Inverse Problems with the Metric of Ky Fan", SFB-Report 2006-31, submitted to Inv. Probl.

# Long-term visitor at RICAM working mainly with the Inverse Problems Group:

# Prof. Vincenzo Capasso, Milano (Long-term visitor)

March 1- June 30, 2006

## **Reasearch Topics**

## **Theory**

- Spatially structured stochastic processes, and related
- Statistical and Inverse Problems
- Stochastic Geometry

## **Applications**

- Social behaviour of swarms,
- Birth-and-growth processes, in material science and medicine.

During my period at RICAM I have had the possibility to complete research work initiated during previous contacts with the Linz scintific system, and during my stay at the Vienna University during October 2005-January 2006, in collaboration with Martin Burger from RICAM and the Institute fuer Industriemathematik, of the Johannes Kepler Universitaet, and collaborators and PhD students from my own university in Milan, during their visits at RICAM.

At RICAM I have initiated a new research field, under the leadership of Professor Heinz Engl, and in collaboration with Dr Stephan Kinderman, on Inverse problems in presence of uncertainty, by extending previous work by them, and by Engl, Burger and myself, to the case of doubly stochastic spatially structured systems. This collaboration is still ongoing and we expect to have first readable results by the end of June. The collaboration will continue via email and exchange of visits; a further stay at RI-CAM is already planned in occasion of the EMS Summer School on "Mathematics in Molecular Cell Biology" which will take place at RICAM in Linz, during September 9-23, 2006. This school has been organized also by myself, together with Martin Burger (RICAM and Johannes Kepler University, Linz), Yasmin Dolak-Struss (University Vienna) and Christian Schmeiser (University Vienna and RICAM).

I have also contributed in designing and planning the RICAM Special Semester on Quantitative Biology Analyzed by Mathematical Methods, to be held during 1 October 2007 – January 2008, within which I have been given responsibility of the topic "Pattern Formation and Functional Morphology" together with R.Anderssen.

I have participated in the seminar activity of RICAM, and delivered myself a talk about my current interests, and have had the opportunity to participate in discussions on current research carried by members of the Institute. As a documentation of my activity at RICAM, for which I have always acknowledged my temporary affiliation to RICAM, a list of papers is provided below, together with a list of invited talks.

Hereby I wish to express all my gratitude to the RICAM Institute, and in particular to its Director, Professor Heinz Engl for offering me such a fruitful period of scientific activity.

### **Publications**

- 1. On an aggregation model with long and short range interactions (in collaboration with M. Burger and D. Morale) Nonlinear Analysis; RWA (2006). In press.
- 2. Mesoscale averaging of nucleation and growth models. (in collaboration with M. Burger and L.Pizzocchero) SIAM J. Multiscale Modeling and Simulation, (2006). In press.
- 3. Some remarks on the continuity of random closed sets (in collaboration with E. Villa) In "S4G Stereology, Spatial Statistics, Stochastic Geometry" (V. Benes, Editor),2006. In press.
- 4. On mean geometric densities arising in inhomogeneous birth-and-growth processes (in collaboration with E. Villa) In "S4G Stereology, Spatial Statistics, Stochastic Geometry" (V. Benes, Editor),2006. In press.
- 5. A Stochastic Model for Price Herding: a Method for Estimation and Prediction. (in collaboration with A. Bianchi and D. Morale). (2006) Submitted.
- 6. Long time behavior of a system of stochastic differential equations modelling aggregation in population dynamics. (In collaboration with Daniela Morale and Matteo Ortisi) (2006). Submitted.
- 7. On the approximation of geometric densities of random closed sets. (In collaboration with Ambrosio, L. and Villa, E.) RICAM Report N. 2006-14,Linz,Austria (2006).2
- 8. On the geometric densities of random closed sets, 2005. (In collaboration with Villa, E.) RICAM Report 13/2006, Linz, Austria.
- 9. An extension of the Kolmogorov-Avrami formula to inhomogeneous birthand-growth processes. (In collaboration with M.Burger and A. Micheletti) Submitted (2006).
- 10. Densities of n-facets of incomplete Johnson.Mehl tessellations generated by inhomogeneous birth-and-growth processes. (In collaboration with M.Burger and A. Micheletti) Submitted (2006).
- 11. On the stochastic geometry of birth-and-growth processes. Application to Material Science, Biology and Medicine. Proceedings of the International Conference on Modelling, Simulation and Optimization of Complex Systems, Hanoi, Vietnam (2006). In preparation.

#### **Invited talks**

- 1. Multiscale Modelling of Random Geometric Birth-and-Growth Processes, for Multi-Physics Problems Occurring in Material Sciences And Biomedicine. (Main Invited Lecture) (Invited Main Lecture) International Conference on Modelling, Simulation and Optimization of Complex Systems, Hanoi, Vietnam, March 6-10, 2006
- 2. Random Geometric Birth-and-Growth Processes -Application to Material Sciences and Biomedicine RICAM Group Seminar on Inverse Problems March 20, 2006
- 3. Multiscale Modelling of Random Geometric Birth-and-Growth Processes: Application to Material Sciences And Biomedicine. Laboratoire "Jacques Luis Lions", Universit Pierre e Marie Curie (Paris VI) Paris, March 26, 2006.
- 4. On the stochastic geometry of birth-and-growth processes Mathematisches Kolloquium TU Graz, Austria, May 12, 2006
- 5. On the Evolution Equations of Mean Geometric Densities for a Class of Space and Time Inhomogeneous Stochastic Birth-and-Growth Processes. Application to Material Science and Biomedicine. (Main Invited Lecture) 6th International Conference on Stereology, Spatial Statistics and Stochastic Geometry Prague, June 26-29, 2006.

# GROUP "SYMBOLIC COMPUTATION"

# **Group Leaders:**

O.Univ.-Prof. Dr.phil. DDr.h.c. Bruno Buchberger

Ao. Univ.-Prof. Dr. Josef Schicho

#### Structure of the Area

The Symbolic Computation Area of RICAM consists of two working groups:

Working Group on Computational Logic ("Theorema"):

Group leader: Professor Bruno Buchberger Working Group on Computational Algebra: Group leader: Professor Josef Schicho

# Researchers funded via ÖAW/Upper Austrian government funds:

Dr. Martin Giese

Dr. Oliver Labs

Dr. Florina Piroi

Dr. Markus Rosenkranz

Ao. Univ.-Prof. Dr. Josef Schicho

Mag. Alexander Zapletal

# Researchers externally funded:

Msc. Michael Barton Dipl.Inf. Tobias Beck

Dr. Pavel Chalmoviansky

Msc. Jose-Manuel Garcia-Vallinas

Msc. Niels Lubbes Msc. Brian Moore Msc. Jana Pilnikova Dr. Georg Regensburger

# Introduction by Group Leader Prof. Josef Schicho

In the first half of the year 2006, the research in the group "Symbolic Computation" has been centered around the special semester of Groebner bases. B. Buchberger, who was co-leader of the group until September, was the organizer and crystallization point of most interactions (discussions, spontaneous workshops, etc.) All other group members participated on the workshops, many gave invited or contributed talks. As an example, the solution of parts of the Casas-Alvero conjecture on univariate polynomials by two group members and two guests of the special semester should be mentioned (details see sections on Labs and Schicho).

In autumn, two quite successful PhD theses have been defended. The thesis of J. Pilnikova contains the development of a new method for solving certain types of Diophantine equations, based on Lie algebras. This method was used for solving the last unresolved cases in the problem of parametrizing rational surfaces over Q. The thesis of T. Beck contains not only a sparse version of algorithms for curve parametrization, but the rudiments for an algorithm for surface parametrization which -- according to first experiments - is expected to be much faster than existing methods.

Three subprojects of the special research area SFB13 have been furthered mainly (but not exclusively) by members of the symbolic group: subproject 1303, where Beck, Pilnikova, and Schicho made various contributions; subproject 1315, with contributions by Barton, Chalmoviansky, and Kapl; and subproject 1322, with the achievements of key results by Regensburger and Rosenkranz (details can be found in the sections describing the achievements of the individual researchers).

# Alexander Zapletal advised by Prof. Bruno Buchberger

#### Scientific Achievements 2006

From February until July 2006 the "Special Semester on Gröbner Bases and Related Methods 2006", jointly organized by RICAM and RISC (Research Institute for Symbolic Computation), took place at RICAM. During this time A. Zapletal was the local organizer and responsible for the daily run of the workshops. For details on the special semester, see the according section in this report.

In the frame of preparing the special semester a database of papers on Gröbner bases was built up. This bibliography was initiated by B. Buchberger and is being built up under his direction. The manof aging editor of the bibliography and the developer the web-interface (http://www.ricam.oeaw.ac.at/Groebner-Bases-Bibliography/) is his scientific assistant A. Zapletal. The database was presented to all visitors of the special semester (approx. 300) and is therefore well known in the community of scientists who work with Gröbner bases.

Additionally, A. Zapletal started to work together with members of the computational logic group at RICAM and RISC on a redesign of the Theorema software system. This is done in a workgroup which is directed by B. Buchberger, who is also the inventor of the Theorema system.

# **Scientific Cooperations**

#### External

Close cooperation with the Research Institute for Symbolic Computation (RISC), Johannes Kepler University of Linz. A. Zapletal participates in the weekly Theorema seminar and also in other seminars which are related to the redesign of the Theorema system.

## Michael Barton advised by Prof. Josef Schicho

### **Scientific Achievements**

Michael Barton is a PhD student of Prof. Karger (Univ. Prag), who spent part of his studying time at RICAM in the frame of the SFB project.

Together with B. Jüttler (Univ. Linz), he generalized the method of Bezier clipping for solving polynomial equations. This has lead to a method with better convergence in singular cases (quadratic Bezier clipping) and to a method for bivariate systems.

He left RICAM in September.

# **Scientific Cooperations**

#### Internal

B. Moore implemented parts of his method.

### External

B. Juettler was his partner in the investigation of Bezier clipping methods.

### Conferences

Sixth International Conference on Curves and Surfaces, 29.6 - 5.7. 2006, Avignon, France: Computing roots of polynomials by quadratic clipping.

26th Conference on Geometry and Computer Graphics, September 11 - 15, 2006, Nové Město na Moravě, Czech Republic: Bivariate linear clipping.

#### Scientific visits and talks

- Workshop on Algebraic Spline Curves and Surfaces, Mai 16-19, 2006, Eger, Hungary:
- Bezier clipping via degree reduction
- SFB meeting, Strobl, April 20-22: Bezier clipping via degree reduction
- FSP meeting, Strobl, June 19-22: Bezier clipping via degree reduction

#### **Publications 2006**

Journal:

### Submitted:

M. Barton, B. Juettler: Computing roots of polynomials by quadratic clipping.

**Procedings:** 

### Accepted:

M. Barton, B. Juettler: Bivariate linear clipping, proceedings of 26th Conference on Geometry and Computer Graphics, September 11 - 15, 2006, Nové Město na Moravě, Czech Republic.

## Brian Moore advised by Prof. Josef Schicho

He joined RICAM in July in order to work in the SFB project 1303.

### Work before

After finishing is master thesis in applied mathematics in Canada, he has worked for several years in research and development in the field of robotics at the Canadian Space Agency. During this period, he has worked mainly on the modeling and simulation of complex mechanical structures used to support robotics research, space operations and astronaut training.

# **Scientific cooperation**

# **External**

There is a cooperation with Bert Juettler (Univ. Linz) and Michael Barton (Univ. Prag) for the development of a Bezier clipping method for the computation of the real roots of two bivariate polynomials.

He initiated a contact with Clement Gosselin, an established expert in the field of parallel robotics at Laval University. A project description was written and a meeting took place in Canada to describe

possible approaches to solve the problem of the classification of family of dynamically balanced parallel robots.

An agreement was signed with the Canadian Space Agency in order to use their robotic modeling and simulation system and the possibility to develop new components.

# Workshops

- "Polynomial equations solving in the context of parallel mechanisms", Workshop on algebraic geometry (Obergurgl, Austria, September 2006).
- "Robotics and sum of squares", Workshop on Algebraic Spline Curves and Surfaces (Eger, Hungary, May 2006).

### Scientific visit

- Visit of Herwig Haueser group and Manfred Husty at the University of Innsbruck to discuss the problem of the forward kinematics of parallel mechanisms.
- Visit of Clement Gosselin, leader of the robotic group at Laval University in Canada to discuss
  possible approaches to the problem of the classification of dynamically balanced parallel mechanisms.

# Dr. Florina Piroi

### **Scientific Achievements**

She did some research in the area of quantum algorithms. Together with A. Winterhof, she studied and quantum algorithm in coding theory (period reconstruction). She also worked on the Theorema system together with B. Buchberger and the Theorema group.

She is currently on childcare (since October 2006).

## **Scientific Cooperations**

## Internal

A. Winterhof: quantum algorithms in conding theory.

### External

B. Buchberger, Theorema group.

Participation at conferences, scientific visits and talks

### Conferences

Formal Groebner Basis Theory, Special semester on Groebner bases (RICAM): Organizational Tools for Formal Mathematics in Theorema

# **Publications 2006**

# Journal papers

1. B. Buchberger, A. Craciun, T. Jebelean, L. Kovacs, T. Kutsia, K. Nakagawa, F. Piroi, N. Popov, J. Robu, M. Rosenkranz, W. Windsteiger. Theorema: Towards Computer-Aided Mathematical Theory Exploration. Journal of Applied Logic, pp. 470-504. 2006.

# **Proceedings**

2. Florina Piroi and Arne Winterhof. "Quantum Period Reconstruction of Binary Sequences". In Marc P. C. Fossorier and Hideki Imai and Shu Lin and Alain Poli, editors. Applied Algebra, Algebraic Algorithms and Error-Correcting Codes, 16th International Symposium, AAECC-16, Las Vegas, NV, USA, February 20-24, 2006, Proceedings. LNCS vol. 3857. Springer.

# Dr. Georg Regensburger

### **Scientific Achievements 2006**

The focal point of G. Regensburger's work was on boundary problems within the SFB project F1322 "Computer Algebra for Pure and Applied Functional Analysis". With M. Rosenkranz he developed a framework for multiplying and factorizing linear ordinary boundary problems and the corresponding Green's operators [5]. Two publications, emphasizing the theoretical and algorithmic aspects, respectively, are in preparation.

He also continued successfully his research on nonlinear first-order ordinary boundary problems and the max-plus algebra, where the addition is replaced by the maximum and the multiplication by the sum [2,6,7]. The implementation of the method for constructing generalized solutions via max-plus interpolation for the computer algebra system Maple was revised and a publication is in preparation. Moreover, G. Regensburger worked, in particular within the Special Semester on Gröbner Bases, on applications of Gröbner bases to the construction of parametrized wavelets [4,9] and with Prof. Josef Schicho to symbolic computation in Witt rings [3].

## **Scientific Cooperations**

#### Internal

G. Regensburger works with Dr. M. Rosenkranz in the SFB project F1322 led by Prof. B. Buchberger and Prof. H. W. Engl. He worked with Prof. J. Schicho on symbolic computation for Witt rings [3].

### External

The cooperation with Prof. M. Burger (now Univ. of Münster) on nonlinear BVPs and max-plus algebra continued. G. Regensburger edits with Prof. Alan Park (Korea Institute for Advanced Study) the proceedings of the workshop "Gröbner Bases in Control Theory and Signal Processing" within the Special Semester on Gröbner Bases.

## Participation at Conferences, Scientific Visits and Talks

#### Conferences

- [1] ICM, International Congress of Mathematicians, Madrid, Spain, August 22 30.
- [2] Mini-Program on the Algebraic Theory of Differential Equations, Heriot-Watt University, Edinburgh, Scotland, July 31 to August 11.
- "Boundary value problems for nonlinear first-order ODEs constructing generalized solutions via the max-plus algebra"
- [3] Special Semester on Gröbner Bases, Workshop D2: Gröbner Bases in Symbolic Analysis, RISC, Hagenberg, RICAM, Linz, May 08 May 17.
- With J. Schicho: "Gröbner Bases and Identities in Witt Rings"

[4] Special Semester on Gröbner Bases, Workshop D3: Gröbner Bases in Control Theory and Signal Processing, RICAM, Linz, Austria, May 18-May 19.

"Parametrizing orthonormal wavelets by moments".

[5] SFB Statusseminar, Strobl, Austria, April 20 – 22.

With M. Rosenkranz: "Factorization and Division in the Realmof Linear Ordinary BVPs".

[6] "Nonlinear first-order ordinary BVPs via Max-plus Interpolation".

[7] GAMM, Berlin, Germany, March 27 – 31.

"Max-plus Linear Algebra and Nonlinear Ordinary BVPs".

[8] Special Semester on Gröbner Bases, RICAM, Linz, Austria:

Workshop C1: Formal Gröbner Bases Theory, March 06 – March 10.

Workshop B2: Efficient Computation of Gröbner Bases, February 27 – March 03.

Workshop B1: Approximate Commutative Algebra, February 20 – February 24.

Workshop A: Gröbner Bases Theory and Applications in Algebraic Geometry, February 06 – February 17.

## **Publications 2006**

#### Submitted

[9] G. Regensburger, "Parametrizing compactly supported orthonormal wavelets by discrete moments, Applicable Algebra in Engineering, Communication and Computing", to appear, 2006.

#### Dr. Martin Giese

# **Scientific Achievements 2006**

Most mathematical texts contain a certain amount of (almost always implicit) meta-mathematical manipulation, where the mathematical symbols are not treated as representing the mathematical entities that are at the center of attention, but simply as symbols, i.e. syntactically. Reasoning about the syntax of a theory instead of inside theory itself is a meta-mathematical activity which can be a tremendously powerful tool for the mathematician.

Based on his preliminary studies in 2005, M. Giese has been collaborating with B. Buchberger and T. Kutsia at the Research Institute for Symbolic Computation (RISC) of the University of Linz, as well as M. Rosenkranz at RICAM to deepen the understanding of the reflection principles necessary to put such meta-mathematical reasoning on a sound formal basis. He has worked on the extension and improvement of a prototypical implementation which now allows to express usual mathematical algorithms and facts on one hand, and algorithms for e.g. proof search and meta-mathematical facts about those in a common framework. M. Giese has presented his findings in this area at two international workshops [1,2], as well as numerous internal seminars.

M. Giese is participating intensely in the process of re-designing the Theorema system currently undertaken at RISC, by contributing to several series of seminars on reflection, on the mechanical construction and representation of mathematical proofs, and on the efficient implementation of logically specified programs through a translation to Java.

Another line of research concerns an extension of analytic free variable tableaux and sequent calculi: standard versions of these formalisms and their corresponding completeness proofs tend to use non-destructive rules. For efficient implementations, destructive rules are preferable, but it is hard to reason about such calculi using the standard techniques. M. Giese was able to adapt the idea of

"saturation up to redundancy"—commonly used in a resolution setting—to analytic calculi and published his results [6].

Furthermore, M. Giese has written an introductory text on first-order logic with subtyping and on formal reasoning for this logic, which is going to appear as a chapter of the upcoming book about the KeY system [8]. He has also published an extended account on some earlier work on equality handling in free variable tableaux [7].

### **Scientific Cooperations**

### External

Cooperation with B. Buchberger, T. Kutsia and other RISC members, concerning the reflection mechanism, questions of the design of a mathematical proof assistant, and generation of Java code.

Cooperation with members of the KeY project at University of Karlsruhe, Germany, University of Koblenz, Germany, and Chalmers University, Göteborg, Sweden in the preparation of the upcoming book about the KeY system [8].

Cooperation with J. Kiniry, University College Dublin, Ireland, in the preparation of a joint project proposal.

### Participation at Conferences, Scientific Visits and Talks

- 1. Talk on "Practical Reflection for Formal Mathematics in Theorema", Workshop on Formal Gröbner Bases Theory, Linz, Austria, March 2006.
- 2. Invited talk "Practical Reflection for Formal Mathematics in Theorema", SCORE Workshop on Proving and Solving, Aizu-Wakamatsu, Japan, March 2006.
- 3. Talk on "A Logic with Subtypes to talk about Java Objects", Systems Research Group, University College Dublin, Ireland, August 2006.
- 4. Invited talk on "A Logic with Subtypes to talk about Java Objects", ESF Exploratory Workshop: Challenges in Java Program Verification, Nijmegen, The Netherlands, October 2006.
- 5. Panelist at Panel Discussion of Intl. Workshop on Implementation of Logics, Phnom Penh, Cambodia, November 2006.

### **Publications 2006**

### **Appeared**

- 1. M. Giese, Saturation up to Redundancy for Tableau and Sequent Calculi, Logic for Programming, Artificial Intelligence, and Reasoning, LPAR06, Springer, LNCS 4246, pages 182–196, 2006.
- 2. M. Giese, Superposition-based Equality Handling for Analytic Tableaux, Journal of Automated Reasoning, appeared online first 2006.

#### To Appear

1. M. Giese, Chapter on First-Order Logic in: Verification of Object-Oriented Software—The KeY Approach, Springer, Lecture Notes in Computer Science, 2006, to appear.

### Dr. Janka Pilnikova

### **Scientific achievements**

Together with W. de Graaf (Univ. Trento), M. Harrison (Univ. Sydney), and J. Schicho (RICAM), she adapted and extended the Lie algebra method for solving (certain types of) Diophantine equations to

the case of Del Pezzo surfaces of degree 6 and 8. The solution of these cases completes the algorithm for surface parameterization over the field of rational numbers, a major project initialized by the solution of the conical case by Schicho in 2000.

She also gave an algorithm for splitting a central simple algebra of degree 4 (the degree 3 case is related to Del Pezzo cases of degree 9 and was solved by her last year).

In October, P. defended her PhD thesis entitled "Parametrizing algebraic varieties using Lie algebras", supervised by Josef Schicho.

After getting a position at Comenius University in Bratislava, Slovakia, she left RICAM in December 2006.

### **Scientific cooperations**

### Internal

J. Schicho was her PhD advisor.

### External

Willem de Graaf, University of Trento, Italy, was partner in the development of the Lie algebra method.

#### Conferences

"Splitting central simple algebras of degree 4", Rhine Workshop on Computer Algebra, March 16-17, 2006, Basel, Switzerland

"Interactions of Geometry, Algebra and Number Theory", Workshop on Algebraic Spline Curves and Surfaces, May 17-18, 2006, Eger, Hungary

"Schubert calculus",

Workshop on Algebraic Geometry and Singularities, September 22-25, 2006, Obergurgl, Austria

# Scientific visits and talks

"On Lie algebras arising from Schubert varieties", seminar talk, October 18, 2006, University of Trento, Italy

### **Publications 2006**

# Journal publications

### **Appeared**

W.A. de Graaf, M. Harrison, J. Pilnikova, J. Schicho, A Lie Algebra Method for Rational Parametrization of Severi-Brauer Surfaces, Journal of Algebra, vol. 303, No. 2, 514-529, 2006

#### <u>Accepted</u>

J. Pilnikova, Splitting a central simple algebra of degree 4 over the rational numbers

#### Submitted

W.A. de Graaf, J. Pilnikova, J. Schicho, Parametrizing Del Pezzo surfaces of degree 8 using Lie Algebras

### José Manuel García Vallinas advised by Prof. Josef Schicho

He works in the SFB project 1303 since August 2005.

#### **Scientific Achievements 2006**

Originally, G.-V. worked on the problem of constructing root parametrizations for algebraic curves. This problem, however, turned out to have unexpected difficulties, so he decided to change the topic and to work on numeric-symbolic problems in computational algebraic geometry.

#### Participation at Conferences, Scientific Visits and Talk

### Conferences

Workshop on algebraic geometry (Obergurgl, Austria, September 2006).

International Congress of Mathematics (Madrid, Spain, August 2006).

Workshop on Algebraic Spline Curves and Surfaces (Eger, Hungary, May 2006).

Groebner Special Semester (Linz, Austria, Febrery/March 2006).

Winter School on Algebraic Geometry (Barcelona, Spain, January 2006).

# Scientific Talks

- "Algebraic Geometry and Clusterings", Workshop on algebraic geometry (Obergurgl, Austria, September 2006).
- "Roots Parametrization", Workshop on Algebraic Spline Curves and Surfaces (Eger, Hungary, May 2006).

"Roots Parametrization", Winter School on Algebraic Geometry (Barcelona, Spain, January 2006).

### Prof. Josef Schicho

### Scientific Achievements 2006

Together with Pilnikova (RICAM), de Graaf (Univ. Trento), and Harrison (Univ. Sydney), S. extended the Lie algebra method for solving (certain types of) Diophantine equations to the case of Del Pezzo surfaces of degree 6 and 8. The solution of these cases completes the algorithm for surface parametrization over the field of rational numbers, a major project initialized by the solution of the conical case (also by S.) in 2000.

Sparse techniques have already been used in computer algebra for various problems in algebraic system solving. Together with T. Beck, S. developed sparse versions for two algorithms for curve parametrization.

S. could also make a contribution to an investigation of S. Widder and P. Schuster (Univ. Wien) of dynamic patterns of gene regulation.

Together with H.-C. Graf von Bothmer (Univ. Hannover), O. Labs (RICAM), C. van de Woestijne (Univ. Leiden), he could prove some cases of the Casas-Alvero conjecture on univariate polynomials.

An idea for a symbolic-numeric method for the analysis of curve singularities has been worked out by S. Kusper in the frame of his diploma thesis: the singularity is analyzed through the topological type of its knot, which can be computed also in the presence of numerical errors.

### **Scientific Cooperations**

### Internal

Johannes Kraus: 1 joint paper.

Georg Regensburger: 1 joint talk, 1 joint paper planned.

(Joint papers with own PhD students are not counted in this list.)

#### External

Bert Jüttler, Linz: 3 joint papers. He is co-investigator in the FWF-funded special research area SFB 13, subproject 15.

Herwig Hauser, Innbruck: 1 joint FWF project (not running under RICAM because it started 2002), plus another FWF project which started in October 2006. 4th joint seminar of a series alternating in Tirol and Upper Austria.

Rafael Sendra, Madrid: 1 special issue in a journal jointly edited (in preparation).

Mike Harrison, Sydney: 1 joint paper.

Peter Schuster and Stephanie Widder: 1 submitted paper.

Günter Landsmann (Linz) and Peter Mayr (Linz): 1 joint paper.

Willem de Graaf (Trento): 1 submitted paper.

# Participation at Conferences, Scientific Visits and Talks.

Gröbner Bases Theory and Applications in Algebraic Geometry (RICAM, Special Semester on Gröbner Bases 2006): Algorithmic Resolution of Singularities, invited talk.

Approximative Commutative Algbra (RICAM, Special Semester on Gröbner Bases 2006): Analysis of Plane Curve Singularities, contributed talk.

SFB Status seminar, Strobl 2006 SeDuMi and potential application, talk.

Gröbner Basis in Symbolic Analysis (RICAM, Special Semester on Gröbner Bases 2006): Formal computations in Witt rings, contributed talk (jointly with G. Regensburger).

Arithmetic and Algebraic Geometry (Clay Summer School, Göttingen 2006): Construction of Rational Points on Rational Surfaces, invited lecture.

International Symposium of Algorithmic and Algebraic Computation (Genua 2006): Rational parametrizations for degree 6 Del Pezzo surfaces using Lie algebras (joint work with M. Harrison), contributed talk.

Algebraic Geometry and Geometric Modeling (AGGM, Barcelona 2006): "Linear Systems of Plance Curves", invited talk.

### Scientific Visits

SFB status seminar (Strobl 2006): project meeting.

Joint Seminar Innsbruck-Linz (Brandenberg 2005): workshop in algebraic geometry and singularities together with collegues from Linz and Innsbruck.

Joint Seminar Eger-Linz (Eger, 2006): workshop with the groups of Jüttler and Miklos Hoffmann (Univ. Miskolc)

#### **Publications 2005**

### Appeared or accepted

Journal papers:

- 1. J. Schicho: The parametric degree of a rational surface. Math. Z. 254, pp 185-198, 2006.
- 2. B. Jüttler, J. Schicho, I. Szilagyi: Local parametrization of cubic surfaces. J. Symb. Comp. 41, pp 30-48, 2006.
- 3. W. A. de Graaf, M. Harrison, J. Pilnikova, J. Schicho: A Lie algebra method for the parametriza tion of Severi-Brauer surfaces. J. Algebra 303/2, pp 514-529, 2006.
- 4. J. Kraus, J. Schicho: Algebraic multigrid based on computational molecules, I: scalar elliptic problems. Computing 77, pp 57-75, 2006.
- 5. G. Landsmann, P. Mayr, J. Schicho: A topological criterion for polynomial functions on GL(2,R). Aequationes, accepted.
- 6. T. Beck, J. Schicho: Parametrization of algebraic curves defined by sparse equations. AAECC, accepted.
- 7. M. Shalaby, B.Jüttler, J. Schicho: Approximate implicitization of planar curves by piecewise rational approximation of the distance function. AAECC, accepted.

## **Proceedings**

- 8. M. Harrison and J. Schicho: Rational parametrisation for degree 6 Del Pezzo surfaces using Lie algebras. Proc. ISSAC 2006, pp 132-137, ACM Press 2006.
- 9. M. Aigner, B. Jüttler, J. Schicho, I. Szilagyi: Implicitization and distance bounds. Proc. AGGM 2004, pp 71-86, Springer 2006.
- 10. T. Beck and J. Schicho: Curve parametrization over optimal field extensions exploiting the Newton polygon. Proc. Compass 2005, Springer 2006.

#### Submitted

- 11. J. G. Alcazar, J. Schicho, J. R. Sendra: Computation of the topological types of the level curves of an algebraic surface.
- 12. H-C. Graf von Bothmer, O. Labs, J. Schicho, C. van de Woestijne: The Casas-Alvero Conjecture for infinitely many primes.

- 13. W. A. de Graaf, J. Pilnikova, J. Schicho: Parametrizing Del Pezzo surfaces of degree 8 using Lie algebras.
- 14. S. Widder, J. Schicho, P. Schuster: Dynamic Patterns of Gene Regulation I: Simple Two Gene Systems.

#### Dr. Oliver Labs

#### **Scientific Achievements**

During his short stay at RICAM, Oliver Labs finished his program (with S. Holzer, see:www.surfex.algebraicsurface.net) for visualization of algebraic curves and surfaces, participated in the special semester on Gröbner bases, and continued his work on constructing surfaces with many singularities.

Together with Graf von Bothmer and van de Woestijne, and Schicho, Oliver Labs could prove some cases of the Casas-Alvero conjecture on univariate polynomials. This work appeared as a preprint on eww.arxiv.org.

Oliver Labs left in March.

# **Scientific Cooperations**

## External

H.-C. Graf von Bothmer (Univ. Hannover), C. van de Woestijne (Univ. Leiden) Stephan Holzer (TU München)

### Internal

J. Schicho

# Participation at conferences, scientific visits and talks

Talks at conferences

February 2006: Gröbner Bases Theory and Applications in Algebraic Geometry (RICAM, Special Semester on Gröbner Bases 2006): "Surfex, a tool for visualizing algebraic varieties."

February 2006: Approximate Commutative Algebra (RICAM, Special Semester on Gröbner Bases 2006): "Surf and Surfaces."

Talks during visits

March 2006: "surfex - Visualisierung algebraischer Flächen." Invited by Herwig Hauser (Innsbruck).

### **Publications 2006**

S. Holzer, O. Labs: "Illustrating the Classification of Real Cubic Surfaces." Proc. of AGGM 04, Springer 2006.

H-C. Graf von Bothmer, O. Labs, J. Schicho, C. van de Woestijne: The Casas-Alvero Conjecture for infinitely many primes (submitted).

## Mario Kapl advised by Prof. Josef Schicho

# Work before joining RICAM

Mario Kapl finished his studies of "Technische Mathematik" in September 2005 at the Johannes Kepler University Linz. Since January 2006 he is working in the frame of the SFB project 1315 as a PhD student advised by Prof. Dr. Bert Jotter (Institute of Applied Geometry, JKU Linz).

#### **Scientific Achievements 2006**

In 2006 the work of Mario Kapl was focused on finding a wavelet representation of implicitly defined spline curves for which the region of interest - the curve - is preserved better than for existing uniform wavelets. For this purpose he constructed the so called weighted spline wavelets. Weighted spline wavelets are wavelets that are adapted to the region of interest by means of a weighted inner product. Furthermore he has constructed lazy wavelets for periodic B-spines of degree d>1. Lazy wavelets are wavelets with poor approximation properties but with simple analysis and synthesis filters.

### Participation at Conferences, Scientific Visits and Talks Conferences (including talks)

SFB-Status seminar 2006, April 20-22, 2006, Strobl, Austria

Workshop on algebraic Spline Curves and Surfaces, May 17-18, 2006, Eger (Hungary) Talk: Spline Wavelets

FSP S092 Workshop on Computional Geometry and Geometric Computing, November 27-29, 2006, Vorau (Austria) Talk: Weighted Wavelets

### Dr. Markus Rosenkranz

#### **Scientific Achievements 2006**

Markus Rosenkranz works on building up an algebraic approach for analyzing various boundary problems, initiated in his dissertation ("A Polynomial Approach to Boundary Value Problems", available as RISC Technical Report 2003-05). Also called **Symbolic Functional Analysis**, this approach is now reformulated in a wider scope (see the two draft articles described in the Scientific Plans), whose leading idea may be expressed in the slogan "Symbolic Functional Analysis = Differential Algebra + Linear Algebra."

Along these lines, Markus Rosenkranz has achieved the following key results in 2006, worked out in close cooperation with Georg Regensburger:

- Codification of a **boundary problem** as differential operator plus finite-dimensional dual sub space.
- Introducing new **multiplication of problems**, antiisomorphic to composition of their Green's operators.
- A factorization algorithm for problems and their Green's operators.
- Adjunction of **problems as inverses** in the ring of Green's operators.
- Extending the classical **Mikusiński calculus** such that it covers boundary and not just initial conditions.

These results have been reported – in various stages of maturity – in the talks listed below. They will be written up in 2007, as two joint articles (see Scientific Plans).

# **Scientific Cooperations**

#### Internal

As a research project, Symbolic Functional Analysis is embedded under the label F1322 within the SFB F013, entitled **Numerical and Symbolic Scientific Computing** and funded by the FWF. This subproject has been co-initiated and is continually co-supervised by Prof. Buchberger from RISC and Prof. Engl. It benefits from stimulating inputs both from the analysis / numerics side (Prof. Engl's group on Inverse Problems) and from the computer algebra / symbolics side; see also talk [2].

In the summer semester of 2006, Markus Rosenkranz has been involved in the interdisciplinary RI-CAM **Special Semester on Gröbner Bases**. In particular, he has chaired – together with Dongming Wang and Viktor Levandovskyy – the D2 workshop "Gröbner Bases in Symbolic Analysis." Together with Dongming Wang, he will also edit a proceedings volume of the D2.2 session, to be published by de Gruyter. For details, see the RICAM homepage.

### External

As a project co-supervised by Prof. Buchberger, the Symbolic Functional Analysis group (currently consisting of Markus Rosenkranz and Georg Regensburger) is in permanent contact with the **Theorema group** at RISC, also conducted by Prof. Buchberger. In fact, there is a stimulating exchange of ideas through the Theorema seminar, based on the idea that symbolic computation (on boundary or other problems) is a form of specialized reasoning; see also talks [6] and [7].

In particular, we are currently preparing a cooperation with a specific project by Professor Buchberger (in the frame of the Theorema group) on the formulation and implementation of **general polynomial domains** in various data structures using Buchberger's conceptual frame of Theorema functors for a generic build-up of mathematics. In these domains, simplification, generalized Groebner bases and other fundamental algorithmic as well as non-algorithmic topics will be studied, including those that arise in the context of symbolic boundary problems [6].

### Participation at Conferences, Scientific Visits and Talk

#### Conferences

- [1] M. Rosenkranz, A Novel Treatment of Linear Two-Point Boundary Value Problems, March, 2006, GAMM, Berlin, Germany.
- [2] M. Rosenkranz, G. Regensburger, Factorization and Division in the Realm of Linear Ordinary BVPs, April, 2006, SFB Status Seminar, Strobl, Austria.
- [3] M. Rosenkranz, Algebraic Methods for Differential Equations and Boundary Value Problems, June, 2006, CNRS-NSF Symposium, Avignon, France.
- [4] M. Rosenkranz, Using Groebner Bases for Solving Linear Two-Point Boundary Value Problems, May, 2006, Special Semester for Groebner Bases, Workshop D2, Hagenberg, Austria.
- [5] M. Rosenkranz, Symbolic Computation with Two-Point Boundary Value Problems, 11 August, 2006, Workshop on the Algebraic Theory of Differential Equations, Edinburgh, United Kingdom.

# Scientific Talks

- [6] M. Rosenkranz, Symbolic Computation with BVPs. Noncommutative Polynomials + Boundary Calculus, October 2006, Theorema seminar, Hagenberg, Austria.
- [7] M. Rosenkranz, The Lausch-Nöbauer Functor: Polynomials in the "Old Style", November 2006, Theorema Seminar, Hagenberg, Austria,

#### **Publications 2006**

#### Appeared

- [8] W. Windsteiger, B. Buchberger, M. Rosenkranz, The Seventeen Provers of the World (ed. Freek Wiedijk), Springer, LNAI 3600, Berlin Heidelberg New York, 2006, ISBN 3-540-30704-4.
- [9] B. Buchberger, M. Rosenkranz, et al., Theorema: Towards Computer-Aided Mathematical Theory Exploration, Journal of Applied Logic, 4, 4, 359-652, December, 2006, ISSN 1570-8683.

## Niels Lubbes advised by Prof. Josef Schicho

He joined RICAM in July 2006 in order to work on the FWF-project P18992 (led by H. Hauser and J. Schicho).

#### Work before

- The topic of his master's thesis was hyperelliptic curves and the discrete logarithm problem.

# Conference(Talk)

- "Divisors and line bundles", Workshop on algebraic geometry (Obergurgl, Austria, September 2006).

### **Scientific visit:**

- Visits of Herwig Haueser group at the University of Innsbruck to follow a intensive course concerning topics in algebraic geometry.

#### Dr. Pavel Chalmoviansky

### **Scientific Achievements**

He worked in the SFB project 1315, mainly on the topics of approximate parametrization and subdivision. He left RICAM by March.

### **Scientific Cooperations**

#### External

With B. Jüttler (Univ. Linz), he investigated approximate parametrization techniques. C. also provided an algorithm for shape design to Dalibor Lukavs (Univ. Prag).

#### **Publications 2006**

Journal papers

### Accepted

D. Lukavs and P. Chalmoviansky,

A Sequential Coupling of Optimal Topology and Multilevel Shape Design Applied to 2-Dimensional Nonlinear Magnetostatics, Comp. and Visualization

B. Juettler and P. Chalmoviansky,

A Predictor-Corrector Method for Approximate Parameterization of Intersection Curves, AAECC.

#### Dr. Tobias Beck

#### Scientific Achievements 2006

Beck and Schicho have continued their work on the efficient parametrization of plane algebraic curves by rational maps. In 2005 an algorithm was developed that benefited from the shape of the Newton Polygon of the defining equation. Its shortcoming was the possibly high degree of algebraic field extensions needed to represent the parametrization. From theory it is known that field extensions of degree at most two are always sufficient. Beck and Schicho were now able to show that one can have both at the same time, an algorithm that is adapted to the shape of the Newton Polygon and produces a parametrization using a field extension of minimal degree.

Beck has handed in and successfully defended his thesis "Contributions to the Parametrization of Algebraic Varieties" on November 22. The thesis comprises three parts: The first part describes the algorithmic treatment of multivariate algebraic power series (dating back to 2004). The second part deals with parametrization of plane curves (see above). Finally the last part gives an algorithm for the computation of adjoint spaces for surfaces. In order to proof correctness of this algorithm, Beck has introduced and thoroughly studied the concept of "formal desingularizations".

### **Conferences**

Winter School on Commutative Algebra and Applications (WSCA), Barcelona, January 30 - February 3, 2006

### **Scientific Talks**

- 10th Rhine Workshop on Computer Algebra (RWCA), Basel, March 16 17, 2006: "Parametrization of Algebraic Curves Defined by Sparse Equations"
- Geometry Workshop, Eger, May 16 19, 2006: "Parametrization of Algebraic Curves Defined by Sparse Equations"
- Magma 2006 conference, Berlin, July 30 August 2, 2006: "Computational Formal Resolution of Surfaces in P3"
- Workshop on Resolution of Algebraic Varieties, Obergurgl, September 22 25, 2006: "On the Concept of Formal Desingularizations"

# **Publications 2006**

### Accepted

Curve Parametrization over Optimal Field Extensions Exploting the Newton Polygon, with Josef Schicho (to appear in the Compass II proceedings)

### 2.3. GROUP "FINANCIAL MATHEMATICS"

# **Group Leaders:**

Prof. Dr. Hansjörg Albrecher

o.Univ.-Prof. Dr. Walter Schachermayer

# Researchers funded via ÖAW/Upper Austrian government funds:

Dr. Jürgen Hartinger

Dr. Gottlieb Pirsic

Dr. Jörn Saß

Dr. Klaus Scheicher

Univ.-Doz. Dr. Arne Winterhof

#### Researchers externally funded:

Mag. Nina Brandstätter

Dr. Domingo Gomez

Dr. Markus Hahn

DI Dominik Kortschak

DI Wolfgang Putschögl

DI Stefan Thonhauser

# Introduction by Group Leader Prof. Hansjörg Albrecher

After its restructuring in 2005, the Financial Mathematics Group was enlarged in 2006 with the start of the FWF project "Mathematical Models for Insurance Risk" led by Doz. Albrecher. Later on during the year Doz. Winterhof raised the new FWF project "Pseudo-Random Sequences", so that together with the on-going FWF-project "Computing optimal portfolios under partial information" led by Dr. Sass, more than half of the group members are currently financed through external funds. Moreover, in March 2007 Philip Ngare (University of Nairobi) will join the group as an additional PhD student, who is financed through a scholarship of the Austrian Exchange Service. During the year 2006, Dr. Hartinger received an offer as an actuary in the insurance industry which he accepted. Starting in January 2007, this Postdoc position will be taken up by Dr. Corina Constantinescu, who received her PhD degree at Oregon State University (USA) working on the analysis of investment strategies in insurance portfolios. At RICAM she will in particular focus on analytical aspects of risk analysis and the interplay between financial and insurance mathematics.

The research of the group is centered around two approaches to mathematical finance, namely stochastic finance and Monte Carlo- and Quasi-Monte Carlo-based simulation methodology. Altogether, in 2006 more than 50 publications of group members appeared or were accepted for publication in journals and refereed conference proceedings and about 20 additional manuscripts were submitted for publication.

For portfolio optimization, in 2006 new results for the existence of optimal trading strategies under transactions costs were obtained. Furthermore, in joint research with the Optimization and Optimal Control Group at RICAM, a semi-smooth Newton method was implemented to find the optimal trading regions for a problem with finite time horizon. Future work will deal with extensions to the multidimensional case, other types of transaction costs, and price systems under transaction costs. In another research activity, the optimal wealth level under certain shortfall constraints was fully characterized and results for partial information were extended to cover certain stochastic volatility models and to allow for consumption. Moreover, Markov chain Monte Carlo methods were developed to estimate the corresponding parameters. Refinement of the estimation procedures and a sensitivity analysis

based on the distribution of the estimated parameters are planned. Here the discussion with the Inverse Problems Group will be intensified.

For the determination of optimal dividend policies in an insurance portfolio, the group succeeded to include certain types of solvency constraints in the calculations, which allows to balance between profitability and safety of dividend strategies. Also, analytical formulae in the presence of particular types of dividend payments could be derived that enable tuning of control parameters to a desired target. Furthermore, explicit formulae for some measures of risk in the classical risk model were developed, when tax payments for profit are taken into account. This also allowed to calculate the optimal collection strategy for a tax authority in this model.

For various types of risk measures the appropriate consideration of dependencies of risks is a crucial issue. In that respect, during 2006 some criteria on the type and degree of dependence structures could be established under which the asymptotic tail of the sum of such risks still behaves in an explicitly calculable way.

In addition, model-independent lower price bounds for Asian options were derived and a long-standing puzzle concerning mispricings of options with long maturity after calibration to vanilla options in the Heston model with stochastic volatility could be resolved in joint work with a group in Belgium. For the pricing of collateralized debt obligations, a unified framework in a Levy setting for several popular models in the market was established. Moreover, in cooperation with the Inverse Problems group, calibration techniques for parameters in local Levy models for asset prices were started to be investigated. These research activities will be further pursued.

For the study of nonlinear pseudorandom number generators, discrepancy was analysed via exponential sums, and linear complexity and related measures of some particular interesting generators as Dickson and Redei generators were investigated. Interesting future research directions are the study of character sums over such generators as well as complementing the results on discrepancy and linear complexity. Moreover, complexity lower bounds for cryptographic functions and sequences were studied. Here hyperelliptic curve cryptosystems provide interesting functions for future research. The expertise of the symbolic computation group may be helpful for solving these problems.

More details on research results can be found on the following pages.

In 2006 the Financial Mathematics Group hosted about 15 visitors and in March 2006 Prof. Hanspeter Schmidli (University of Cologne) gave a lecture series on "Optimal Stochastic Control in Risk Theory" at the institute. In May 2007, an "International Workshop on Financial and Actuarial Mathematics for Young Researchers" will be organized at RICAM. It intends to gather young PostDocs and PhD students from Austria and other European countries to exchange research ideas. This event will also make the activities of the institute in this research field known to a broader community.

At present, there are collaborations with the Inverse Problems group, the Optimization and Optimal Control group and the Symbolic Computation group within RICAM. In addition to these internal cooperations, there are numerous international collaborations as presented in the individual reports of the researchers. Together with the Inverse Problems group, a mini-symposium on "Bregman distances and their applications" will be organized at the ICIAM in Zürich, taking place in July 2007. Also, a jointly organized international workshop on Inverse Problems in Finance is planned at RICAM for late spring 2007.

# Prof. Hansjörg Albrecher

#### **Scientific Achievements 2006**

Apart from conducting and participating in research activities within the Financial Mathematics group (described at other places in this report), H. Albrecher continued to work on extensions of results on risk measures in collective risk theory. The asymptotic behaviour of ruin probabilities was investigated for arbitrary dependence structure between the interclaim time and claim size distribution with J.

Teugels in [3] and for dependence of shot-noise type among interclaim times with S. Asmussen in [4]. The determination of optimal dividend strategies in various contexts of practical relevance in finance and insurance was investigated in [6],[7],[10],[11],[12] and [14] in joint work with J. Hartinger and S. Thonhauser. For the classical collective risk model, together with C. Hipp, in [15] the payment of taxes was for the first time incorporated in calculations of ruin probabilities of insurance companies, resulting in transparent identities between this model and the one without tax. This also gave rise to a calculation technique for the optimal collection strategy of a tax authority.

As a complement of the results in [1], weak limit laws for certain popular measures of variation were established as a function of the number of existing moments of the underlying distributions together with S. Ladoucette and J. Teugels in [13]. These results allow to more efficiently reveal misuses of such measures when assessing risks in practice.

Together with P. Mayer and W. Schoutens, in [16] model-independent lower price bounds for Asian options were derived that solely depend on the prices of traded vanilla options and it was shown how these bounds can be tightened under mild additional assumptions. In [8] a long-standing puzzle concerning mispricings of options with long maturity after calibration to vanilla options in the Heston model with stochastic volatility could be resolved by a refined study of the involved Fast Fourier transforms using complex analysis techniques. Together with S. Ladoucette and W. Schoutens, a unified framework in a Levy setting for several popular models to price synthetic collateralized debt obligations could be established, allowing deeper insight into the relations between these models and the resulting prices.

Moreover, in cooperation with the Inverse Problems group, calibration techniques for parameters in local Levy models for asset prices were started to be investigated.

Parts of the above research activities were carried out via the FWF research project P18392 "Mathematical Models for Insurance Risk" led by H. Albrecher. In 2006, he supervised four Master students and currently has four PhD students (S. Haas, D. Kortschak, P. Mayer and S. Thonhauser).

On from 2007, H. Albrecher will act as Associate Editor of the journals "Mathematical Methods of Operations Research" and "Blätter der deutschen Gesellschaft für Versicherungs- und Finanzmathematik".

### **Scientific Cooperations**

#### Internal

In addition to cooperations within the Financial Mathematics group and the FWF project P18392, also with:

Dr. S. Kindermann and Prof. H. Engl: Inverse problems for local Levy models

### External

Prof. S. Asmussen (University of Aarhus): Dependence in Risk Theory

Dr. A. Badescu (University of Toronto): Dependence in Risk Theory

Prof. O. Boxma (TU Eindhoven): Ruin Models with Dependency

Dr. M. Claramunt (Universitat de Barcelona): Dividend barrier models

Prof. K. Eisele (Universite Louis Pasteur Strasbourg): Multivariate Phase-Type Distributions

Prof. C. Hipp (University of Karlsruhe): Risk processes with tax

Prof. R. Korn (Kaiserslautern): Stochastic control in finance

Dr. S. Ladoucette (K.U. Leuven): Risk Measures in Reinsurance

Dr. D. Landriault (University of Waterloo): Risk Theory

Dr. C. Macci (University Tor Vergada, Rome): Large deviation techniques

Prof. W. Schoutens (K.U. Leuven): Hedging of Exotic Options

Prof. J. Teugels (K.U. Leuven): Actuarial Aspects of Reinsurance

Prof. R. Tichy (TU Graz): QMC Techniques in Risk Theory

Dr. D. Vyncke (University of Gent): Simulation Techniques

Prof. G. Wilmott (University of Waterloo): Discounted Penalty Functions

### Research Visits, Conferences and Talks

AMaMeF Worskhop on Numerical Methods in Finance, INRIA-Rocquencourt, February 3-7: Talk: "Semi-static hedging strategies for strongly path-dependent options"

EURANDOM Workshop on Risk Measures & Risk Management for High-Frequency Data, Eindho-

Johannes-Kepler-Symposium, JKU Linz:

Invited Talk: "Bewertung von Risiken in der Versicherungsmathematik", March 22, 2006.

Radon Institute, Linz:

ven, March 6-8, 2006

Invited Talk at the Kuratorium Meeting: "On Measuring and Hedging Risk in Finance and Insurance", April 6, 2006.

Int. Workshop on Applied Probability, Connecticut (USA), May 15-18, 2006:

Invited Talk: "Dividend Payment Strategies in the Sparre Andersen Ruin Model"

Austrian Financial Market Authority, Vienna:

Invited Talk: "Bewertung von Risiken in der Versicherungsmathematik", May 24, 2006.

Department of Mathematics, University of Tübingen, Germany:

Invited Talk: "Erweiterungen des Cramer-Lundberg-Modells in der kollektiven Risikotheorie", May 30, 2006.

21st European Conference on Operational Research, Reykjavik, July 2-5, 2006:

Invited Talk: "Characteristics of the collective risk process in the presence of dividend payments and dependent risks"

Department of Mathematics, Humboldt University Berlin, Germany:

Invited Talk: "Zur Bewertung und Steuerung von Risiken in der Finanz- und Versicherungsmathematik", July 13, 2006.

10th Congress on Insurance: Mathematics & Economics. Leuven, July 20-22, 2006:

Talk: "Ruin probabilities and aggregate claims distributions for shot noise Cox processes"

1<sup>st</sup> Int. Workshop on Gerber-Shiu Functions, Concordia University, Montreal, August 7-8, 2006: Invited Talk: "On the discounted penalty function in the presence of dependence and dividend payments"

41st Actuarial Research Conference, Universite de Montreal, August 10-12, 2006.

Department of Statistics and Actuarial Science, University of Waterloo, Canada:

Research visit: August 13-16, 2006,

Invited Talk: "Ruin Probabilities for an Insurance Portfolio with Dependent Risks", August 15, 2006.

Department of Applied Mathematics, University of Porto, Portugal:

Research visit: September 2-9, 2006,

Series of Lectures on "Mathematical Techniques in Insurance"

Invited Talk: "The Quasi-Monte Carlo Method: Theory and Applications", September 8, 2006.

Int. Workshop on Credit Risk under Levy Models, Edinburgh, September 18-22, 2006: Invited Talk: "Static hedging strategies for Asian options"

Fraunhofer Zentrum Kaiserslautern, Germany:

Research visit: October 11-13, 2006.

Invited Talk: "Model-independent bounds for Asian options prices"

Department of Statistics and Decision Support Systems, University of Vienna:

Invited Talk: "Ruin Probabilities for an Insurance Portfolio with Dependent Risks", October 16, 2006.

Department of Mathematical Stochastics, Leibniz University Hannover:

Invited Talk: "Erweiterungen des Cramer-Lundberg-Modells in der kollektiven Risikotheorie", December 8, 2006.

# Lectures at TU Graz:

- 1. Seminar on Financial and Actuarial Mathematics, Winter 2005/6
- 2. Mathematics for Finance and Insurance 1, Summer 2006
- 3. Advanced Insurance Mathematics, Winter 2006/7

#### **Publications 2006**

## **Appeared**

- 1. H. Albrecher, J.L. Teugels: Asymptotic Analysis of a Measure of Variation. Theory of Probability and Mathematical Statistics 74 (2006), 1-9.
- 2. H. Albrecher, R.E. Burkard, E. Cela: An asymptotical study of combinatorial optimization problems by means of statistical mechanics. Journal of Computational and Applied Mathematics 186 (2006), No.1, 148-162.
- 3. H. Albrecher, J.L. Teugels: Exponential behavior in the presence of dependence in risk theory. Journal of Applied Probability 43 (2006), No. 1, 257-273.
- 4. H. Albrecher, S. Asmussen: Ruin probabilities and aggregate claims distributions for shot noise Cox processes. Scandinavian Actuarial Journal (2006), No. 2, 86-110.
- 5. H. Albrecher, S. Asmussen, D. Kortschak: Tail asymptotics for the sum of two heavy-tailed dependent risks. Extremes 9 (2006), 107-130.
- 6. H. Albrecher, S. Thonhauser, Discussion of "Optimal Dividends in the Compound Poisson Model", North American Actuarial Journal, 10 (2006), No. 3, 68-71.
- 7. H. Albrecher, J. Hartinger, On the non-optimality of horizontal barrier strategies in the Sparre Andersen model, Hermis J. Comp. Math. Appl., 7 (2006), 1-14.

# Accepted

- 8. H. Albrecher, P. Mayer, W. Schoutens, J. Tistaert, The little Heston trap, WILMOTT, to appear.
- 9. H. Albrecher, S. Ladoucette, W. Schoutens, A generic one-factor Levy model for pricing synthetic CDOs. In: Advances in Mathematical Finance, Birkhaeuser, to appear.
- 10. H. Albrecher, S. Thonhauser, Discussion of "On the merger of two companies", North American Actuarial Journal, to appear.
- 11. S. Thonhauser, H. Albrecher, Dividend maximization under consideration of the time value of ruin, Insurance: Mathematics & Economics, to appear.

#### Submitted

- 12. H. Albrecher, J. Hartinger, S. Thonhauser, Exact solutions for dividend strategies of threshold and linear barrier type in a Sparre Andersen model, submitted.
- 13. H. Albrecher, S. Ladoucette, J. Teugels, Asymptotics of the Sample Coefficient of Variation and the Sample Dispersion, submitted.
- 14. H. Albrecher, J. Hartinger, A risk model with multi-layer dividend strategy, submitted.
- 15. H. Albrecher, C. Hipp, Lundberg's risk process with tax, submitted.
- 16. H. Albrecher, P. Mayer, W. Schoutens, Model-independent lower bounds for arithmetic Asian option prices, submitted.

# Dominik Kortschak advised by Prof. Hansjörg Albrecher

#### **Scientific Achievements 2006**

In 2006 the work of DI Kortschak was focused on the asymptotic study of the probability that the sum of dependent random variables exceeds a given threshold where the main attention was given to subexponential marginal distributions. This is a problem that arises for instance in financial mathematics when one wants to evaluate the probability of high losses in a portfolio. In joint work with H. Albrecher and S. Asmussen, a condition on the copula could be established such that the behaviour of the dependent sum of two random variables asymptotically behaves like the independent sum for all continuous subexponential marginal distributions; furthermore some general bounds were given and examples were provided for which the exact asymptotic behaviour can be evaluated. It was shown that asymptotic independence is not equivalent to the case that the behaviour of the sum is like in the independent case for all marginal distributions that are in the maximum domain of attraction of the Gumbel distribution. The connection with multivariate extreme value theory was studied and borderline cases were discussed, such as cases where the tail of one summand is significantly lighter than the tail of the others. Furthermore DI Kortschak worked on conditions under which the asymptotic behaviour exists at least for all regularly varying marginal distributions and solved the problem for diagonal copulas.

In the year 2006, in Berlin DI Kortschak received the "2. Preis für Aktuarswissenschaften 2006" of the SCOR reinsurance group for his Diploma thesis, and furthermore he was awarded a "Würdigungspreis" of the Graz University of Technology for excellent achievement in his diploma studies.

### **Scientific Cooperations**

#### Internal

Dr. H. Albrecher (Financial Mathematics)

Dr. J. Hartinger (Financial Mathematics)

#### External

Prof. S. Asmussen (University of Aarhus): Dependence in Risk Theory

#### Participation at Conferences, Scientific Visits and Talks

- Workshop on Asymptotics: Particles, Processes and Inverse Problems, Lorentz Center, Leiden, Netherlands, July 10-14, 2006.
- 4th Conference in Actuarial Science and Finance at Samos, Greece, September 14-17, 2006. Talk: "Tail asymptotics for the sum of two dependent risks".
- Short Course Simulation in Insurance and Finance, Samos, Greece, September 18-20, 2006.
- LMS/EPSRC Short Course "Stability, Coupling and Rare Events", Heriot-Watt University, Edinburgh, United Kingdom September 4-9, 2006.

- 6th International Workshop on Rare Event Simulation (RESIM) at Bamberg, Germany October 8-10, 2006. Talk: "On the efficiency of the Asmussen-Kroese-estimator and its application to stoploss transforms".
- Oberwolfach-Seminar "Dependence and Tail Modelling with Application to Finance, Insurance, Teletraffic and Climate", Oberwolfach, Germany, November 19-25 2006. Student presentation: "Tail asymptotics for the sum of two dependent risks".

#### **Publications 2006**

### Appeared

1. H. Albrecher, S. Asmussen, D. Kortschak, Tail asymptotics for the sum of two heavy-tailed dependent risks, Extremes, 9, 107-130, 2006.

#### Submitted

- 2. J. Hartinger and D. Kortschak, Quasi-Monte Carlo techniques and rare event sampling, submitted.
- 3. J. Hartinger and D. Kortschak, On the efficiency of the Asmussen-Kroese-estimator and its application to stop-loss transforms, submitted.

#### **Preprint**

4. D. Kortschak and H. Albrecher, On the asymptotic behaviour of the sum of dependent random variables.

# Stefan Thonhauser advised by Prof. Hansjörg Albrecher

# **Scientific Achievements 2006**

In 2006 the work of DI Stefan Thonhauser was mainly concentrated on the calculation of explicit solutions for problems arising in actuarial mathematics. One part dealt with a traditional dividend maximization problem involving also solvency considerations in the objective function, both in the classical Cramer-Lundberg as well as in a diffusion risk model. Another field of activity was the extension of an algorithmic method for obtaining analytical expressions for probability of ruin and expected dividends in a Sparre Andersen risk model with predefined dividend strategies. Furthermore, the analysis of the dividend maximization problem for a modified risk process including interest force was started.

# **Scientific Cooperations**

#### Internal

Prof. Albrecher Dr. Hartinger

### Participation at Conferences, Scientific Visits and Talks

Summer School on Risk Measurement and Optimal Investment, Munich, Germany, June 29-30.

IME 2006, Leuven, Belgium, July 18-20.

Talk: "Dividend maximization under consideration of the time value of ruin".

4th Conference in Actuarial Science & Finance on Samos, Karlovassi, Greece, September 14-17.

Talk: "Exact solutions for dividend strategies of threshold and linear barrier type in a Sparre Andersen model".

Short course on Simulation in Insurance and Finance, Karlovassi, Greece, September 18-20.

#### **Publications 2006**

### **Appeared**

1. H. Albrecher, S. Thonhauser: Discussion of "Optimal Dividends in the Compound Poisson Model". North American Actuarial Journal, 10(3):68-71, 2006.

#### Accepted

- 2. S. Thonhauser, H. Albrecher: Dividend maximization under consideration of the time value of ruin, to appear in Insurance: Mathematics & Economics.
- 3. H. Albrecher, S. Thonhauser: Discussion of "On the Merger of Two Companies", to appear in North American Actuarial Journal.

### **Submitted**

4. H. Albrecher, J. Hartinger, S. Thonhauser: Exact solutions for dividend strategies of threshold and linear barrier type in a Sparre Andersen model, submitted.

## Prof. Walter Schachermayer

#### **Research Visits, Conferences and Talks**

Colloquium in honor of Professor F. Delbaen, ETH Zurich, Switzerland;

Research Visit: November 22-24, 2006;

Invited talk: "The Mathematics of Arbitrage", November 23, 2006.

Research with Prof. Ioannis Karatzas and Dr. Peter Bank, Probability Seminar at Columbia University, and Thirteenth Annual CAP Workshop on Derivative Securities and Risk Management, November 3, 2006, of the Center for Applied Probability, New York, U.S.A.;

Research Visit: October 21 - November 3, 2006;

Mini course of four lectures: "Functional-Analytic Methods in Finance", October 24 - November 1, 2006;

Invited talk at the Probability Seminar: "A Super-Replication Theorem in Kabanov's Model of Transaction Costs", October 27, 2006;

Invited talk at CAP workshop: "Optimal risk sharing for law invariant monetary utility functions", November 3, 2006.

Erlebniswelt Forschung - 10 Jahre Wittgenstein-Preis, September 21, Vienna, Austria;

Invited Talk: "Wie verlässlich ist der Zufall? Mathematik und Finanzmärkte", September 21, 2006.

Journées de Probabilité, September 18-22, 2006, Marseille Luminy, France;

Research Visit: September 18-20, 2006;

Invited talk: "A Super-Replication Theorem in Kabanov's Model of Transaction Costs", September 19, 2006.

2006 IMS Annual Meeting, July 30 - August 4, 2006, Institute of Mathematical Statistics, Rio de Janeiro, Brazil;

Research Visit: July 29 - August 4, 2006;

Invited talk: "Optimal risk sharing for law invariant monetary utility functions", August 3, 2006.

9th International Vilnius Conference on Probability Theory and Mathematical Statistics, June 25-30, 2006, Vilnius, Lithuania;

Research Visit: June 25-30, 2006;

Invited talk: "Optimal risk sharing for law invariant monetary utility functions", June 30, 2006.

CAIMS-MITACS 2006 Joint Annual Conference, June 15-20, 2006, York University, Toronto, Canada;

Research Visit: June 15-18, 2006;

Invited talk: "Optimal risk sharing for law invariant monetary utility functions", June 17, 2006.

Workshop 'Optimization problems in financial economics', Banff Research Institute, Banff, Canada; Research Visit: May 20-26, 2006;

Invited Talk: "Optimal risk sharing for law invariant monetary utility functions", May 24, 2006.

International Symposium Mathematics for the 21st Century (Matemáticas para el siglo XXI), May 3-4, 2006, Madrid, Spain;

Research Visit: May 3-4, 2006;

Invited talk: "The Notion of Arbitrage and Free Lunch in Mathematical Finance", May 3, 2006.

2006 Seminar on Stochastic Processes, March 23-25, 2006, Princeton University, Princeton, NJ, USA; Research Visit: March 22-25, 2006;

Invited talk: "A Super-Replication Theorem in Kabanov's Model of Transaction Costs", March 23, 2006.

Research with Prof. Dmitry Kramkov, Department of Mathematical Sciences, Carnegie Mellon University, Pittsburgh, PA, 15213-3890, USA;

Research Visit: March 19-21, 2006;

Invited talk: "A Super-Replication Theorem in Kabanov's Model of Transaction Costs", March 20, 2006.

ICAM 2006, International Congress on the Applications of Mathematics, March 13-17, 2006, Universidad de Chile, Santiago de Chile, Chile;

Research Visit: March 13-18, 2006;

Plenary talk: "Optimal risk sharing for law invariant monetary utility functions", March 16, 2006.

10. Internationale Tagung über Schulmathematik, February 26 to March 1, 2006, TU Vienna, Austria; Invited talk: "Die Rolle der Mathematik auf den Finanzmärkten", February 27, 2006.

VII Workshop on Quantitative Finance, January 26-27, 2006, Università di Perugia, Italy; Research Visit: January 25-28, 2006; Invited talk: "Optimal risk sharing for law invariant monetary utility functions", January 26, 2006.

### **Publications 2006**

#### Appeared:

1. F. Delbaen, W. Schachermayer:

The Mathematics of Arbitrage.

Springer Finance, xvi+371 p., ISBN 3-540-21992-7 (2006).

2. D. Rokhlin, W. Schachermayer:

A note on lower bounds of martingale measure densities.

Illinois Journal of Mathematics, Vol. 50 (2006), No. 4, pp. 815-824.

3. E. Jouini, W. Schachermayer, N. Touzi:

Law invariant risk measures have the Fatou property.

Advances in Mathematical Economics, Vol. 9 (2006), pp. 49-71.

4. W. Schachermayer:

The Notion of Arbitrage and Free Lunch in Mathematical Finance.

(expanded version of [118]), Aspects des mathématiques financières (actes de colloque, Paris, le 1er février 2005), Académie des Sciences (2006), pp. 19-29.

### Accepted:

5. W. Schachermayer, J. Teichmann:

How close are the Option Pricing Formulas of Bachelier and Black-Merton-Scholes? to appear in Mathematical Finance.

6. W. Schachermayer, J. Teichmann:

Characterization of optimal Transport Plans for the Monge-Kantorovich-Problem. to appear in Proceedings of the A.M.S.

7. L. Campi, W. Schachermayer:

A Super-Replication Theorem in Kabanov's Model of Transaction Costs.

to appear in Finance and Stochastics

### Submitted:

8. W. Schachermayer, U. Schmock, J. Teichmann:

Non-monotone convergence in the quadratic Wasserstein distance, submitted.

9. E. Jouini, W. Schachermayer, N. Touzi:

Optimal risk sharing for law invariant monetary utility functions, submitted.

### Other scientific achievements 2006

• W. Schachermayer, J. Teichmann;

"Final Workshop of the Research Training Network 'Evolution Equations for Deterministic and Stochastic Systems'";

Vienna University of Technology, June 5-8, 2006;

• W. Schachermayer, U. Schmock;

"Workshop Aktuarausbildung";

Vienna University of Technology, February 28, 2006;

### Dr. Jürgen Hartinger

# **Scientific Achievements 2006**

In 2006 J. Hartinger finished several projects on theoretical and applied aspects of Quasi-Monte Carlo theory in financial and actuarial mathematics. In particular, corner avoidance properties of randomized Quasi-Monte Carlo methods (in cooperation with V. Ziegler, e.g. [2]) and applications of these methods to rare event sampling (in collaboration with D. Kortschak, e.g. [3]) were investigated.

Another focus of research was laid on various aspects of ruin theory. In [2] and [6] (in cooperation with H. Albrecher and S. Thonhauser) the goal was to contribute to the discussion on optimal dividend strategies in a Sparre Andersen model, i.e. a risk model where the claim inter-arrival times are generalized Erlang distributed. Heuristically, in this model an optimal barrier has to depend on the time elapsed since the last claim arrival. In [2] the non-optimality of horizontal barriers is shown. Closed formulae for suboptimal dividend strategies are discussed in [6]. A central project in 2006 was the

development of closed formulae for various key variates, such as ruin probabilities, moments of discounted dividends, in a Cramer Lundberg risk model with surplus-dependent parameters (see [5]). At the end of May, Dr. Hartinger accepted an actuarial position in the insurance industry and left RI-CAM.

# **Scientific Cooperations**

### Internal

Hansjörg Albrecher (Financial Mathematics): ruin theory, discounted penalty and dividend strategies. Dominik Kortschak (Financial Mathematics): QMC – rare event sampling Stefan Thonhauser (Financial Mathematics): ruin theory, discounted penalty and dividend strategies

### External

Reinhold Kainhofer (Vienna): QMC – corner avoidance properties, financial applications Robert F. Tichy (Graz): various aspects of QMC theory and ruin theory Volker Ziegler (Vienna/Graz): QMC – corner avoidance properties

# **Participation at Conferences**

Summer School Risk Measurement and Optimal Investment, Munich (Germany).

### **Publications 2006**

### **Appeared**

- 1. J. Hartinger and R. Kainhofer: Non-uniform low-discrepancy sequence generation and integration of singular integrands, 2006, H. Niederreiter & D. Talay, eds, Proceedings of MCQMC 2004, Juan-Les-Pins France, June 2004, Springer Verlag, Berlin.
- 2. H. Albrecher and J. Hartinger: On the non-optimality of horizontal barrier strategies in the Sparre Andersen model, 2006, Hermis J. Comp. Math. Appl., 7:1-14.

# Accepted

3. J. Hartinger and V. Ziegler: A note on corner avoidance of random start-Halton sequences, to appear in SIAM Journal on Numerical Analysis.

### Submitted

- 4. J. Hartinger and D. Kortschak: On the efficiency of the Asmussen-Kroese estimators and its application to stop-loss transforms, submitted.
- 5. J. Hartinger and D. Kortschak, Quasi-Monte Carlo techniques and rare event sampling, submitted.
- 6. H. Albrecher and J. Hartinger: A risk model with multi-layer dividend strategy, submitted.
- 7. H. Albrecher, J. Hartinger and St. Thonhauser: Exact solutions for dividend strategies of threshold and linear barrier type in a Sparre Andersen model, submitted.

#### Dr. Gottlieb Pirsic

#### Introduction

The main focus of work this year lay in finding and working in areas that try to combine viewpoints and techniques of discrete mathematics and algebra with topics of financial and actuarial mathematics.

# **Scientific Activities 2006**

Regarding Quasi-Monte Carlo methods, (due to stimulation by the Workshop D1 of the Special Semester on Groebner Bases) some attempts were made to transfer the approach to coding theory via Groebner bases to digital net theory, especially the computation of the minimal code distance to the computation of the t-parameter seen as the minimal distance in the dual space. The idea is to encode the vector space as an appropriate polynomial ideal, then the minimum distance arises as the minimum degree of elements in this ideal. This was the subject of the talk given at the Antalya Algebra Days conference.

For the discrete Malliavin calculus approaches of Leitz-Martini and Privault, further comparisons were made. E.g., in discussion with Privault it emerged that there is a common generalization that is closer to Privault's approach, though. Privault's approach to pricing and hedging of options was made more explicit, in particular for the case of European and digital options.

In collaboration with H. Albrecher, inspired by an approach of S. Gerhold, generalizations of the Panjer recursions were studied. These arise in insurance mathematics, when the probability distributions of aggregate claim sizes are considered as the compound probabilities of given (discrete) claim size and claim number distributions. Now if the claim number distribution fulfils some recurrence equation with coefficients polynomial in the index (i.e., if it is holonomic, also called P-recursive), then the same will hold for the aggregate claims distribution, though this need then in general not be a finite recursion. If additional conditions are imposed on the claim size distribution, it can be shown that the aggregate claim distribution is again holonomic and thus fulfils a (computationally preferable) finite recursion. The methods strongly involve the use of generating functions.

The aims of the research are to find a general framework for the existing literature, according to the holonomic and generating-function viewpoint, to find relations of the claim size and number distributions to the recursion length of the aggregate claims and to try to extend the classes as far as possible. The obtained results (mainly concerning the first part and partly the second) are currently contained in a preliminary note (10 pages).

As a by-product of the work on holonomic recursions, a (multivariate) inversion of Faa di Bruno's formula (a higher-order chain rule) was derived. This is contained in the submitted paper [3].

# **Scientific Cooperations**

## <u>Internal</u>

H. Albrecher

### **External**

N. Privault, Universite de La Rochelle, Discrete Malliavin calculus

# Participation at Conferences, Scientific Visits and Talk

### Conferences

30 April – 6 May, Special Semester on Groebner Bases and Related Methods 2006, Workshop D1: Groebner Bases in Cryptography, Coding Theory, and Algebraic Combinatorics, Linz

17 May – 21 May, Antalya Algebra Days VIII, Antalya

### Scientific Talks

20 May, 2006, Antalya Algebra Days: Sudokus, quasi-Monte Carlo methods and Gröbner bases: various views on digital nets.

#### Scientific Visits

11 April - 14 April, N. Privault, Univ. de Evry-Courcouronne

#### **Publications 2006**

### **Appeared**

- 1. G. Pirsic, J. Dick, F. Pillichshammer, Cyclic digital nets, hyperplane nets and multivariate integra tion in weighted Sobolev spaces, SIAM J. Numer. Anal., 44, 1, 358-411, 2006.
- 2. G. Pirsic, A small taxonomy of integration node sets, Österreich. Akad. Wiss. Math.-Natur. Kl. Sitzungsber. II, 214, 133-140, 2006.

# Submitted

3. G. Pirsic, An inverse of the Faà di Bruno formula, submitted to American Mathematical Monthly, 2006

#### Dr. Jörn Sass

# **Scientific Achievements 2006**

In 2006 Dr Sass continued his work on portfolio optimization under transaction costs, under partial information, under risk constraints and on parameter estimation in Markov switching models.

In the continuous time Black-Scholes model, [2] deals with a combination of fixed and proportional transaction costs. For a general class of impulse control strategies the existence of an optimal strategy for maximizing the asymptotic growth rate is proved under very weak conditions. For a finite time horizon and proportional costs, a semi-smooth Newton method has been applied in a joint work with Prof Kunisch [5] to solve the free boundary problem which determines the optimal trading regions. Also for proportional transaction costs, but in a general discrete-time model, it is shown - in a cooperation with Prof Schäl - that a numeraire portfolio exists.

In [9] the utility maximization problem under a shortfall risk constraint is solved and strategies are derived, in [4] the results are applied to a hidden Markov model for the drift of the stock returns. This is a model with partial information where the underlying drift process has to be filtered from the observations. In [3] models with unobservable drift and non-constant volatility models (e.g. Hobson-Rogers-model) are considered and a Markov chain Monte Carlo method (MCMC) to estimate the relevant parameters is derived, generalized in [6]. The papers [1] and [7] deal with convex constraints on the trading strategies (including the case of stochastic volatility models) which leads to an incomplete market.

This is partly joint work with Dr Hahn and DI Putschögl in the FWF project P17947, led by Dr. Sass. Another part of the project includes parameter estimation in Markov switching models. In [8] a method of moments combined with a linear regression is used to estimate parameters, providing very good estimates for large sample sizes. For less observations and critical parameter ranges MCMC methods in [10] can improve the widely used expectation maximization algorithm. Further improvements are discussed with the Inverse Problems Group.

### **Scientific Cooperation**

#### Internal

- 1. M. Hahn, parameter estimation in Markov switching models, [3,6,10], continued.
- 2. R. Griesse, K. Kunisch, numerical solution of free boundary problems arising in finance, [5], continued.
- 3. W. Putschögl, portfolio optimization for stochastic volatility and partial information, [3,6], continued.
- 4. E. Resmerita, EM algorithm for infinite dimensional filters, discussed

### External

- 5. R.J. Elliott, University of Calgary, method of moments for Markov switching models, [8].
- 6. S. Frühwirth-Schnatter, JKU Linz, MCMC methods for Markov switching models, [10], continued.
- 7. A. Gabih, Universität Leipzig, utility maximization under risk constraints, [4,9].
- 8. U.G. Haussmann, UBC Vancouver, portfolio optimization with partial information and Lévy noise, advanced.
- 9. A. Irle, C. Prelle, Universität Kiel, portfolio optimization under transaction costs, [2], continued.
- 10.V. Krishnamurthy, UBC Vancouver, method of moments for Markov switching models, [8].
- 11.M. Schäl, Universität Bonn, numeraire portfolio under transaction costs, advanced.
- 12.R. Wunderlich, FH Zwickau, utility maximization under risk constraints, [4,9], continued.

### Participation at Conferences, Scientific Visits and Talks

### Conferences

- 1. AMaMeF 2006, Side/Antalya, Turkey, April 26-29, invited talk: Utility Maximization under Partial Information and Levy Noise
- 2. Frankfurter Stochastik Tage, March 14-17, talk: Utility maximization in a hidden Markov model with Levy noise.
- 3. 9th Vilnius International Conference on Probability and Mathematical Statistics, June 26-30, talk: Utility maximization with convex constraints and partial information.
- 4. Bachelier Finance Society 2006 Fourth World Congress, Tokyo, August 17-20, talk: Portfolio Optimization with Partial Information: A Hidden Markov Model for Stock Returns with Jumps.
- 5. Operations Research 2006, September 6-8, talk: Trading Regions under Proportional Transaction Costs
- 6. DMV Tagung, Bonn, September 17-23, invited talk: Utility maximization with partial information and further constraints.

# Scientific Visits and Colloquium Talks

- 1. Institute for Operations Research, ETH Zürich, June 13-16, invited talk: Maximizing Expected Utility Under Convex Constraints and Partial Information.
- 2. Actuarial Mathematics and Statistics Department, Heriot-Watt University, Edinburgh, October 27, invited talk: Optimal Portfolio Policies Under Transaction Costs.
- 3. Mathematisches Seminar, University of Kiel, October 31 November 3, invited talk: Optimale Handels-strategien bei Transaktionskosten.

#### Guests

- Dr. A. Gabih, University of Leipzig, March 6-10.
- Prof. R. Wunderlich, University of Applied Sciences Zwickau, March 6-10.
- DiplMath. C. Prelle, University of Kiel, March 20-31.

## Lectures

- 1. Personenversicherungsmathematik (life insurance mathematics), winter 2005/6, JKU Linz
- 2. Stochastische Differentialgleichungen (SDEs), summer 2006, JKU Linz
- 3. Schadenversicherungsmathenatik (non-life insurance, risk theory), winter 2006/7, JKU Linz

### **Publications 2006**

### Appeared

- 1. J. Sass, Portfolio optimization under partial information and convex constraints in a hidden Markov model, H.-D. Haasis, H. Kopfer, J. Schönberger, Operations Research 2005 Proceedings, Springer, Berlin, 223-228, 2006.
- 2. Irle, J. Sass, Optimal portfolio policies under fixed and proportional transaction costs, Advances in Applied Probability, 38, 916-942, 2006.

#### Accepted

- 3. M. Hahn, W. Putschögl, J. Sass, Portfolio optimization with non-constant volatility and partial information, Brazilian Journal of Probability and Statistics.
- 4. R. Wunderlich, J. Sass, A. Gabih, Optimal portfolios under bounded shortfall risk and partial information, Operations Research Proceedings 2006.
- 5. K. Kunisch, J. Sass, Trading regions under proportional transaction costs, Operations Research Proceedings 2006.
- 6. M. Hahn, W. Putschögl, J. Sass, Parameter estimation for stock models with non-constant volatility using Markov chain Monte Carlo Methods, Operations Research Proceedings 2006.
- 7. J. Sass, Utility maximization with convex constraints and partial information, Acta Applicandae Mathematicae.

#### Submitted

- 8. R.J. Elliott, V. Krishnamurthy, J. Sass, Moment based regression algorithm for drift and volatility estimation in continuous time Markov switched models, revised version submitted.
- 9. Gabih, J. Sass, R. Wunderlich, Utility maximization under bounded expected loss, submitted (RI-CAM Report 2006 24).
- 10.M. Hahn, S. Fruehwirth-Schnatter, J. Sass: Markov chain Monte Carlo Methods for parameter estimation in multidimensional continuous time Markov switching models, revised version submitted.

#### Dr. Markus Hahn

#### **Scientific Achievements 2006**

In 2006, Dr Hahn mainly worked on calibration of continuous time stock models using Markov chain Monte Carlo methods; in particular, he studied Markov switching models and non-constant volatility models. In cooperation with Prof Frühwirth-Schnatter, DI Putschögl and Dr Sass he developed different estimation algorithms, focusing on application to financial time series. He also finished his Ph.D. studies in December 2006.

# **Scientific Cooperation**

#### Internal

DI Putschögl

Dr Sass

### **External**

Prof. Frühwirth-Schnatter, IFAS, JKU Linz, on MCMC methods for Markov switching models.

### Participation at Conferences, Scientific Visits and Talks

# Conferences (including talks)

- Frankfurter Stochastik Tage, Frankfurt, Germany, March 14-17, talk: MCMC Methods for Parameter Estimation in Hobson-Rogers-Type Volatility Models.
- Workshop on Statistical Inverse Problems, University of Göttingen, March 23-25.
- Volatility Models, Young Statisticians Meeting 2006, Edinburgh, April 19-20, talk: MCMC Methods for Parameter Estimation in Hobson-Rogers-Type Volatility Models.
- Summer School on Risk Measurement and Optimal Investment, LMU, Munich, June 29-30.
- Operations Research 2006, Karlsruhe, September 6-8, talk: Parameter Estimation for Stock Models with Non-Constant Volatility Using MCMC Methods.

# Scientific visits (including talks)

October 18-19, 2006, TU Munich, SFB 386, invited talk: Markov Chain Monte Carlo Methods for Parameter Estimation in Markov Switching Models.

#### Lectures

Financial Mathematics project at "Applied mathematics week" for intellectually gifted high school pupils organised by "Stiftung Talente", February 2006.

### **Publications 2006**

#### Ph.D. thesis

1. MCMC Calibration of Continuous Time Stock Models with Regime Switching and Stochastic Volatility.

# Accepted

- 2. M. Hahn, W. Putschögl, J. Sass, Portfolio optimization with non-constant volatility and partial in formation, Brazilian Journal of Probability and Statistics.
- 3. M. Hahn, W. Putschögl, J. Sass, Parameter estimation for stock models with non-constant volatility using Markov chain Monte Carlo Methods, Operations Research Proceedings 2006.

### Submitted

4. M. Hahn, S. Frühwirth-Schnatter, J. Sass: Markov chain Monte Carlo Methods for parameter esti mation in multidimensional continuous time Markov switching models, revised version submitted.

## Wolfgang Putschögl advised by Dr. Jörn Sass

Scientific Achievements 2006

In 2006 the work of DI Putschögl was focused on portfolio optimization under partial information. In [1] explicit representations of the optimal trading strategy using Malliavin calculus have been derived in a hidden Markov model for the drift and non-constant volatility; [2] deals with the parameter estimation for this model. Furthermore optimal consumption strategies have been considered under partial information. Currently, explicit consumption and investment strategies are derived under fairly general conditions.

### **Scientific Cooperations**

#### Internal

Dr Hahn

Dr Sass

# Participation at Conferences, Scientific Visits and Talks

# Conferences (including talks)

- Frankfurter Stochastik Tage, Frankfurt, Germany, March 14-17, talk: Optimizing the Terminal Wealth under Partial Information for Non-Constant Volatility.
- Spring School of Finance, Bologna, Italy, May 18-19.
- Summer School on Risk Measurement and Optimal Investment, LMU, Munich, Germany, June 29-30.
- Operations Research 2006, Karlsruhe, Germany, September 6-8, talk: How to make Portfolios more robust.

## Scientific visits (including talks)

- University of Bologna, Italy, May 25, invited talk: On Multidimensional Asset Management using Non-Constant Volatility.
- University Roma Tor Vergata, Italy, May 23, invited talk: A Multidimensional Generalization of the Hobson-Rogers Model Applied to Portfolio Optimization.

# **Teaching**

Seminar Financial mathematics (together with Prof Larcher), winter 2006, JKU Linz Lecture Financial mathematics and statistics 1, winter 2006, University of Applied Sciences Linz Lecture Financial mathematics and statistics 2, summer 2006, University of Applied Sciences Linz

#### **Publications 2006**

- 1. M. Hahn, W. Putschögl, J. Sass, Portfolio optimization with non-constant volatility and partial in formation, Brazilian Journal of Probability and Statistics, to appear.
- 2. M. Hahn, W. Putschögl, J. Sass, Parameter Estimation for Stock Models with Non-Constant Vola tility using Markov Chain Monte Carlo Methods, Operations Research Proceedings 2006, to appear.

#### Dr. Klaus Scheicher

#### Scientific Achievements 2006

In 2006, Dr. Scheicher studied applications of quasi Monte Carlo algorithms in ruin theory. For the Poisson model, the non-ruin probability is given by the classical Pollaczeck-Khinchine formula, which is an exponential weighted sum of convolution integrals. The weights of the integrals are exponentially decreasing with growing dimension. Therefore, the variables of the high-dimensional integrals are, in some sense, less important than the variables occurring in the low-dimensional integrals. This fact gives rise to the suggestion that quasi Monte Carlo techniques can lead to improvements for numerical determination of these expressions. This suggestion has already been hardened by numerical simulations. In [6], the development of a corresponding theory for such applications has been started. In particular, the case of Pareto distributed claims has been studied.

In [4] and [5], some collaborations in number theory have been continued. In [4], the set of all three-dimensional shift radix systems has been completely characterized. This result was obtained by implementing an algorithm of Akiyama and Scheicher which was given in a preceding paper from 2005. In [5], the set of numbers in an algebraic function field has been characterized which admit a purely periodic beta-expansion. Such expansions have been introduced by Scheicher in 2005.

# Participation at Conferences, Scientific Visits and Talks

### Conferences

Frankfurter Stochastik Tage, 2006. Talk: Efficient simulation of Levy areas. Numerical Methods for Finance, Dublin 2006. : Efficient simulation of Levy areas.

### Scientific Visits:

6.2-24.2. Faculté des Sciences de Sfax (Tunisia)

Invited Talk: From number systems to shift radix systems.

Invited Talk: On the efficiency of numerical Integration with Applications in Finance.

# **Scientific Cooperations**

# **Internal Cooperations**

H. Albrecher

T. Beck (Symbolic Computation Group)

### **External Cooperations**

A. Huszti, University of. Debrecen

M. Jellali, Faculté des Sciences de Sfax

M. Mkaouar, Faculté des Sciences de Sfax

P. Surer. MU Leoben

J. Thuswaldner, MU Leoben

#### **Publications 2006**

### **Accepted**

- 1. K. Scheicher, \$beta\$-expansions in algebraic function fields over finite fields, Finite Fields and Their Applications, to appear.
- 2. K. Scheicher, Complexity and effective dimension of discrete Levy areas, Journal of Complexity, to appear.

### **Submitted**

- 3. S. Akiyama, K. Scheicher, Symmetric shift radix systems and finite expansions, submitted.
- 4. A.Huszti, K.Scheicher, P.Surer, J.Thuswaldner, Three dimensional symmetric shift radix systems, submitted
- 5. M.Jellali, M.Mkaouar, K.Scheicher, Purely periodic beta-expansions with Pisot unit bases in function fields, submitted.

# Work in progress

6. K. Scheicher, Computation of ruin probabilities by quasi Monte Carlo Simulation.

#### Dr. Arne Winterhof

#### **Scientific Achievements 2006**

Dr. Winterhof has raised a new FWF project (P19004, "Pseudorandom sequences").

With Prof. Topuzoglu (Istanbul) he wrote a book chapter on recent developments on pseudorandom sequences for quasi-Monte Carlo methods and cryptography [2].

In cooperation with the symbolic computation group (Dr. Piroi, [8]) and Prof. Shparlinski (Sydney, [23]), Dr. Winterhof proved the existence of a polynomial time quantum algorithm for the period finding problem for all sequences with moderate autocorrelation.

In 2006 Dr. Winterhof's research focused on

- 1. pseudorandom number generation (in view of quasi-Monte Carlo applications for financial mathematics) [1,4,6,12-14,20,21] in joint work with Prof. Shparlinski, E. ElMahassni (Sydney), Prof. Aly (Cairo), Prof. Niederreiter (Singapore) and Dr. Meidl (Istanbul).
- 2. cryptographic functions and sequences [3,7,9-11,15-19,22] in joint work with N. Brandstätter (RI CAM), Prof. Aly, Prof. Garaev and Prof. Luca (Mexico), Prof. Shparlinski, Dr. Meidl, Dr. Kiltz (Amsterdam), Dr. Adelmann (Braunschweig) and Prof. Lange (Kopenhagen).

He supervised a bachelor thesis (K. Nachbagauer) and has two current PhD-students (N. Brandstätter, H. Schön).

He is co-editor of Finite Fields and Their Applications.

### **Scientific Cooperations**

#### Internal

- N. Brandstätter: Cryptography and pseudorandom numbers
- F. Piroi (Symbolic Computation): Quantum period reconstruction

# **External**

- H. Aly (Cairo): Cryptographic functions and sequences
- C. Adelmann (Braunschweig): Cryptographic functions
- E. Kiltz (California): Cryptographic functions
- T. Lange (Kopenhagen): Boolean functions
- E. El Mahassni (Sydney): Pseudorandom numbers
- M. Garaev (Mexico): Sidelnikov sequences
- F. Luca (Mexico): Sidelnikov sequences
- W. Meidl (Istanbul): Cryptography, pseudorandom numbers
- H. Niederreiter (Singapore): Pseudorandom numbers
- I. Shparlinski (Sydney): Cryptography, pseudorandom numbers, quantum algorithms
- A. Topuzoglu (Istanbul): Pseudorandom numbers

### Lectures, Conferences, Scientific Visits and Talks

#### Lectures

Winter term 05/06: Cryptography (JKU Linz)

Summer term 06: Algorithmic number theory (JKU Linz)

Winter term 05/06: Coding theory (JKU Linz)

#### Conferences

invited: Complexity measures for binary sequences, Antalya Algebra Days 2006 contributed: On the discrepancy and linear complexity of some counter-dependent recurrence sequences, SETA 2006

### Scientific Visits

Hungarian Academy of Sciences Budapest:one week

University of Santander: 2 weeks

### **Invited Scientific Talks**

Cyclotomic R-orthomorphisms over finite fields, TU Vienna Pseudorandom sequences, Hungarian Academy of Sciences

#### **Publications 2006**

### <u>Appeared</u>

- 1. Shparlinski and A. Winterhof, On the discrepancy and linear complexity of some counter-dependent recurrence sequences, Proceedings of Sequences and their Applications 2006, Lecture Notes in Computer Sciences 4086 (2006), 295—303.
- 2. Topuzoglu and A. Winterhof, Pseudorandom sequences, in Topics in Geometry, Cryptography and Coding Theory, Springer, Berlin, 2006.
- 3. N. Brandstätter and A. Winterhof, Linear complexity profile of binary sequences with small correlation measure, Periodica Mathematica Hungarica 52 (2006), 1—8.
- 4. E.D. El Mahassni and A. Winterhof, On the distribution and linear complexity of counter-dependent nonlinear congruential pseudorandom number generators, JP Journal of Algebra, Number Theory and Applications 2 (2006), 1—6.
- 5. Shparlinski and A. Winterhof, Constructions of approximately mutually unbiased bases, Proc. LATIN'06, Lecture Notes in Computer Sciences 3886 (2006), 793—799.
- 6. E.D. El-Mahassni, I. Shparlinski and A. Winterhof, Distribution of nonlinear congruential pseudorandom numbers for almost squarefree integers, Monatshefte für Mathematik 148 (2006), 297—307.

- 7. H. Aly and A. Winterhof, On the k-error linear complexity over F\_p of Legendre and Sidelnikov sequences, Designs, Codes and Cryptography 40 (2006), 369—374.
- 8. F. Piroi and A. Winterhof, Quantum period reconstruction of binary sequences, Proceedings AAECC 16, Lecture Notes in Computer Sciences 3857 (2006) 60-67.
- 9. M. Garaev, F. Luca, I. Shparlinski and A. Winterhof, On the lower bound of the linear complexity over F\_p of Sidelnikov sequences, IEEE Transactions on Information Theory 52 (2006), 3299-3304.
- 10. H. Aly and A. Winterhof, Polynomial representations of the Lucas logarithm, Finite Fields and Their Applications 12 (2006), 413—424.
- 11. N. Brandstätter and A. Winterhof, Approximation of the discrete logarithm in finite fields of even characteristic by real polynomials, Archivum Mathematicum (Brno) 42 (2006), 43—50.
- 12. E. D. El-Mahassni and A. Winterhof, On the distribution of nonlinear congruential pseudorandom numbers in residue rings, International Journal of Number Theory 2 (2006), 163—168.
- 13. Winterhof, On the distribution of some new explicit inversive pseudorandom numbers and vectors, Proceedings MC2QMC 2004,487--499, Springer, Berlin, 2006.
- 14. H. Aly and A. Winterhof, On the linear complexity profile of nonlinear congruential pseudorandom number generators with Dickson polynomials, Designs, Codes and Cryptography 39 (2006), 155—162.
- 15. Shparlinski and A. Winterhof, On the nonlinearity of linear recurrence sequences, Applied Mathematics Letters 19 (2006), 340—344.
- 16. W. Meidl and A. Winterhof, Some notes on the linear complexity of Sidelnikov-Lempel-Cohn-Eastman sequences, Designs, Codes and Cryptography 38 (2006), 159—178.
- 17. E. Kiltz and A. Winterhof, Polynomial interpolation of cryptographic functions related to Diffie-Hellman and discrete logarithm problem, Discrete Applied Mathematics 154 (2006), 326—336.
- 18. Adelmann and A. Winterhof, Interpolation of functions related to the integer factoring problem, Lecture Notes Computer Science 3969 (2006), 144-154.
- 19. N. Brandstätter and T. Lange and A. Winterhof, On the non-linearity and sparsity of Boolean functions related to the discrete logarithm in finite fields of characteristic two, Lecture Notes Computer Science, 3969 (2006), 135—143.

#### Accepted

- 20. H. Niederreiter and A. Winterhof, Exponential sums for nonlinear recurring sequences, Finite Fields and Their Applications, to appear.
- 21. W. Meidl and A. Winterhof, On the linear complexity profile of nonlinear congruential pseudorandom number generators with Redei functions, Finite Fields and Their Applications, to appear.

#### Submitted

- 22. H. Aly, W. Meidl and A. Winterhof, On the k-error linear complexity of cyclotomic sequences, submitted.
- 23. Shparlinski and A. Winterhof, Quantum period reconstruction of noisy sequences, submitted.

# Nina Brandstätter advised by Dr. Arne Winterhof

## **Scientific Achievements 2006**

In 2006 Mag. Brandstätter's research focused on cryptographic functions and sequences.

In [1,3] Mag. Brandstätter, Prof. Lange (Kopenhagen) and Dr. Winterhof proved complexity lower

bounds on functions approximating the discrete logarithm in a finite field of characteristic two complementing earlier results for odd characteristic. The main mean in the odd characteristic case are bounds on quadratic character sums. In particular a compensation for the quadratic character was introduced.

In [2] Mag. Brandstätter and Dr. Winterhof proved an interesting relation between linear complexity and correlation measure, two quality measures for sequences which have been considered independent before.

In [4] Mag. Brandstätter and Dr. Meidl analyzed some particularly promising cryptographic sequences, the Sidelnikov sequences.

#### **Scientific Cooperations**

#### Internal

Dr. Winterhof (Financial Mathematics): Cryptographic functions and sequences

### **External**

T. Lange (Kopenhagen): Boolean functions W. Meidl (Istanbul): Cryptographic sequences

I. Shparlinski (Sydney): Cryptography

A. Topuzoglu (Istanbul): Pseudorandom numbers

### **Conferences: Talks**

Antalya Algebra Days: Sidel'nikov Sequences over F d

Sequences and Their Applications (Beijing): On the Linear Complexity of Sidel'nikov Sequences over F d

#### **Publications 2006**

#### Appeared

- 1. N. Brandstätter and A.Winterhof, Approximation of the discrete logarithm in finite fields of even characteristic by real polynomials, Archivum Mathematicum, 42(1):43--50, 2006.
- 2. N. Brandstätter and A. Winterhof, Linear complexity profile of binary sequences with small correlation measure, Periodica Mathematica Hungarica, 52(2):1--8, 2006.
- 3. N. Brandstätter, T. Lange and A. Winterhof, On the non-linearity and sparsity of Boolean functions related to the discrete logarithm in finite fields of characteristic two, Lecture Notes Computer Science, 3969, pages 135--143, 2006.
- 4. N. Brandstätter and W. Meidl, On the linear complexity of Sidel'nikov Sequences over F\_d, Lecture Notes Computer Science, 4086, 47--60. Springer, 2006.

# **Submitted**

5. N. Brandstätter, Quality measures for pseudorandom number generators, PhD thesis.

#### Dr. Domingo Gomez advised by Dr. Arne Winterhof

Dr. Gomez is a former PhD student of J. Gutierrez (Santander) and joined RICAM in October 2006. He was supported by a grant of the Spanish ScienceFund and will be employed in Dr. Winterhof's FWF project in 2007.

#### **Scientific Achievements 2006**

In joint work with Prof. Blackburn (London), Prof. Gutierrez (Santander), Prof. Shparlinski and A. Ibeas (Santander) Dr. Gomez analyzed the predictability of several pseudorandom number generators for cryptographic applications [1,2,4] and analyzed exponential sums of nonlinear pseudorandom number generators with Dickson polynomials [3].

# **Scientific Cooperations**

#### Internal

A. Winterhof (Financial Mathematics)

### External

S.Blackburn (London)

J. Gutierrez (Santander)

A. Ibeas (Santander)

I. Shparlinski (Sydney)

### **Publications 2006**

## **Appeared**

- 1. S. R. Blackburn, D. Gómez Pérez, J. Gutierrez and I. Shparlinski, Reconstructing noisy polynomial evaluation in residue rings, Journal of Algorithms. 61-12, 45-58, 2006.
- 2. D. Gómez, J. Gutierrez and A. Ibeas, Integer factoring with extra information, Proc. RECSI 2006. Barcelona, Spain. 573—583.
- 3. D. Gómez, J. Gutierrez and I. Shparlinski, Exponential sums with Dickson polynomials, Finite Fields and Their Applications, 12 (2006), 16-15.
- 4. D. Gómez, J. Gutierrez, Alvar Ibeas, Attacking the Pollard generator, IEEE Trans. Information Theory, 52(12) 1-7, 2006.

#### Submitted

5. D. Gómez, J. Gutierrez and A. Ibeas, An algorithm for finding small roots of multivariate polynomials over the integers, University of Cantabria, Preprint 2006.

# 2.4. GROUP "ANALYSIS OF PARTIAL DIFFERENTIAL EQUATIONS"

# **Group Leaders:**

o.Univ.-Prof. Dr. Peter Markowich ao.Univ.-Prof. Dr. Christian Schmeiser

# Researchers funded via ÖAW/Upper Austrian government funds:

Dr. Keith Anguige

Dr. Shun-Yin Henry Chu

Dr. Massimo Fonte

Dr. Massimo Fornasier

Dr. Arjan Kuijper (half-time employed at RICAM 01.01.2006-31.10.2006, full-time since 01.11.2006)

Dr. Lukas Neumann

## Introduction by Group Leader Prof. Christian Schmeiser

Three new PostDocs have been hired in 2006 for several reasons. Firstly, to continue the activities of the group in Mathematical Biology. For this purpose Keith Anguige has been hired. Massimo Fornasier is strengthening the activities in the analysis of PDE methods for image processing. Finally, Massimo Fonte represents the third research direction of the group in conservation laws and kinetic transport models.

The scientific achievements include modelling work on the macroscopic description of ensembles of biological cells with an emphasis an short range interactions such as cell-cell adhesion. The models considered there have several qualitative properties in common with another subject of research: the Cahn-Hilliard equation, which models phase change processes and is also used in image processing. The image processing activity includes work on PDE methods for mathematical inpainting as well as contributions to shape analysis. The work on existence result for the Camassa-Holm equation (a model for water waves) and on the long time behaviour of semiclassical kinetic models for quantum particles can be seen as PDE analysis in the classical sense.

From the organisational point of view, the EMS summer school on *Mathematics in Molecular Cell Biology* has been coorganized by C. Schmeiser and took place at RICAM in September 2006. During two weeks, about 50 participants attended the following short courses:

- Willi Jäger (Universität Heidelberg): Multiscale Models of Cells
- Alex Mogilner (University of California Davis): Quantitative Approaches to Cell Motility and Division
- Wolfgang Nonner (University of Miami): Modeling and Simulation of Ion Channels
- Hans Othmer (University of Minnesota): Analysis of Complex Reaction Networks
- Christoph Schütte (Free University Berlin, MATHEON): Metastability in Biological Systems as well as a number of additional lectures.

Results of the research work of the PostDocs are detailed in the following sections.

### Dr. Keith Anguige

### Work before joining RICAM

Before joining RICAM, Keith Anguige held a Leverhulme Special Research Fellowship in `modelling bacterial behaviour' at the University of Nottingham. The purpose of his work was to investigate anti-bacterial therapies targeted at the quorum-sensing system of Pseudomonas aeruginosa colonies.

The main part of the project consisted of analysing topically-applied anti-quorum-sensing and antibiotic treatments in the context of a multi-compartment continuum model of a P. aeruginosa biofilm. The resulting model equations comprised a coupled hyperbolic-parabolic system for the relevant bacterial growth dynamics and reaction kinetics, and some light could be shed on the efficacy of various treatment strategies by using a combination of mathematical analysis (Maximum Principle, characteristics) and numerical simulations.

#### **Scientific Achievements 2006**

At RICAM, continuing his work in Mathematical Biology, but in a slightly different specialisation, Dr. Anguige has been collaborating with Christian Schmeiser on a specific adhesion-diffusion problem in cell motility. In particular, a discrete 1-d model for the motion of a system of particles which can to some extent move randomly, but whose movements are restricted by volume filling and cell-to-cell adhesion has been written down and subjected to numerical and mathematical investigation - the motivation for the modelling is to gain an understanding of structure formation in processes such as gastrulation and vasculogenesis in the early embryo.

For small values of the adhesion coefficient, the continuum limit of the model (a nonlinear diffusion equation for the cell density) has a positive diffusivity, and numerical solutions of the discrete model closely mimic the behaviour of this equation; in particular, all initial inhomogeneities in the density distribution smooth out over time, leaving a uniform profile at steady state.

On the other hand, for large values of the adhesion coefficient a number of rather more interesting phenomena, such as plateau formation, fine spatial oscillations, and coarsening behaviour become possible. These phenomena are related to the ill-posedness of the limiting equation in this case, and can be understood with a combination of linear stability analysis of the discrete model and steady-state analysis of the limiting continuum equation (and higher-order corrections thereof).

One version of the corrected equation, which is rather similar to the viscous Cahn-Hilliard model for phase separation in alloys, has been shown to be well-posed, and, by analogy, it is expected that the slow coarsening behaviour observed in solutions of the discrete model may be understood by carrying out an appropriate asymptotic analysis of this higher-order equation.

# **Scientific Cooperations**

#### Internal

Prof. Chrisitian Schmeiser

# Participation at Conferences, Scientific Visits and Talks

June 20th, 2006: Talk at RICAM Workshop - Mathematics in Biosciences: Honouring the 60th Birthday of Vincenzo Capasso, Linz.

September, 2006: Attendance at the EMS Summer School `Mathematics in Molecular Cell Biology'.

### **Publications**

# **Appeared**

K. Anguige, J. R. King and J. P. Ward: A multi-phase mathematical model of quorum sensing in a maturing Pseudomonas aeruginosa biofilm, Mathematical Biosciences, 203(2), pp 240-276, 2006.

#### Submitted

K. Anguige, C. Schmeiser: A one-dimensional model of cell diffusion and aggregation, incorporating volume filling and cell-to-cell adhesion.

# Dr. Shun-Yin Henry Chu

#### Scientific Achievements 2006

He obtained new results on stability/instability and asymptotic behaviour for transition solutions of the Cahn-Hilliard equation with M.Burger, P.Markowich, and C.B.Schoenlieb. More precisely, they proposed an analytic description of stability of the solution in time via the Willmore functional and discussed various kinds of small perturbations on some interesting profiles by numerical exhibition. They found in their various numerical computations that the high frequency, small amplitude oscillating perturbations with respect to kink solutions play an important role on the evolution of the Willmore functional so that the instabilities of the problem can be understood in a new sense. Moreover, the rate of asymptotic convergence to stable solution in \$H^{-2}(\Omega)\$ can be controlled implicitly by the variation of the Willmore functional, which might be computed numerically for some particular initial data.

He considered no-slip boundary layer problems of fluid mechanics. In the process of his previous works, he obtained a partial regularity criterion of three-dimensional self-similar weak solutions of transformed Prandtl's problem with both stagnation point flows and positive swirls.

Some topics such as regularity, blowup, well-posedness and asymptotic behaviour of Camassa-Holm equation had being explored with Y.Zhou. In particular, they worked on the characterization of the blowup solution by initial data.

#### **Scientific Cooperations**

#### Internal

Prof. Dr. Martin Burger(Now in Westfaelische Wilhelms Universitaet Muenster, Germany)

Prof. Dr. Peter Markowich

Prof. Dr. Christian Schmeiser

# External

Carola Schoenlieb, Technische Universität Wien, Austria Dr. Yong Zhou, East China Normal University, China

# Participation at Conferences, Scientific Visits and Talk

#### Conferences

The 3<sup>rd</sup> East China Partial Differential Equations Conference, Contemporary Partial Differential Equations – Frontier and Prospect, East China Normal University, Shanghai, China, 3 July – 7 July, 2006

#### Scientific Visits

East China Normal University, Shanghai, China, 26 – 30 June, 28 – 29 July, 2006 Zhejiang University, Hangzhou, China, 1 July – 2 July, 2006 University of Science and Technology of China, Hefei, Anhui, China, 6 July – 10 July, 2006

# Scientific Talks

Discussion of unstable states of the Cahn-Hilliard equation, Zhejiang University, 1 July, 2006

#### **Publications 2006**

#### Submitted

- 1. Shun-Yin Chu, Global Existence of Weak Solutions to 3-D Axisymmetric Prandtl's System with both Stagnation Point Flow and Positive Swirls
- 2. M. Burger, S.-Y. Chu, P. Markowich and C.B. Schoenlieb, The Willmore Functional and Instabilities in the Cahn-Hilliard Equation

#### Dr. Massimo Fonte

# Work before joining RICAM

Before joining RICAM, Massimo Fonte obtained a Ph.D. in Mathematical Analysis in the sector of "Functional Analysis and Application" at S.I.S.S.A./I.S.A.S. Trieste (Italy) at the end of October 2005. The title of his thesis is "Analysis of singular solution for two nonlinear wave equations".

Dr. Fonte's research area concerns non-linear partial differential equations of hyperbolic type. In his thesis, he studied some non-linear models arising from mathematical physics and, in particular, the issue of blow-up for a non-linear shallow water wave equation in 1-D and for a discrete model of the Boltzmann equation in 2-D. He mainly devoted his research to the construction of solutions which are stable with respect to a Wasserstein-like metric. He is also interested in conservation laws in 1-D and multi-D.

# **Scientific Achievements 2006**

Dr. Fonte's research work in 2006 was mainly dedicated to the study of the Camassa-Holm equation, which is an analytic model of the water waves in a shallow water regimen. This non-linear P.D.E. has a Hamiltonian structure and it was widely studied by several authors in the nineties, but a general result of existence and continuous dependence with respect to the initial data could not be found. In collaboration with Prof. A. Bressan, a first result was proved for spatially periodic initial data by introducing a distance, defined in term of optimal transportation. Recently, Dr. Fonte has extended this result to a wider class of initial data. A key role is played by the solitary waves of the system, because of their persistence in time. Starting from the P.D.E., a Hamiltonian system of O.D.E. for the coefficients of the solitary waves was constructed. This system was well studied in the literature whenever blow-up does not occur, but classical solutions cannot be extended in presence of the wave breaking. The solutions are thus obtained by performing a change of variable, in order to resolve all the singularities which appear in a finite time. All these results can be applied only for solutions which conserve the energy of the model.

The second part of the work by Dr. Fonte is focused on the study of the so-called "dissipative solutions" of the Camassa-Holm equation. In this case, this equation has the physical meaning as "hyperlastic-rod wave equation". He performed the construction of a semigroup of dissipative solutions, via resolution of a discontinuous system of O.D.E., and the definition of a metric space (X, d) for which continuous dependence fits well. This work is still in progress.

#### **Scientific Cooperations**

#### External

Prof. A. Bressan, Pennsylvania State University (USA).

# Dr. F.S. Priuli, S.I.S.S.A./I.S.A.S. (Italy) & NTNU Trondheim (Norway)

# Participation at Conferences, Scientific Visits and Talk

#### Conferences

Boltzmann Equation and Fluidodynamic Limits. Honouring the memory of L. Boltzmann (1844-1906). S.I.S.S.A./I.S.A.S., Trieste (Italy), June 12-17, 2006.

Eleventh International Conference on Hyperbolic Problems. Theory, Numeric, Applications. École Normale Supérieure de Lyon, Lyon (France), July 17-21, 2006.

# Scientific Talks

February 2006, Talk in the Group Seminar at RICAM.

#### **Publications 2006**

#### Submitted

M. Fonte, Conservative solutions of the Camassa-Holm Equation on the real line, submitted.

#### Dr. Massimo Fornasier

# Work before joining RICAM

The research activity of Dr. Fornasier has been focused on developments of the theory of frames, i.e., stable redundant non-orthogonal expansions in function spaces, and their use in modelling, PDE, and numerical analysis. Introduced by Duffin and Schaeffer in 1952 in the study of nonharmonic Fourier series, frames play an important role in wavelet theory as well as in Gabor (time-frequency) analysis. Besides already traditional and relevant applications of frames in signal processing, image processing, data compression, pattern matching, sampling theory, communication and data transmission, recently the use of frames also in numerical analysis for the solution of operator (PDE and integral) equations is investigated. Dr. Fornasier contributed to the formulation of a general theory for the characterization of Banach function spaces by means of frames [A1,A4,S2]. Once functions can be represented by a frame in a stable way, one may question how such expansions can be used for the solution of operator equations. The paper [A5] presents the foundations of adaptive methods for the numerical solution of certain linear and nonlinear equations by means of frame discretizations on overlapping domain decompositions. Frames in image processing have been used for the formulation of fast and accurate pattern recognition methods in [A3]. These methods have been implemented for the development of the Mantegna Project, i.e., the complete restoration of the famous A. Mantegna's frescoes in Padua (Italy).

Before joining RICAM, Dr. Massimo Fornasier was Ph.D. student at the University of Padua in Italy (1999-2002), he was co-author and scientific responsible of the Mantegna Project (<a href="www.progettomantegna.it">www.progettomantegna.it</a>), he joined the EU-Research Training Network HASSIP (Harmonic Analysis and Statistics for Signal and Image Processing, University of Vienna, Austria, and University of Marburg, Germany, 2003-2004), and he obtained an EU-Invidual Marie Curie Fellowship, project Flexible Time-Frequency Decompositions and Adaptive Treatment of Operator Equations by Frames, at the University of Vienna (2004-2006).

# **Scientific Achievements 2006**

The construction of bases on domains with complicated geometry is usually very cumbersome and finally it may conclude with unstable results. The use of overlapping domain decompositions avoids

the problem of interfacing bases through boundaries, but it creates regions of redundancy and it results in a frame instead of a basis. Some relevant results in 2006 are concerned with adaptive numerical schemes for PDE based on frame discretizations [A7,S1] on overlapping domain decompositions. Emphasis is given to linear elliptic problems and magneto-hydrodynamic models. A new model based on variational calculus and the solution of a system of nonlinear PDE for color image processing, and in particular for re-colorization, is proposed in [A2]. The model is analyzed in [S6-7] where existence of solutions and efficient numerical schemes for their approximation are presented. Applications to the re-colorization of the Mantegna's frescoes are included, see [A3].

Two major Dr. Fornasier's external projects were approved in Oct.-Nov. 2006: 2006 WWTF "Five Senses - Call 2006" (4 years, 400 kEuro), "Mathematical Methods for Image Analysis and Processing in Visual Arts" (joint project with Prof. Dr. P. Markowich), and 2006 Outgoing International Marie Curie Fellowship (18 months, 120 kEuro) "Sparse Approximation for Blind Source Separation" (individual project). The first project is concerned with variational and PDE methods for image analysis in visual arts, and in particular for the *mathematical inpainting* of the Neidhart frescoes in Vienna (1.,Tuchlauben 19). The second project is focused on the solution of inverse problems with sparsity constraints (see [S5]), and applications in neuroimaging (fMRI and magnetoencephalography). Dr. Fornasier joined RICAM on June 1, 2006 and, with an unpaid leave of 1 year, started a cooperation within the Program in Applied and Computational Mathematics (PACM), Princeton University, USA, on the basis of this second individual project.

# **Scientific Cooperations**

#### Internal

Prof. Dr. Peter Markowich

Dr. Arjan Kuijper

PD. Dr. Ronny Ramlau (Inverse Problems)

#### External

Dr. Maria Charina, Institute for Applied Mathematics, University of Dortmund Germany

Prof. Costanza Conti, Energetic Department "Sergio Stecco", University of Florence Italy

Prof. Stephan Dahlke, AG Numerik/Wavelet-Analysis Group, Philipps-University of Marburg Germany

Prof. Ingrid Daubechies, Program in Applied and Computational Mathematics, Princeton University USA

Prof. Hans G. Feichtinger,, Numerical Harmonic Analysis Group, University of Vienna Austria

Prof. Karlheinz Groechenig, Numerical Harmonic Analysis Group, University of Vienna Austria

Prof. Laura Gori, Department of Math. Methods and Models for Appl. Sci., University of Rome "La Sapienza Italy"

Dr. Riccardo March, IAC "Mauro Picone" Rome, National Council of Research Italy

Prof. Francesca Pitolli, Department of Math. Methods and Models for Appl. Sci., University of Rome "La Sapienza Italy"

Dr. Holger Rauhut, Numerical Harmonic Analysis Group, University of Vienna Austria

Prof. Gabriele Steidl, Faculty of Mathematics and Computer Sciences, University of Mannheim Germany

Prof. Rob Stevenson, Department of Mathematics, University of Utrecht Holland

Dr. Gerd Teschke, Konrad-Zuse-Zentrum fuer Technomathematik Berlin Germany

Prof. Domenico Toniolo, Department of Physics "G. Galilei", University of Padua Italy

# Participation at Conferences, Scientific Visits and Talk

### Conferences

[C1] Adaptive algorithms. Mobile digital signal transmission, Int. Conf. MathMod, 8-10 Feb. 2006, Vienna, Austria.

- [C2] *Metodi di campionamento non uniforme e variazionali per il restauro di immagini*, Convegno nazionale GNCS, 14-16 Feb. 2006, Dipartimento di Matematica "F. Enriques", Università di Milano.
- [C3] Fast algorithms for inverse problems with joint sparsity constraints, Int. Conf. Recent Progress in Spline and Wavelet Approximation, 14-16 Jun. 2006, Università di Roma "La Sapienza".
- [C4] Linear inverse problems with joint sparsity constraints, Mini-workshop "Sparsity and Applications", 21 Jun. 2006, Radon Institute for Computational and Applied Mathematics (RICAM), Linz, Austria.
- [C5] Variational methods, inpainting, and art restoration, Int. Conf. "Nonlinear PDEs: Homogenization and Kinetic Equations", 26-30 Jun. 2006, Vienna, Austria.
- [C6] Fast reconstruction algorithm for sparse multivariate and vector valued data, 1<sup>st</sup> Dolomites workshop on constructive approximation and applications, 8-12 Sept. 2006, Alba di Canazei, Italia.
- [C7] Recovery algorithms for vector valued data with joint sparsity constraints, Sparse Approximation Workshop, 10-12 Nov. 2006, Princeton University, USA.

#### Scientific Visits

AG Numerik/Wavelet-Analysis Group, Fachbereich Mathematik und Informatik der Philipps-Universitaet Marburg, Germany, 16-20 Gen. 2006, 24-20 Sett. 2006.

Program in Applied and Computational Mathematics, Princeton University, USA, Oct. 2006-Oct. 2007.

# Scientific Talks

- [T1] *Variational calculus, wavelets, and image processing,* Radon Institute for Computational and Applied Mathematics (RICAM), 7 Feb. 2006, Linz, Austria.
- [T2] Faithful recovery of vector valued functions from incomplete data. Recolorization and art restoration, Colloquium, Program in Applied and Computational Mathematics, Princeton University, 20 Nov. 2006, Princeton, USA.
- [T3] Faithful recovery of vector valued functions from incomplete data. Recolorization and art restoration, Colloquium, Department of Mathematics, University of Goettingen, 19 Dec. 2006, Goettingen, Germany.

#### **Publications 2006**

#### Appeared [A]

- 1. H. G. Feichtinger, M. Fornasier: *Flexible Gabor-wavelet decompositions for L2 Sobolev Spaces*, Annali di Matematica Pura e Applicata, **185(1)**, 2006, pp. 105-131.
- 2. M. Fornasier: *Nonlinear projection recovery in digital inpainting for color image restoration*, Journal of Mathematical Imaging and Vision, **24(3)**, 2006, pp. 359 373.
- 3. R. Cazzato, G. Costa, A. Dal Farra, M. Fornasier, D. Toniolo, D. Tosato, C. Zanuso: *Il Progetto Mantegna: storia e risultati* (Italian), in "Andrea Mantegna. La Cappella Ovetari a Padova" (Eds. Anna Maria Spiazzi, Alberta De Nicolo' Salmazo, Domenico Toniolo), Skira, 2006.
- 4. M. Fornasier: *Banach frames for alpha-modulation spaces*, **to appear** in Applied and Computational Harmonic Analysis.
- 5. S. Dahlke, M. Fornasier, T. Raasch: *Adaptive frame methods for elliptic operator equations*, **to appear** in Advances in Computational Mathematics.
- 6. M. Fornasier: *On some stability results of localized atomic decompositions*, to appear in Matematica e delle sue Applicazioni.
- 7. S. Dahlke, M. Fornasier, T. Raasch, R. Stevenson, M. Werner: *Adaptive frame methods for elliptic operator equations: the steepest descent approach*, **to appear** in IMA Journal of Numerical Analysis.

#### Submitted [S]

- 1. Charina, C. Conti, M. Fornasier: *Adaptive frame methods for nonliear variational problems*, arXiv:math.NA/0503381, 2006.
- 2. S. Dahlke, M. Fornasier, H. Rauhut, G. Steid, G. Teschke: *Generalized coorbit theory, Banach frames, and the relation to alpha-modulation spaces,* Bericht Nr. 2005-6, Philipps-Universitaet Marburg, 2006.
- 3. M. Fornasier, L. Gori: Sampling theorems on bounded domains, ArXiv math.NA/0604624, 2006.
- 4. M. Fornasier, S. Dahlke, K. Groechenig: *Optimal adaptive computation in the Jaffard algebra and localized frames*, RICAM report no. 2006-28, Aug. 2006.
- 5. M. Fornasier, H. Rauhut: Recovery algorithms for vector valued data with joint sparsity constraints, RICAM report no. 2006-27, Aug. 2006.
- 6. M. Fornasier, R. March: Restoration of color images by vector valued BV functions and variational calculus, RICAM report no. 2006-30, Sept. 2006.
- 7. M. Fornasier, Faithful recovery of vector valued functions from incomplete data. Recolorization and art restoration, RICAM report no. 2006-31, Oct. 2006.

# Dr. Arjan Kuijper

#### **Scientific Achievements 2006**

Arjan Kuijper studied the structure of images changing under influence of two classes of partial differential equations. The first class consists of the p-Laplacians, while the second one contains weighted combinations of second order derivatives in gauge coordinates [4,10]. These classes have Gaussian scale space in common. In this framework, an analysis of the topological multi-scale structure and a method to derive it efficiently has been presented [8].

He continued his work on shape analysis using the Symmetry Set [1], including relations to the Medial Axis [9], its multi-scale structure [3], and matching algorithms using various variants of the Symmetry Set [2, 5, 6] in collaboration with people from the IT University, Denmark and the University of Liverpool, UK.

His research has been presented at various conferences, workshops, and scientific meetings.

He was participant in the "Wittgenstein 2000 Award" grant of the Austrian Science Fund (FWF), awarded to Prof. P. Markowich, Dept. of Mathematics, University of Vienna, as well as in the project "Analyse Digitaler Bilder mit Methoden der Differenzialgleichungen" (2006) of the FFG - the Austrian National Science Foundation – yielding collaboration with the University of Vienna, the University of Linz, UCLA in Los Angeles, and the Ecole Normale e Superieur in Cachan, as well as the industrial partners Phase One and Nikon Austria.

He was involved in the successful WWTF Proposal (Five senses-Call 2006), "Mathematical Methods for Image Analysis and Processing in the Visual Arts" (funding volume: 400,000 € / project duration: 4 years).

He has been teaching an course on "Image Analysis and Processing" at Kepler University Linz in fall 2006, attended by people of various RICAM groups (Inverse Problems, Analysis of PDEs, and Mathematical Imaging) and the Department of Knowledge-Based Mathematical Systems - Fuzzy Logic Laboratorium Linz-Hagenberg.

He was referee for international peer reviewed journals & conferences:

- IEEE Transactions on Pattern Analysis and Machine Intelligence,
- IEEE Transactions on Image Processing,
- Journal of Mathematical Imaging and Vision,
- Electronic Letters in Computer Vision and Image Analysis,
- 9th European Conference on Computer Vision (ECCV06),

- 13th International Conference on Image Processing (ICIP06),
- 1st joint Scale-Space and Variational Methods Conference (SSVM 07),.
- 31st annual workshop of the Austrian Association for Pattern Recognition, OEAGM07, and chairman of a session of the 30th annual workshop of the Austrian Association for Pattern Recognition (OAGM/AAPR), OEAGM06, Obergurgl, Austria.

# **Scientific Cooperations**

#### Internal

Prof. Dr. Peter Markowich, RICAM/ Dept. of Mathematics, Vienna, Austria

Dr. Peter Elbau, RICAM

Dr. Bastian Gebauer, RICAM

Dr. Massimo Fornasier, RICAM

#### External

Dr. Ole Fogh Olsen, Prof. Dr. Mads Nielsen, Dr. Marco Loog, Image group, IT University of Copenhagen, Denmark.

Dr. Philip Bille, Theory group, IT University of Copenhagen, Denmark.

Prof. Dr. Peter Giblin, Dept. of Mathematics, University of Liverpool, United Kingdom.

Dr. Luc Florack, Prof. Dr. Bart Ter Haar Romeny, Biomedical Image Analysis, Technical University of Eindhoven, the Netherlands.

Leila Muresan, Dr. Peter Bauer, Department of Knowledge-Based Mathematical Systems - Fuzzy Logic Laboratorium Linz-Hagenberg, Austria.

Dr. Norayr Matevosyan, Carola Schoenlieb, Dept. of Mathematics, University of Vienna, Austria

Dr. Khoa N. Le, Griffith University, Australia.

Dr. Ilkka Havukkala, Knowledge Engineering and Discovery Research Institute, Auckland University of Technology, New Zealand.

#### Participation at Conferences, Scientific Visits and Talk

#### Conferences

30th annual workshop of the Austrian Association for Pattern Recognition (OAGM/AAPR), OEAGM06, Obergurgl, Austria, March 2-3, 2006.

European Conference on Computer Vision (ECCV), Graz, Austria, May 7 - 13, 2006

SIAM Conference on Imaging Science, Minneapolis, USA, May 15-17, 2006.

International Conference on Pattern Recognition (ICPR) 2006, 20 - 24 August 2006, Hong Kong.

Workshop on Variational and PDE Level Set Methods, September 1st - 3rd, 2006, Obergurgl, Austria.

Workshop on Image Analysis and Inverse Problems, December 11th - 13th, 2006, Eindhoven, the Netherlands.

#### Scientific Visits

ECCV Colloquium, Graz, 09.01.2006

Seminar Medical Image Analysis, Rotterdam, the Netherlands, 13.01.2006

Mathematical Image Group in Innsbruck (Prof. Dr. Scherzer), 01.03.2006.

Dept. of Mathematics, Vienna: Markowich, Moreysan, Schoenlieb (several times)

Fuzzy lab, Hagenberg: Muresan, Heise, Bauer (regularly)

# Scientific Talks

"PDE-based topological image segmentation", Workshop on Image Analysis and Inverse Problems, December 11th - 13th, 2006, Eindhoven, the Netherlands.

"Geometrical & p-Laplacian PDEs in Image Analysis", Workshop on Variational and PDE Level Set Methods, September 1st - 3rd, 2006, Obergurgl, Austria.

#### **Publications 2006**

# **Appeared**

- 1) Alternative 2D Shape Representations using the Symmetry Set, A. Kuijper, O. F: Olsen, P. J. Giblin, and M. Nielsen. Journal of Mathematical Imaging and Vision, 26 (1/2): 127-147, 2006.
- 2) Matching 2D Shapes using their Symmetry Sets, A. Kuijper, O. F.Olsen, P. Giblin, and Ph. Bille International Conference on Pattern Recognition 2006, 20 24 August 2006, Hong Kong.
- 3) Multi-Scale Shape Analysis Using Symmetry Sets, A. Kuijper, O. F.Olsen, SIAM Conference on Imaging Science, Minneapolis, USA, May 15-17, 2006.
- 4) p-norm PDE's, A. Kuijper, P. Markowich, SIAM Conference on Imaging Science, Minneapolis, USA, May 15-17, 2006.
- 5) Describing and Matching 2D Shapes by Their Points of Mutual Symmetry, A. Kuijper, O.F. Olsen 9th European Conference on Computer Vision (Graz, Austria, May 7 13, 2006), Part III, LNCS 3953, pages 213-225, 2006.
- 6) Shapes, Symmetry Sets, and Matching, A.Kuijper, O.F. Olsen, 30th annual workshop of the Austrian Association for Pattern Recognition (OAGM/AAPR), OEAGM06, (Obergurgl, Austria, March 2-3, 2006), pages 65--74, 2006.
- 7) Book review: Handbook of Mathematical Models in Computer Vision by Paragios, Chen, and Faugeras (Editors), IAPR newsletter, 24 (4), 20--21, October 2006

#### Submitted

- 8) An Analysis of Scale Space Saddles, A. Kuijper, journal paper, submitted, 2006
- 9) Deriving the Medial Axis with Geometrical Arguments, A. Kuijper, journal paper, submitted, 2006
- 10) Image Processing with Geometrical and Variational PDEs, A. Kuijper, conference paper, submitted, 2006
- 11) Minisymposium "The role of scale and orientation in mathematical image analysis" at the 6th International Congress on Industrial and Applied Mathematics, ICIAM 2007, Zürich, Switzerland, accepted.

#### Dr. Lukas Neumann

#### **Scientific Achievements 2006**

Lukas Neumann is mainly studying equations arising from mathematical physics. Among these, kinetic equations (for example describing the motion of the density of a gas in phase space) are his main interest.

Lukas Neumann (in collaboration with C. Sparber) studied the long time behaviour of Fokker-Planck type equations describing Fermions or Bosons in a semiclassical setting. In collaboration with C. Schmeiser he studied equations describing transport and reaction of chemical components. The main interest in this case is the asymptotics for large time as well as in the hydrodynamic regime. He also supervised the exercise class for the lecture "Integralgleichungen und Randwertprobleme" at the University of Linz.

# **Scientific Cooperations**

#### Internal

o.Univ.-Prof. Dr. Peter Markowich ao.Univ.-Prof. Dr. Christian Schmeiser

#### External

Miguel Escobedo, Universidad del País Vasco Clément Mouhot, Université Paris Dauphine Christof Sparber, Universität Wien

# Participation at Conferences, Scientific Visits and Talk

#### Conferences

27.2.-5.3. 2006 "Fluid Dynamic Equations", Short course by C. Bardos, Vienna 2.7.-10.7. 2006 WK-Summercamp, Weissensee

# Scientific Visits

12.2.-19.2. 2006: UPV, Bilbao 19.7.-21.7. 2006 Universität Wien 12.10.-13.10. 2006 Universität Wien

# Scientific Talks

February 2006 Talk in the Seminar of the Institute for Mathematics of the UPV

# **Publications 2006**

#### **Appeared**

C. Mouhot, LN "Quantitative perturbative study of convergence to equilibrium for collisional kinetic models in the torus", Nonlinearity (19), Nr. 4, 2006

#### Submitted

LN, C. Sparber "Stability of steady states in kinetic Fokker-Planck equations for Bosons and Fermions", RICAM Preprint, 2006-34, submitted to M3AS

# 2.5. GROUP "OPTIMIZATION AND OPITIMAL CONTROL"

# **Group Leaders:**

o.Univ.-Prof. DI. Dr. Karl Kunisch

# Researchers funded via ÖAW/Upper Austrian government funds:

Dr. Samuel Amstutz (until July 31, 06)

Dr. Roland Griesse

Dr. Boris Vexler

#### Researchers externally funded:

Dipl. Math. Techn. Olaf Benedix

Mag. Nataliya Metla

# Introduction by Group Leader Prof. Karl Kunisch

The focus of the group is on infinite dimensional optimization problems with partial differential equations as constraints. The present research topics include optimal control of large-scale systems, including control of magneto-hydrodynamical systems and the sensitivity analysis of constrained optimal control problems. Efficient adaptive numerical realizations and the development of a-priori and a-posteriori error estimators, as well as efficient numerical treatment of pointwise inequality constraints on the control and or the state variables are of particular importance to our work.

While not yet submitted, the first successful computations for optimal control of the magneto-hydrodynamical system, which is joint work between the optimal control and the numerical analysis group (Drs. Discacciati and Griesse) was one of the highlights in 06. Moreover the functional analytic treatment of time-dependent optimal control related to MHD systems was significantly advanced.

Topology optimization played a significant role from the middle of 05, due to Dr. Amstutz who, however, left the group again in the middle of 06, due to the fact that he was offered a permanent academic position in France. Dr. Amstutz not only finished his work on the combining level-set ideas with topology optimization, but also, jointly with Dr. Vexler, the possibly first paper on topological sensitivity analysis of time-dependent problems was published. Moreover, the foundation of work on topology optimization in the context of inequality constraints was laid.

Another important issue that was addressed in 06 especially in the work of Dr. Vexler are numerical methods in optimal control of PDE's for which the issue first "optimize" and then "discretize" or vice versa become vacuous since theses two approaches commute. Discontinuous Galerkin discretizations in time and special stabilized finite elements is space play an essential role here. — A general methodology for Dirichlet boundary control with state constraints was developed jointly with the group leader. Development of adaptive algorithms for solution ofparabolic problems was further investigated. Separation of the discretization errors with respect to time, space and control discretization, and separate refinement of spacial meshes in each time step were enabled, which allow efficient treatment of problems with complex dynamic behavior.

While collaboration on the level of exchange of ideas and basic know-how is going on with all other RICAM groups, concrete collaborations are carried out with the groups "Inverse Problems", "Computational Methods for Direct Field Problems", and "Financial Mathematics."

The collaboration with the group "Inverse Problems" is concentrated on two joint FWF-Projects. One project deals with the analysis of SQP methods for problems with mixed state constraints (PD. Dr. Roesch and Dr. Griesse). In the second project we develop discretization strategies for optimal control problem with singularities (PD Dr. Roesch and Dr. Vexler). The collaboration with with "Computational Methods for Direct Field Problems" is centered around the numerical realization of optimal control of MHD, as mentioned above, and research with "Financial Mathematics" focuses on semismooth Newton methods for portfolio optimization. A first joint paper on the latter has recently been accepted.

As group leader I announce most of my papers through the University of Graz, where I have my permanent position. I shall attempt to specifically dedicate one paper per year to the Radon Institute:

K. Ito and K. Kunisch: Optimal Bilinear Control of an Abstract Schrödinger Equation" SIAM J. Control and Optimization, to appear. (for 05)

K. Ito and K. Kunisch: Optimal Control of Obstacle Problems by H^1-Obstacles, Appl. Math. and Optim., to appear. (for 06)

As for the plans for the following two years Dr. Griesse and Dr. Vexler, as well as the externally funded collaborators should follow their successful research projects. Dr. Griesses work will expand into treating optimal control of free boundary value problems in a level set context. Dr. Vexler will expand into optimal control of second order hyperbolic equations for which very little numerical work has been done so far.

The successor to Dr. Amstutz will be Dr. Lu, who will start in July 06. Possible research topics for him include the numerical treatment of Hamilton Jacobi Bellman equations for closed loop control and semi-smooth Newton methods in portfolio optimization.

#### Dr. Samuel Amstutz

### **Scientific Achievements 2006**

<u>1.Topological sensitivity analysis for time-dependent problems</u> (in cooperation with Dr. T. Takahashi and Dr. B. Vexler) This work, initiated in 2005, was completed. A paper on this topic has been accepted.

2, Regularization / filtering techniques and mesh adaptation in topology optimization A numerical study on the regularization of topology optimization problems has been carried out. The techniques which have been experimented are:- an adaptation of the perimeter regularization- a filtering othe sensitivity by a smoothing operator, - the use of successive meshes where each refinement is performed in relation with a posteriori error estimates. This latter technique proved to be the most promising. But the choice of the functional involved in the error indicator needs to be clarified. This research will be continued.

#### 3. Topology optimization with constraints:

The goals of this work are:- the derivation of optimality conditions for topology optimization problems with constraints (possibly infinite dimensional),- the design of an algorithm to solve them,- the application of this algorithm to deal with structural optimization problems subject to a local stress constraint (typically a bound on the Von Mises stress). The first item is well advanced. A related paper is in preparation. The basic idea of the algorithm consists in adapting known methods dedicated to the search of saddle points. However, in the case of an infinite-dimensional set of constraints, the non-smoothness of the Lagrange multiplier requires the use of regularization techniques. Further research is needed in this direction before addressing the third item.

# **Scientific Cooperations**

#### Internal

Dr. Boris Vexler, group "Optimization and Optimal Control"

#### External

Dr. Takéo Takahashi, INRIA & Institut Elie Cartan de Nancy (France)

#### Participation in Conferences, Scientific Visits and Talk

#### Conferences

Journées de Metz "Geometric aspects of PDE and applications", April 13-15, 2006 (Metz, France).

#### Scientific Talks

- 1. Topological sensitivity analysis for time-dependent problems (Journées de Metz)
- 2. Shape optimization using topological sensitivity analysis (seminar at the university of Graz, invited by Prof. Kunisch)

#### **Publications 2006**

#### **Appeared**

- [1] S. Amstutz. Topological sensitivity analysis for some nonlinear PDE systems. J. Math. Pures Appl. 85(4), pp. 540-557, 2006.
- [2] S. Amstutz, H. Andrä. A new algorithm for topology optimization using a level-set method. J. Comput. Phys. 216(2), pp. 573-588, 2006.
- [3] S. Amstutz. Sensitivity analysis with respect to a local perturbation of the material property. Asymptotic Analysis 49(1,2), pp. 87-108, 2006.

#### Accepted

- [4] S. Amstutz, N. Dominguez. Topological sensitivity in the context of ultrasonic nondestructive testing. Accepted in Engineering Analysis with Boundary Elements (special issue, invited paper).
- [5] S. Amstutz, T. Takahashi, B. Vexler. Topological sensitivity analysis for time-dependent problems. Accepted in ESAIM:COCV.

#### Dr. Roland Griesse

#### Introduction

Dr. Roland Griesse conducts research in the field of optimal control of coupled systems of partial differential equations (PDEs). His interests extend from the mathematical analysis to the numerical solution of control- and state-constrained problems. The most recent application areas cover in particular magnetohydrodynamic (MHD) as well as crystal growth phenomena. The stability and perturbation analysis of optimal solutions under parameter perturbations, which is also essential to prove the convergence of iterative optimization methods of SQP type, continues to be another of his areas of expertise.

In July 2006, Dr. Griesse received an offer from Chemnitz University of Technology for a temporary full (W3) replacement professorship. He accepted this position and is on leave from RICAM effective October 2006 through the end of February 2007.

#### **Scientific Achievements 2006**

In 2006, Dr. Griesse has worked on the following topics:

# <u>Sufficient Second-Order Optimality Conditions and Convergence Analysis for SQP Methods for</u> Mixed Constrained Optimal Control Problems

Cooperation with Dr. Arnd Rösch and Dipl.-Math. Nataliya Metla

In 2006, we were able to prove an essential stability result for the solution and its corresponding adjoint states and Lagrange multipliers for linear-quadratic elliptic optimal control problems with mixed control-state constraints. This result was obtained in cooperation with Prof. Dr. Walter Alt (University of Jena, Germany), and a manuscript was submitted for publication. Using this result, a convergence proof for the SQP method applied to semilinear problems is currently being worked out.

# Simulation and Optimal Control in Magnetohydrodyhamics

Dr. Griesse has worked on the analysis of time-dependent MHD optimal control problems. The cooperation with Dr. Marco Discacciati concerning the implementation of numerical algorithms for MHD simulation and control was continued. A paper with the tentative title "Finite Element Solution of a Stationary Optimal Control Problem in Magnetohydrodynamics: Stokes Case" is in preparation.

# Robustness and Sensitivity Analysis in PDE-Constrained Optimization

Dr. Griesse has worked with Dr. Daniel Wachsmuth (TU Berlin, Germany) and Dipl.-Math. Thomas Grund (TU Chemnitz, Germany) on update schemes to recover perturbed optimal solutions from unperturbed ones. Using an adjoint approach, an error estimate with respect to the norm of uniform convergence was shown and numerically confirmed. A joint publication was submitted.

In addition, Dr. Griesse is supervising the master's thesis of Martin Bernauer (Johannes Kepler University, Linz), titled "A Robustification Approach in Unconstrained Optimization and its Application in Optimal Control".

# Optimal Control of Stefan Problems

Dr. Griesse has continued his cooperation with Dr. Stefan Volkwein (Karl-Franzens University of Graz, Austria) and Dr. Axel Voigt (Caesar Research Center, Bonn, Germany) on the optimal control of a Stefan problem arising in crystal growth. In addition, he has submitted a proposal for an FWF project, jointly with Prof. Dr. Karl Kunisch, in this area.

#### A Pathfollowing Method for Nonlinear Complementarity Problems

Dr. Griesse has continued his collaboration with Dr. Moritz Diehl (now with the Katholieke Universiteit Leuven, Belgium) and Dr. Martin Weiser (ZIB Berlin, Germany) on a pathfollowing method for the solution of nonlinear complementarity problems. A publication is in preparation.

# **Scientific Cooperations**

#### Internal

- 1) Prof. Dr. Karl Kunisch, Research Group "Optimization and Control", RICAM and University of Graz
- 2) Dr. Marco Discacciati, Research Group "Computational Methods for Direct Field Problems", RI-CAM
- 3) PD Dr. Arnd Rösch, Research Group "Inverse Problems", RICAM
- 4) Dipl.-Math. Nataliya Metla, Research Group "Inverse Problems", RICAM
- 5) Dr. Boris Vexler, RICAM

## External

- 1) Prof. Dr. Walter Alt, Friedrich-Schiller University Jena, Germany
- 2) Dr. Juan Carlos de los Reyes, Quito, Ecuador
- 3) Dr. Daniel Wachsmuch, Berlin University of Technology, Germany
- 4) Dipl-Math. Thomas Grund, Chemnitz University of Technology, Germany
- 5) Dr. Martin Weiser, ZIB Berlin, Germany
- 6) Dr. Moritz Diehl, Katholieke Universiteit Leuven, Belgium
- 7) Ao. Prof. Stefan Volkwein, University of Graz, Austria
- 8) Dr. Axel Voigt, Caesar Research Center, Bonn, Germany
- 9) Martin Bernauer, Johannes Kepler University Linz, Austria
- 10) Dipl.-Math.Kerstin Brandes, University of Bayreuth, Germany

# Participation in Conferences, Scientific Visits and Talks

#### Conferences

1) February 7-10, 2006	5 <sup>th</sup> MATHMOD Vienna, Austria
2) March 6-10, 2006	Intl. Conference on High Performance Scientific Computing, Hanoi,
	Vietnam
3) March 27-31, 2006	GAMM Annual Scientific Meeting, Berlin, Germany
4) April 6, 2006	Talk at RICAM Scientific Board Meeting, Linz, Austria
5) May 30, 2006	Colloquium Talk at Darmstadt University of Technology, Germany
6) June 13-16, 2006	MAFELAP Uxbridge, United Kingdom
7) July, 20, 2006	Colloquium Talk at Kaiserslautern University of Technology,
	Germany
8) July 24-27, 2006	GAMM-SIAM Conference on Applied Linear Algebra, Düsseldorf,
	Germany
9) September 17-23, 2006	DMV Annual Meeting, Bonn, Germany
10) September 25-27, 2006	Chemnitz FEM Symposium, Chemnitz, Germany (invited speaker)

# Activities as Organizer

1) February 7-10, 2006 Co-organization of a special session on *Optimal Control of Applications Governed by Differential Equations* at the 5<sup>th</sup> MATHMOD Conference in Vienna (together with PD Dr. Kurt Chudej, University of Bayreuth, Germany)

# Scientific Visits

1) January 9-20, 2006	University of Bremen (invitation by Prof. Dr. Peter Maaß), held a short course
	on "Infinite-Dimensional Optimization"
2) March 30-31, 2006	Berlin University of Technology, Germany (cooperation with Dr. Daniel
	Wachsmuth)
3) May 29-30, 2006	Darmstadt University of Technology, Germany (invitation by Prof. Dr. Stefan
	Ulbrich)
4) Sept. 28-29, 2006	Berlin University of Technology, Germany (cooperation with Dr. Juan Carlos
· -	de los Reyes)

#### Scientific Talks

- 1) "Modeling of an MHD Free Surface Problem Arising in CZ Crystal Growth" (Mathmod Vienna, Austria)
- 2) "Optimal Control in Magnetohydrodyhamics" (GAMM Berlin, Germany)
- 3) "Postcorrection Strategies for Perturbed Nonsmooth Equations" (High Performance Scientific Computing Hanoi, Vietnam)
- 4) "Optimal Control in Magnetohydrodyhamics" (RICAM Scientific Board Meeting, Linz, Austria)
- 5) "Numerical Methods in PDE-Constrained Optimization" (Darmstadt University of Technology, Germany)
- 6) "Optimal Control in Magnetohydrodynamics" (MAFELAP Uxbridge, United Kingdom)
- 7) "Continuous Optimization--Applications and Prospects" (Kaiserslautern University of Technology, Germany)
- 8) "Preconditioning of Linear Systems Arising in the Optimal Control of Magnetohydrodyhamics" (GAMM-SIAM Conference on Applied Linear Algebra, Düsseldorf, Germany)
- 9) "Elliptic Optimal Control Problems with Mixed Constraints" (DMV Bonn, Germany)
- 10) "Finite Elements in Magnetohydrodyhamics and its Optimal Control" (Chemnitz FEM Symposium, Chemnitz, Germany, invited speaker)

#### **Publications 2006**

#### **Appeared**

- [1] A. Borzi, R. Griesse, Distributed Optimal Control of Lambda-Omega Systems, Journal of Numerical Mathematics, 14, 1, 17-40, 2006
- [2] R. Griesse, S. Volkwein, Parametric Sensitivity Analysis for Optimal Boundary Control of a 3D Reaction-Diffusion System, Large-Scale Nonlinear Optimization, Springer, 127-149, 2006
- [3] R. Griesse, A.J. Meir, Modeling of an MHD Free Surface Problem Arising in CZ Crystal Growth, 5th IMACS Symposium on Mathematical Modelling (5th MATHMOD Vienna), ARGESIM Report 30, 2006

#### Accepted

- [4] R. Griesse, K. Kunisch, Optimal Control for a Stationary MHD System in Velocity-Current Formulation, accepted for publication in: SIAM Journal on Control and Optimization, 2006
- [5] R. Griesse, B. Vexler, Numerical Sensitivity Analysis for the Quantity of Interest in PDE-Constrained Optimization, accepted for publication in: SIAM Journal on Scientific Computing, 2006 [6] K. Brandes, R. Griesse, Quantitative Stability Analysis of Optimal Solutions in PDE-Constrained Optimization, accepted for publication in: Journal of Computational and Applied Mathematics, 2006
- [7] R. Griesse, Lipschitz Stability of Solutions to Some State-Constrained Elliptic Optimal Control Problems, Journal of Analysis and its Applications, 25, 4, 435-355, 2006
- [8] C. Büskens, R. Griesse, Computational Parametric Sensitivity Analysis of Perturbed PDE Optimal Control Problems with State and Control Constraints, accepted for publication in: Journal of Optimization Theory and Applications (JOTA), 2006

#### **Submitted**

[9] R. Griesse, T. Grund, D. Wachsmuth, Update Strategies for Perturbed Nonsmooth Equations, submitted, 2006

[10] W. Alt, R. Griesse, N. Metla, A. Rösch, Lipschitz Stability for Elliptic Optimal Control Problems with Mixed Control-State Constraints, submitted, 2006

[11] J.C. de los Reyes, R. Griesse, State-Constrained Optimal Control of the Stationary Navier-Stokes Equations, submitted, 2006

#### Dr. Boris Vexler

#### Introduction

The research area of Dr. Boris Vexler is the development and analysis of efficient numerical methods for solution of optimization problems governed by partial differential equations. He works on the development of problem-adjusted discretization and solution concepts based on a priori and a posteriori error analysis. The fields of applications are fluid dynamics, chemical reaction systems, and multidimensional reactive flows.

#### Scientific Achievements 2006

In 2006, Dr. Vexler has worked on the following topics:

- 1) Adaptivity with dynamical meshes for space-time finite elements discretizations (in cooperation with D. Meidner and M. Schmich). We continued our work on the development of adaptive techniques for finite element discretization of parabolic optimization problems, see [5], [9]. The proposed adaptive algorithm allows for construction of efficient discretizations by balancing different types of discretization errors (due to space, time and control discretization). Moreover, separate refinement of the spacial mesh in each time step leads to dynamic meshes, which are important for numerical optimization of processes with complex dynamic behaviour.
- 2) Optimal control of the convection-diffusion equation using stabilized finite element method (in cooperation with R. Becker). We investigated discretization of optimal control problems governed by convection-diffusion equations which are subject to pointwise control constraints, see [8]. We presented a stabilization scheme which leads to improved approximate solutions even on coarse meshes in the convection dominated case. Moreover, in general different approaches ``optimize-then-discretize" and ``discretize-then-optimize" coincide for the proposed discretization scheme. This allows for a symmetric optimality system on the discrete level and optimal order of convergence.
- 3) Analysis, solution and discretization techniques for Dirichlet optimal control problems governed by parabolic equations (in cooperation with K. Kunisch). We analyzed optimal Dirichlet boundary control based on the very weak solution of a parabolic state equation, see [10]. This approach allows to consider the boundary controls in L^2 which has advantages over approaches which consider control in Sobolev spaces involving (fractional) derivatives. We incorporated point-wise constraints on the boundary by the primal-dual active set strategy and proved its global and local super-linear convergence. We proposed a discretization concept based on space-time finite elements and studied numerical examples.
- 4) <u>Topological sensitivity analysis for time-dependent problems</u> (in cooperation with S. Amstutz and T. Takahashi). We developed asymptotic expressions describing the behaviour of a given functional depending on the solution of a time-dependent partial differential equation, when the topology of the domain is perturbed by the nucleation of a small hole, see [6]. This notion forms the basic ingredient of different topology optimization / reconstruction algorithms. Such topology sensitivity expressions are known for some elliptic problems. We achieved theoretically justified formulas for the heat and the wave equations.

#### Founded research projects

In 2006, FWF and DFG granted support for the joint project "Numerical analysis and discretization strategies for optimal control problems with singularities" applied for jointly by Th. Apel, A. Rösch, and B. Vexler. A PhD-position in the FWF-part of the project (FWF Project P18971-N18) was appointed to Dipl. Math. Olaf Benedix, who started to work in the project in September 2006. The DFG part of this project is supported within the priority program 1253 "Optimierung mit partiellen Differentialgleichungen". The corresponding PhD-position (at Universität der Bundeswehr München) was appointed to Dipl.-Tech. Math. Dieter Sirch.

#### Activities as organizer

- Minisymposium "Finite Elements in Optimal Control" at MAFELAP (London), 2006 (joint with A. Rösch)
- Minisymposium "Multigrid for Optimal Control" at GAMM 2006 (joint with A. Borzi)

#### **Teaching**

January 15-27,2006 Compact Course "Optimization with PDEs: Theory, Numerical Methods and Applications", University of Heidelberg, Germany

Summer-Semester 2006 Course "Numerical Optimization with PDEs", University of Linz, Austria

July 3-14, 2006, Course "Optimization with PDEs" at ICE-EM Australian Graduate School in Mathematics, Brisbane, Australia

Winter-Semester 06/07 Course "Adaptive Finite Element Methods", University of Linz, Austria

#### **Scientific Cooperations**

#### Internal

- 1) Prof. Dr. Karl Kunisch, Research Group "Optimization and Control", RICAM and University of Graz.
- 2) Dr. Roland Griesse, Research Group "Optimization and Control", RICAM
- 3) Dr. Samuel Amstutz, Research Group "Optimization and Control", RICAM
- 4) PD Dr. Arnd Rösch, Research Group "Inverse Problems", RICAM

# **External**

- 1) Prof. Dr. Rolf Rannacher, University of Heidelberg, Germany
- 2) Prof. Dr. Roland Becker, University of Pau, France
- 3) Prof. Dr. Thomas Apel, Universität der Bundeswehr München, Germany
- 4) Prof. Dr. Barbara Kaltenbacher, University of Stuttgart, Germany
- 5) Ao. Prof. Dr. Alfio Borzi, University of Graz, Austria
- 6) Dipl. Math. Dominik Meidner, University of Heidelberg, Germany
- 7) Dipl. Math. Michael Schmich, University of Heidelberg, Germany
- 8) Dr. Takeo Takahashi, Université Henri Poincaré Nancy, France
- 9) Dipl. Math. Winnifried Wollner, University of Heidelberg, Germany
- 10) Dipl. Math. Anke Griesbaum, University of Heidelberg, Germany

#### Participation in Conferences, Scientific Visits and Talks

# Conferences

February 6-8, 2006	Application Workshop of the DFG priority program 1253, Bad Honef,
	Germany
March 27-31, 2006	GAMM Annual Meeting 2006, Berlin, Germany
April 27-28, 2006	Second Austrian Numerical Analysis Day, Graz, Austria
June 13-16, 2006	MAFELAP 2006, London, UK
November 20-21, 2006	Kick of meeting of the DFG priority program 1253, Thurnau, Germany

#### Scientific Visits

February 3-4, 2006	University of Bonn (invited by Prof. Dr. Angela Kunoth)
April 10-21, 2006	Oberwolfach, Research in Pairs (RiP)
April 26-27, 2006	University of Graz (invited by Prof. Dr. Karl Kunisch)
May 3-5, 2006	University of Erlangen (invited by PD Dr. Barbara Kaltenbacher)
June 6-7, 2006	University of Göttingen (invited by Prof. Dr. Gert Lube)
June 19-23, 2006	TU Berlin (invited by Prof. Dr. Fredi Tröltzsch) & WIAS(invited by Prof. Dr.
	Dietmar Hömberg)
June 27-28, 2006	University of Darmstadt (invited by Prof. Dr. Stefan Ulbrich)
November 7-10, 2006	Universität der Bundeswehr München, Germany (invited by Prof. Dr. Thomas
	Apel)

#### Scientific Talks

- 1. Adaptive Space-Time Finite Element Methods for Parabolic Optimization Problems, February, 2006, University of Bonn
- 2. Adaptive Space-Time Finite Element Methods for Parabolic Optimization Problems, March, 2006, GAMM
- 3. Discretization of Optimal Control Problems by Stabilized Finite Element Methods, April, 2006, University of Graz
- 4. Adaptive Space-Time Finite Element Methods for Parabolic Optimization Problems, April 2006, Second Austrian Numerical Analysis Day, Graz
- 5. Adaptive Space-Time Finite Element Methods for Parabolic Optimization Problems, May, 2006, University of Erlangen
- 6. Adaptive Finite Element Methods for Optimization Problems governed by PDEs, June, 2006, University of Göttingen,
- 7. Adaptive Finite Element Methods for Optimization Problems governed by PDEs, June, 2006, WIAS, Berlin,
- 8. Optimal Dirichlet Boundary Control of Elliptic and Parabolic Equations, June, 2006, TU Berlin,
- 9.A Posteriori Error Estimation for Optimal Control Problems with Pointwise Inequality Constraints, June, 2006, MAFELAP, London
- 10. Adaptive Finite Element Methods for Optimization Problems governed by PDEs, June, 2006, University of Darmstadt
- 11. Adaptive Finite-Elemente-Verfahren für Optimierungsprobleme mit partiellen Differentialgleichungen, September, 2006, University of Bonn
- 12. Adaptive Finite-Elemente-Verfahren für Optimierungsprobleme mit partiellen Differentialgleichungen, October, 2006, University of Mainz
- 13. Adaptive Finite Element Methods for Optimization Problems governed by PDEs, Munich, November, 2006

#### **Publications 2006**

#### **Appeared**

- [1] A. Rösch, B. Vexler "Optimal control of the Stokes equations: A priori error analysis for finite element discretization with postprocessing", *SIAM Journal Numerical Analysis*, 44, 5, 1903--1920, 2006
- [2] R. Becker, M. Braack, D. Meidner, R. Rannacher, and B. Vexler "Adaptive Finite Element Methods for PDE-Cons-trained Optimal Control Problems", Reactive Flows, Diffusion and Transport, W. Jäger, R. Rannacher, J. Warnatz (eds.), Springer Verlag, Berlin, 2006.
- [3] B. Vexler "Finite Element Approximation of Elliptic Dirichlet Optimal Control Problems", accepted for publication in: *Numerical Functional Analysis and Optimization*, 2006
- [4] R. Griesse, B. Vexler "Numerical Sensitivity Analysis for the Quantity of Interest in PDE-Constrained Optimization", accepted for publication in: SIAM Journal on Scientific Computing, 2006
- [5] D. Meidner, B. Vexler "Adaptive Space-Time Finite Element Methods for Parabolic Optimization Problems", accepted for publication in: *SIAM Journal on Control and Optimization*, 2006
- [6] S. Amstutz, T. Takahashi, B. Vexler "Topological sensitivity analysis for time-dependent problems", accepted for publication in: ESAIM: Control, Optimisation and Calculus of Variations, 2006
- [7] K. Kunisch, B. Vexler "On the choice of the cost functional for optimal vortex reduction for instationary flows", accepted for publication in Proc. of Conference on Active Flow Control, Berlin, 2006

#### Submitted

- [8] R. Becker, B. Vexler "Optimal Control of the Convection-Diffusion Equation using Stabilized Finite Element Methods", submitted, 2006,
- [9] M. Schmich, B. Vexler "Adaptivity with Dynamic Meshes for Space-Time Finite Element Discretizations of Parabolic Equations", submitted, 2006
- [10] K. Kunisch, B. Vexler "Constrained Dirichlet Boundary Control in L^2 for a Class of Evolution Equations", submitted, 2006

#### Olaf Benedix, advised by Dr. Boris Vexler and Dr. Arnd Rösch

#### Work before joining RICAM

The year's part prior to September 2006 was used to write my Diploma thesis at the Faculty of Mathematics of the Chemnitz University of Technology (Germany). My field of work was a finite element mortar method of the Nitsche type for parabolic partial differential equations. The stability of the derived algorithm could be shown, and convergence rates were proven in two different norms; both showing the same convergence order as the standard finite element method without mortaring.

#### **Scientific Achievements 2006**

Starting from September 2006 literature studies were done to familiarize with the topic of optimal control with partial differential equations in general, which is the field of work of the FWF-DFG project "Numerical analysis and discretization strategies for optimal control problems with singularities". Especially problems under the presence of additional state constraints were taken care of. An interior-point method using adaptive mesh-refinement to solve these kinds of optimal control problems was implemented into an existing C++-library.

# **Scientific Cooperations**

#### Internal

Dr. Boris Vexler (Group Optimal Control)

PD Dr. Arnd Rösch (Group Inverse Problems)

# Participation in Conferences, Scientific Visits and Talks

Talks

"Finite-Elemente-Mortaring nach Nitsche für parabolische Anfangsrandwertaufgaben", June '06, Linz, Austria

# **Publications 2006**

"Finite-Elemente-Mortaring nach Nitsche für parabolische Anfangsrandwertaufgaben", Diploma thesis, Chemnitz University of Technology

# Nataliya Metla advised by Dr. Roland Griesse and Dr. Arnd Rösch

see group "Inverse Problems"

# 2.6. GROUP "MATHEMATICAL IMAGING"

**Group Leader:** 

Univ.-Prof. Dr. Otmar Scherzer

# Researchers funded via ÖAW/Upper Austrian government funds:

Dr. Peter Elbau Dr. Bastian Gebauer

# Introduction by Group Leader Prof. Otmar Scherzer

The group "Mathematical Imaging" is relatively new and started with the appointment of Dr. Elbau and Dr. Gebauer joining RICAM on October 1<sup>st</sup>, 2006. Dr. Elbau was formerly at the ETH Zürich working in the group of Prof. G. Felder and Dr. Gebauer came from the group of Prof. M. Hanke (Mainz).

The scope of this new group is the study of mathematical techniques for data acquisition and mathematical theory for image analysis. As mentioned in the proposal the research shares joint scientific interests with other working groups at RICAM, especially with the Inverse Problems and Analysis of Partial Differential Equations working groups.

In his PhD thesis, Markus Grasmair from the Infmath Imaging group in Innsbruck has developed existence theory of non convex variational optimization problems in image analysis. The original motivation of this topic was to derive variational problems approximating evolution equations for which just viscosity solutions exist. If successful such an approach can be generalized to derive novel image analysis techniques for higher dimensional data, such as color image data or diffusion tensor imaging data in medicine. At the present research, when analyzing higher dimensional data, we are confronted with a paradox, that the variational optimization problems are know to attain a generalized solution but cannot be minimized efficiently, while the evolution equations can be solved relatively easily with explicit or semi implicit methods, but there is no solution theory available. To close the gap between non convex variational problems and associated PDEs is the core theme of work of Dr. Elbau. There several problems have to be tackled:

- 1. A solution theory of evolutionary equations has to be derived. A very suitable approach has been discovered recently (joint work of Dr. Elbau with Prof. Dziuk (Freiburg) and the Infmath Imaging group in Innsbruck). We call it "Non Convex Semigroup Theory". The approach generalizes convex (linear and nonlinear) semigroup theory, and is based on employing variational relaxation techniques. We have made some success in this area recently, and shown that solutions can be well—defined, and could provide some analytical examples showing that there is in fact a relation to viscosity solutions of evolutionary equations.
- 2. In order to proceed with the ideas of non-convex semigroups we will conduct further analytical studies on explicit solution of case examples of partial differential equations and non convex variational problems. Mathematically the topic of analytical solution is extremely challenging, and tedious calculations are necessary, to get more insight in the nature of such problems. However the analytical studies are necessary to derive adequate solution concepts of evolutionary equations.
- 3. On the theoretical side the existence theory of non convex variational problems has to be extended and novel characterization of the energy functional based on the quasi-convex hull should be provided, using duality arguments or convex characterization arguments. Moreover, the results have to be generalized to general metric spaces.
- 4. On the practical side the numerics of the evolution equations has to be developed. At the present status of research, based on our preliminary solution concept it is not even known what the terminology stability, consistency, and approximation properties actually mean. The appropriate numerical concepts are currently not available, although the efficient numerical implementation is quite straight forward for the models under considerations. We think that it

- is necessary to study this theory in combination with an appropriate analytical theory.
- 5. Several applications have been investigated in the INFMATH group in Innsbruck, concerning filtering of vector valued data, ranging from Video enhancements and enhancement of compressed color images. Several other applications can be considered with variational techniques we developed as well, such as for instance Inverse Problems applications.

For the acquisition of medical images new tomography techniques have the potential of being less harmful for the patient and of showing a better contrast in soft tissue. In thermoacoustic tomography a body is illuminated by a short electromagnetic pulse. This leads to the emission of a sound wave, which is then measured to gain information on the interior of the body. Previous work in the Infmath Imaging in Innsbruck group has been done on reconstruction techniques and novel sensor configurations for this problem. The group leader has initialized an Austrian network on this topic and submitted an NFN draft proposal to the Austrian Science Foundation on thermoacoustic imaging where the Radon Imaging group is intended to actively participate. Several novel mathematical problems have been formulated already, and will also be considered by Dr. Gebauer at Radon. Thermoacoustic tomography is a long term project which has impact from medicine and experimental physics, and is considered a long term project within the research interests of Radon Imaging.

Dr. Gebauer also intends to further develop his successful work on sampling methods for inverse problems applications.

The group is also actively participating in the "bioimaging" semester, to be held this year at Radon, and organizing several events.

#### Dr. Peter Elbau

#### Work before joining RICAM

My work before first of October was mainly dominated by finishing my PhD-thesis at ETH Zurich. Together with my supervisor Prof. Giovanni Felder, I considered the random normal matrix models proposed by L.-L. Chau and Y. Yu with some polynomial potential and concretized the result from P. Wiegmann and A. Zabrodin that the eigenvalues of the matrices in the large matrix limit tend to become homogeneously distributed inside some polynomial curve specified by its harmonic moments which enter the model in the form of coefficients of the potential. Moreover, we considered the corresponding orthogonal polynomials and showed under some technical assumptions that the density of their zeros in the large matrix limit is concentrated on the branch cuts of the Schwarz function of the polynomial curve and is given there by the discontinuity of the Schwarz function times some constant.

#### Scientific work at RICAM

Together with Prof. Scherzer, I am trying to continue the work of Markus Grasmair from the University of Innsbruck considering non-convex variational problems for image-enhancing. The aim would be to identify the solution of the Euler-Lagrange equations of such a problem as the asymptotic limit of the iterative solution of the relaxation of the original functional.

# **Scientific Cooperations**

#### Internal

Prof. Otmar Scherzer, University of Innsbruck and RICAM

#### External

Prof. Giovanni Felder, ETH Zurich

# Participations at Conferences, Scientific Visits, and Talks

#### Conferences

Workshop on "Image Analysis and Inverse Problems", EURANDOM, Eindhoven, the Netherlands, December  $11th-13^{th}$ 

#### Talks

- Random normal matrices and polynomial curves, Mathematical Physics and Random Matrices Seminar, Brunel University, January 25th
- What is a matrix model, Zurich Graduate School in Mathematics, ETH Zurich, April 4th

#### **Publications**

PhD-thesis "Random normal matrix models and polynomial curves" at ETH Zurich

#### Dr. Bastian Gebauer

#### Work before joining RICAM

I received the degree of doctor rerum naturalium (doctor of natural science) from the Johannes Gutenberg-University Mainz, Germany in July 2006. My dissertation "Gebietserkennung mit der Faktorisierungsmethode" (obstacle detection using the factorization method) was supervised by Prof. Dr. Martin Hanke-Bourgeois from the University of Mainz. The second and third referee were Prof. Dr. Andreas Kirsch, University of Karlsruhe and Prof. Dr. Rainer Kress, University of Goettingen. In my thesis I studied the factorization method for the localization of inclusions inside a body from measurements on its surface. The method relies on a range identity that relates the measurements to the range of an auxiliary operator that characterizes the inclusions. In my thesis I developed a general framework for the method to extend the range identity to general real elliptic problems and deduced several known as well as new applications of the method. For the special problem of detecting magnetic or perfect electrically conducting objects by low-frequency electromagnetic waves, I showed the unique solvability of the underlying forward problem and the convergence against the elliptic equations of magnetostatic. Using the general theory for the factorization method the objects could then be reconstructed from the measurements. Also the detection of inclusions described by a parabolic equation in a background described by an elliptic equation was studied. The unique solvability of the underlying parabolic-elliptic forward problem was shown and an extension of the factorization method was derived for this problem.

I had a position as a teaching and research assistant at the Institute of Mathematics at the University of Mainz until September 2006. I started to work at RICAM in October 2006.

# **Scientific Achievements 2006**

In a joint work with Prof. Hanke-Bourgeois and Christoph Schneider we studied the use of sampling methods for low-frequency electromagnetic imaging. Particular results beyond the scope of my thesis deal with the relation of the linear sampling method to the factorization method and the necessary modifications in the physically relevant case of divergence-free currents. A research article about these results is currently prepared.

At RICAM I started to work at the problem of thermoacoustic tomography. I develop the functional analytic setting to include spatially discontinuous sound velocities in the forward problem. Preliminary results show that the direct problem can be treated with a new variational approach, which we expect to be a valuable tool also for the inverse problem.

# **Scientific Cooperations**

#### <u>Internal</u>

Prof. Otmar Scherzer, University of Innsbruck, Austria and RICAM

#### External

Florian Frühauf, Department of Computer Science, University of Innsbruck, Austria Prof. Martin Hanke-Bourgeois, Institute of Mathematics, Joh. Gutenberg University, Mainz, Germany Christoph Schneider, Institute of Mathematics, Joh. Gutenberg University, Mainz, Germany

# Participations at Conferences, Scientific Visits and Talks

#### Conferences

- 77<sup>th</sup> Annual Meeting of the Gesellschaft für Angewandte Mathematik und Mechanik e.V.
   (GAMM), Technische Universität Berlin, Germany, March 27<sup>th</sup> 31<sup>st</sup>, 2006. Talk: "Detecting objects by low-frequency electromagnetic imaging".
- SIAM Conference on Imaging Science, Radisson University Hotel, Minneapolis, Minnesota, USA, May 15<sup>th</sup> – 17<sup>th</sup>, 2006. Talk: "Detecting Interfaces in a Parabolic-Elliptic Problem from Surface Measurements".
- Compactseminar Numerische Mathematik, Höchst im Odenwald, Germany, August 30<sup>th</sup> September 1<sup>st</sup>, 2006.
- Colloquium "There is nothing more practical than a good theory." Fraunhofer Institut Techno- und Wirtschaftsmathematik, Kaiserslautern, Germany, September 14<sup>th</sup> 15<sup>th</sup>, 2006.
- Workshop on "Image Analysis and Inverse Problems", EURANDOM, Eindhoven, The Netherlands, December 11<sup>th</sup> – 13<sup>th</sup>, 2006.

# Scientific Visits

- General Membership at the IMA 2005 2006 annual program on "Imaging", Institute for Mathematics and Its Applications, University of Minnesota, Minneapolis, USA, May 11<sup>th</sup> – June 11<sup>th</sup>, 2006.
- Fachbereich Mathematik, TU Darmstadt, Germany, July 6<sup>th</sup>, 2006. Talk:"Gebietserkennung in einem parabolisch-elliptischen Problem".
- Institut für Numerische und Angewandte Mathematik, University of Göttingen, Germany, August 2<sup>nd</sup>, 2006.

#### Talks

- Talks at conferences and during scientific visits are listed above.
- "Gebietserkennung mit der Faktorisierungsmethode", Dissertation colloquium/defense, University of Mainz, July 28<sup>th</sup>, 2006.

#### **Publications**

#### Appeared

1. The Factorization Method for real elliptic problems, Z. Anal. Anwend. 25 (2006) 81-102.

Accepted
2. with F. Frühauf and O. Scherzer) Detecting interfaces in a parabolic-elliptic problem from surface measurements, SIAM J. Numer. Anal., to appear.

# 3. SPECIAL SEMESTER, CONFERENCES, COLLOQUIA

# 3.1. OVERVIEW

The number of external visitor to the institute, both within the special semesters and independent of them, has grown even more. As in the previous years, the talks have been structured in three groups:

# Radon-Colloquia:

In these talks, prominent external scientists should present overviews over important fields dedicated also to non-specialists. All RICAM employees are expected to attend these colloquia.

#### Radon-Seminars:

These are a bit more specialized talks, both by our own scientists and by external visitors. They should not strictly focus on a specialized topic but have connections to the work of a least two groups in RI-CAM and should therefore be attended by all RICAM scientists.

#### **Group-Seminars:**

These are specialized talks by internal and external scientists intented mostly for members of the organizing group(s), although, of course, members of other groups are also welcome.

In 2007 we will strictly limit the number of Radon-Colloquia and Radon-Seminars, since otherwise, the number of talks to be attended by everybody would just be too large.

In 2006, the following talks were given in these three groups:

# Radon Colloquia

Prof. Gabriel Wittum

Simulation in Technology, University of Heidelberg

Thursday, February 23, 15:30, HS9

# Title: Towards Simulation of Neuronal Signal Processing

Abstract: The crucial feature of neuronal ensembles is their high complexity and variability. This makes modelling and computation very difficult, in particular for detailed models based on first principles. The problem starts with modelling geometry, which has to extract the essential features from those highly complex and variable phenotypes and at the same time has to take in to account the stochastic variability. Moreover, models of the highly complex processes which are living on these geometries are far from being well established, since those are highly complex too and couple on a hierarchy of scales in space and time. Simulating such systems always puts the whole approach to test, including modeling, numerical methods and software implementations. In combination with validation based on experimental data, all components have to be enhanced to reach a reliable solving strategy.

To handle problems of this complexity, new mathematical methods and software tools are required. In recent years, new approaches such as parallel adaptive multigrid methods and corresponding software tools have been developed allowing to treat problems of huge complexity. In the lecture we present an approach for the simulation of signal processing in neurons. This is an outline of work to be done in this highly complex field. Part of this approach is a method to reconstruct the geometric structure of neurons from data measured by 2-photon microscopy in vivo. Being able to reconstruct neural geometries and network connectivities from in vivo measured data

Prof. Olivier Pironneau University of Paris VI

Friday, April 7, 15:00, HF9901

Title: Computation and Calibration of European and American Options

Abstract:

In this talk we present fast algorithms for the computation of European and American options and a least-square approach for the calibration of the volatility with market data for these. Optimal control methods are applied and differentiability of American option with respect to volatility is studied.

Prof. Fredi Tröltzsch

TU Berlin

Wedenesday, May 10, 16:00, HF9901

Title: Optimal Control of Partial Differential Equation – Examples and Methods

Abstract: The mathematical optimization of processes modeled by partial differential equations is attracting rapidly growing interest. Chemical reaction-separation, crystal growth, fluid flow, local hyperthermia in cancer therapy, and thermal treatment of steel are some typical fields of application. The associated mathematical theory of optimization in function space rises interesting questions and requires special answers. The talk illustrates some characteristic examples, introduces basic ideas of optimality conditions and explains some related numerical techniques. Special emphasis is placed on the presence of pointwise state constraints. For instance, in cooling or heating processes, strict bounds on the temperature are often indispensable. Some recent results of numerical analysis are briefly sketched.

Prof. Wolfgang Hackbusch

Max-Planck-Institut

Wednesday, June 7, 15:30, HF9901

Title: Efficient evaluation of coalescence integrals in population balance models

Abstract: The population balance model describes a particle density function f(t,r,x) in space (r) and time (t) with an additional property coordinate x.

The right-hand side of the differential equation contains an integral operator, which is quadratic in f and describes the coalescence of the particles. Since the coordinate x increases the number of dimensions, quite efficient numerical algorithms are unavoidable. The lecture will show how to replace the complexity n2 for the naive evaluation of the integral by  $O(n \log n)$ . This results holds even in the case of non-uniform meshes.

# Radon Seminars

Dr. Oliver Labs

**RICAM** 

Wednesday, January 11, 16:00, HF136

Title: Hypersurfaces with many singularities --- From Classical Constructions to Recent Algorithms

Abstract: A hypersurface in P<sup>n</sup> is the zeroset of a homogeneous polynomial in n+1 variables.

One of the first questions that one can ask on these seemingly simple objects is which and how many singularities can occur on them.

This dates back at least to 1863 when Schlaefli classified all cubic surfaces (i.e. hypersurfaces of degree 3 in P^3) with respect to the singularities occurring on them. Their maximum number  $\mu(3)$ =4 is attained by the four-nodal Cayley cubic. On a surface of degree 4, the maximum possible number of singularities is  $\mu(4) = 16$  which is the number of nodes of the well-known Kummer surfaces (1864). The problem turned out to be very difficult for higher degrees. For degree d>6 there still only exist upper and lower bounds for  $\mu(d)$ .

In the talk, we give an introduction to the problem and the developments up to now — illustrated with many pictures.

See also: www.AlgebraicSurface.net

We close by showing how we used computer algebra to improve the knowledge on this classical question:  $\mu(7) \ge 99$  and  $\mu(9) \ge 226$ .

Our algorithm uses the nice feature of algebraic numbers that they can be "approximated" by reducing them modulo different prime numbers, and that the exact numbers can be "recovered" from these prime field approximations. This method is not restricted to our case: It can actually be applied to many other construction problems in algebraic geometry.

Dr. Jürgen Hartinger

**RICAM** 

Wednesday, January 18, 16:00, HF136

Title: Finance, Simulation, Insurance.

A journey through aspects of quantitative risk management

Abstract: To establish and implement sound quantitative risk models is vital concern for nearly all financial institutions. The aim of financial and actuarial mathematics is to lay a comprehensive base to solve these real-world problems. In this talk we discuss two aspects of basic research supporting this goal:

- (Quasi-)stochastic simulation has become an essential tool in various parts of quantitative risk management. After reviewing and comparing the basic concepts of Monte and Quasi-Monte Carlo techniques, it is planned to give concrete examples were financial applications stimulated research in new and renewed interest in old simulation techniques.
- The first attempts to model non-life insurance portfolios go back more than a century. In the beginning the calculation of the probability of ruin was of main interest. Nowadays, one is most interested in management strategies for such portfolios, e.g. in establishing optimal dividend streams to shareholders or investment strategies to minimize the probability of ruin based on stochastic optimal control techniques. After a short introduction, we survey recent results and open questions in this area.

Dr. Massimo Fonte

International School of Advanced Studies, Trieste

Wednesday, Feb. 8, 16:00, HF136

Title: An optimal transportation metric for singular solutions of a nonlinear water wave equation

Abstract: In this talk we construct a global, continuous flow of solutions to the Camassa-Holm equation on the space H^1. The solutions are conservative, in the sense that the total energy remains a.e. constant in time. Distances defined in term of convex norm performs well in connection with linear problems, but occasionally fail when nonlinear features become dominant.

The new approach is based on the construction of a distance, related on a optimal transportation problem, which provides the ideal tool to measure continuous dependence on the initial data for solutions to the Camassa-Holm equation. Using this new distance functional, we can construct arbitrary solutions as the uniform limit of multi-peakon solutions, and prove a general uniqueness result.

Dr. Ronny Ramlau

**RICAM** 

Wednesday, March 1, 16:00, HF136

Title: Inverse Problems in Rotordynamics

Abstract: In this talk, we consider the identification of imbalances in rotating systems. An imbalance is an asymmetrical mass distribution that leads to vibrations of the system. In the worst case the system can be destroyed. Thus, rotating systems have to be balanced after mounting and in regular intervals. Currently, the balancing process is mostly done by expert knowledge only.

We will present model-based methods that allow the reconstruction of an imbalance from measurements of the system oscillations. Using a finite element ansatz, the connection between a given imbalance f and the resulting oscillations for a fixed rotation frequency  $\Omega$  is given by an ordinary differential equation.

The direct problem consists in the computation of the vibrations u, while the inverse problem

requires the computation of f from a few measurements of u.In many applications, the damping of the

system depends on the oscillation, and therefore we have to solve a nonlinear problem. In our talk, we will present a fast method that allows a stable identification of the imbalance even in the case of high noise in the data.

In some applications it is not of interest to identify the imbalance but to reduce the remaining vibrations of the systems as much as possible by placing a set of balancing weights. As for this task the location of the balancing weights is fixed, we will present an algorithm that determines an optimal mass distribution for a given set of fixed balancing locations.

Our method will be illustrated with three applications: We will consider aircraft engines (in cooperation with Rolls Royce), generators (in cooperation with Siemens AG) and wind power stations (in cooperation with Fielax GmbH).

Dr. Samuel Amstutz

**RICAM** 

Wednesday, March 22, 16:00 HF 136

Title: Topology optimization via topological sensitivity analysis

Abstract: The concept of topological gradient, also called topological derivative, measures the sensitivity of a shape functional with respect to the creation of a small hole inside the domain. It was introduced in the context of structural optimization by Schumacher in 1995 in order to overcome the limitations of the ''classical" shape optimization methods which, at least from the theoretical point of view, cannot handle any topology changes. Several authors contributed to its development, providing sensitivity formulas in many situations. In the same time, its efficiency to deal with academic or industrial problems was demonstrated on various examples.

In this talk, I will first present some basic results concerning the topological gradient and discuss the related optimality conditions. Then I will illustrate by numerical examples different ways of using this information in shape optimization. The following areas should be

addressed: defects detection, optimal design in incompressible fluid dynamics, optimization of wave guides, structural optimization.

Hui Cao,

Shuai Lu and

Sergei Pereverzyev (Joint work with Raytcho Lazarov (Texas A&M University))

**RICAM** 

Thursday, April 6, 18:00, HF9901

Title: Balancing principle for choosing penalty parameters in ill-posed and well-posed problems

Abstract: We discuss a choice of weights in penalization methods. The motivation for the use of penalization in Computational Mathematics is to improve the conditioning of the numerical solution. One example of such improvement is a regularization, where a penalization substitutes ill-posed problem for well-posed one. In modern numerical methods for PDE a penalization is used, for example, to enforce a continuity of approximate solution on non-matching grids.

A choice of a penalty weight should provide a balance between error components related with convergence and stability, which are usually unknown.

In the talk we propose the adaptive strategy for the choice of a penalty weight which does not rely on a priori estimates of above mentioned components.

It is shown that under natural assumptions the accuracy provided by our adaptive strategy is worse only by a constant factor than one could achieve in the case of known stability and convergence rates.

We demonstrate the application of our strategy for the self-regularization of severely ill-posed problems, such as sideway heat equation or elliptic Cauchy problem, and for the choice of a weight in interior penalty discontinuous approximation on non-matching grids. Numerical experiments on a series of model problems support theoretical results.

Dr. Roland Griesse

**RICAM** 

Thursday, April 6, 18:40, HF9901

Title: Optimal Control in Magnetohydrodynamics

Abstract: Magnetohydrodynamics, or MHD, deals with the mutual interaction of electrically

conducting fluids and magnetic fields. In particular, the magnetic fields interact with the electric currents in the fluid and exert a Lorentz force. This feature renders it so phenomenally attractive for exploitation especially in processes involving liquid metals, and in crystal growth. Therefore MHD technology is used routinely today by engineers, for instance to stir molten metals during solidification, to dampen their undesired convectiondriven flow during casting, to filter out impurities, and to melt and even levitate metals.

The tayloring of currents and magnetic fields offers the possibility to drive the fluid in a desired way. In this presentation, we apply an optimal control approach to an incompressible MHD model. Recent numerical results, obtained in cooperation with the group Computational Methods for Direct Field Problems, will be shown.

Univ.-Doz. Dr. Hansjörg Albrecher

**RICAM** 

Thursday, April 6, 19:20, HF9901

Title: On Measuring and Hedging Risk in Finance and Insurance

Abstract: In this talk I will present some of my recent research activities including the determination of ruin-related quantities in collective risk models that incorporate dividend payments and dependencies as well as valuation issues for insurance derivatives. Moreover, static hedging techniques for Asian options are discussed.

Dr. Martin Giese

**RICAM** 

Wednesday, April 12. 13:30, HF136

Title: An Introduction to the Tableau Calculus

Abstract: I will introduce classical first-order logic, a simple formal logic that is used in many applications, and is also the basis of many more complicated logics. I will give a meaning to this logic by a so called "model semantics". I will then introduce a version of the tableau calculus, and explain the connection between derivability in the calculus and semantic validity.

Dr. Arjan Kuijper

**RICAM** 

Wednesday, April 26, 15:00, HF136

Title: Image analysis from biological, computational, and mathematical perspectives

Abstract: The analysis of computer images is a challenging task. Humans are capable of "understanding" and interpreting what they see, but this is still far from being automated. Secondly, operators on images must be capable of treating their discrete nature.

One such operator is a Gaussian filter. Applied to the image one yields a continuous so-called scale space image. An extra dimension is obtained since the filter has a variable width, the scale.

This filter not only mimics the human visual system, but is also obtained as the results of uncommitted axioms one can state on physically obtained images.

Within this scale space image a user-independent hierarchical structure is present, defined by the paths of spatial critical points in scale space, combined with iso-intensity manifolds. The structure can be represented as a binary tree. As an application one finds a topological segmentation of the original image.

The scale space can be written as the traditional heat equation acting on the image as initial data at all time instances. The heat equation forms the center of a large family of PDE approaches in image analysis. The

scale spaces of two special sub-families with potential descriptive power will be discussed: the p-Laplacians and weighted geometrical second order derivatives.

Dr. Marco Discacciati

**RICAM** 

Wednesday, May 31, 16:30, HF136

Title: Multiphysic problems and domain decomposition methods

Abstract: Mathematical modeling of real-life problems may lead to consider different kind of boundary values problems in subregions of the computational domain.

Indeed, one may be obliged to consider truly different models to account for the presence of distinct physical phenomena within the same domain.

This case is usually indicated as multi-physic or multi-field problems.

These problems may be cast in the common framework provided by the so-called heterogeneous domain decomposition method, which extends the classical domain decomposition theory whenever two (or more) kinds of boundary values problems hold in subregions of the computational domain.

In this talk, we will illustrate the basic ideas of heterogeneous domain decomposition considering two examples of multi-physic problems arising in different application areas, namely, magnetohydrodynamics and fluid-structure interaction in hemodynamics. We will show how domain decomposition techniques can be applied in order to set up effective

(parallelizable) algorithms for computing their solution, and present some numerical results.

Dr. Markus Rosenkranz

RICAM

Wednesday, June 14, 13:30, HF136

Title: The Algebra of Boundary Value Problems:

A Symbolic Computation Perspective on Linear Two-Point BVPs

Abstract: We describe a new algebraic way of dealing with Linear Two-Point Boundary Value Problems. The methodology is based on operators (both for the problem statement - differential and boundary operators - and the solution - Green's operator), which are modelled as noncommutative polynomials. The technique of Groebner bases is invoked for obtaining an operator-based solution for any BVP of the type described; the solution algorithm is implemented in the Theorema system. - On a higher level, we regard all regular BVPs as a monoid that is anti-isomorphic to the corresponding Green's operators. Further algebraic investigations of this monoid reveal interesting and useful structures, which lead to "factoring and dividing" BVPs. The notion of division turns out to yield a natural generalization of the so-called Mikusinski calculus, which was up to now bound to initial value problems.

Prof. Axel Munk

Universität Göttingen

Tuesday, June 27, 10:00, HF136

Title: Inverse Jumps

Abstract: We provide an asymptotic theory for penalized least squares estimators of locally constant functions with finitely many jumps which are observed blurred by an operator with random noise. Differences to the direct case are highlighted, particularly, it turns out that a √n-rate of convergence is generic. Moreover, locations of jumps are jointly asymptotic normal, which allows to costruct confidence regions in these function classes. A minimax result shows that our penalized least squares estimators are rate optimal. Various applications are discussed. This is joint work with L. Boysen.

Dr. Eva Sincich

INRIA

Thursday, June 29, 15:15, HF136

Title: Stability and reconstruction for the determination of nonlinear corrosion

Abstract: We deal with an inverse problem arising in corrosion detection. We prove a stability estimate for a nonlinear term on the inaccessible portion of the boundary by electrostatic measurements on the accessible one.

Furthermore we propose a method for the approximate reconstruction of such a nonlinearity.

# **Group Seminars**

Dr. Oliver Labs

**RICAM** 

Wednesday, January 11, 16:00, HF136

Title: Hypersurfaces with many singularities --- From Classical Constructions to Recent Algorithms

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One of the first questions that one can ask on these seemingly simple objects is which and how many singularities can occur on them.

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Wednesday, May 31, 16:30, HF136

Title: Multiphysic problems and domain decomposition methods

Abstract: Mathematical modeling of real-life problems may lead to consider different kind of boundary values problems in subregions of the computational domain.

Indeed, one may be obliged to consider truly different models to account for the presence of distinct physical phenomena within the same domain.

This case is usually indicated as multi-physic or multi-field problems.

These problems may be cast in the common framework provided by the so-called heterogeneous domain decomposition method, which extends the classical domain decomposition theory whenever two (or more) kinds of boundary values problems hold in subregions of the computational domain.

In this talk, we will illustrate the basic ideas of heterogeneous domain decomposition considering two examples of multi-physic problems arising in different application areas, namely, magnetohydrodynamics and fluid-structure interaction in hemodynamics. We will show how domain decomposition techniques can be applied in order to set up effective

(parallelizable) algorithms for computing their solution, and present some numerical results.

Dr. Markus Rosenkranz

**RICAM** 

Wednesday, June 14, 13:30, HF136

Title: The Algebra of Boundary Value Problems:

A Symbolic Computation Perspective on Linear Two-Point BVPs

Abstract: We describe a new algebraic way of dealing with Linear Two-Point Boundary Value Problems. The methodology is based on operators (both for the problem statement - differential and boundary operators - and the solution - Green's operator), which are modelled as noncommutative polynomials. The technique of Groebner bases is invoked for obtaining an operator-based solution for any BVP of the type described; the solution algorithm is implemented in the Theorema system. - On a higher level, we regard all regular BVPs as a monoid that is anti-isomorphic to the corresponding Green's operators. Further algebraic investigations of this monoid reveal interesting and useful structures, which lead to "factoring and

dividing" BVPs. The notion of division turns out to yield a natural generalization of the so-called Mikusinski calculus, which was up to now bound to initial value problems.

Prof. Axel Munk

Universität Göttingen

Tuesday, June 27, 10:00, HF136

Title: Inverse Jumps

Abstract: We provide an asymptotic theory for penalized least squares estimators of locally constant functions with finitely many jumps which are observed blurred by an operator with random noise. Differences to the direct case are highlighted, particularly, it turns out that a √n-rate of convergence is generic. Moreover, locations of jumps are jointly asymptotic normal, which allows to costruct confidence regions in these function classes. A minimax result shows that our penalized least squares estimators are rate optimal. Various applications are discussed. This is joint work with L. Boysen.

Dr. Eva Sincich

**INRIA** 

Thursday, June 29, 15:15, HF136

Title: Stability and reconstruction for the determination of nonlinear corrosion

Abstract: We deal with an inverse problem arising in corrosion detection. We prove a stability estimate for a nonlinear term on the inaccessible portion of the boundary by electrostatic measurements on the accessible one.

Furthermore we propose a method for the approximate reconstruction of such a nonlinearity.

# Conferences co-organized by RICAM

- 17th International Conference on Domain Decomposition Methods (DD17), Strobl, Austria, July 3 7, 2006
- The Conference of the International Association for Boundary Element Methods (IABEM 2006), Graz, Austria, July 10 12, 2006
- 4th Workshop on Fast Boundary Element Methods in Industrial Applications, Soellerhaus (Kleinwalsertal), Austria, September 29 October 2, 2006
- 3rd International Joint Conference on Automated Reasoning, IJCAR, Seattle, August 17 20, 2006
- Organization of a special session on "Optimal Control of Applications described by DAEs/PDEs/PDAEs", MATHMOD, Vienna, Austria (together with Kurt Chudej, Bayreuth, Germany), February 2006
- Workshop on Algebraic Spline Curves and Surfaces, Eger, Hungary, May 2006
- Workshop on Algebraic Geometry and Singularities, Obergurgl, September 2006

# 3.2. SPECIAL SEMESTER ON GROEBNER BASES

# Overview by Prof. Bruno Buchberger

# **Background**

The Groebner bases theory and algorithmic methodology was introduced by Bruno Buchberger in his PhD thesis 1965 and journal publication 1970 (B. Buchberger, "An Algorithmic Criterion for the Solvability of Algebraic Systems of Equations"). In the meantime, Groebner bases have found wide applications in many areas of mathematics and science reflected by over 1000 publications and 10 textbooks on Groebner bases, an extra entry "Groebner Bases" in the AMS classification index (13P10), and Groebner bases software implementations in all major mathematical software systems like Mathematica, Maple, Derive, Magma, Axiom etc.

#### **Scientific Director**

The special semester on Groebner bases, jointly organized by RICAM (Radon Institute for Computational and Applied Mathematics, Austrian Academy of Science, Linz, Austria) and RISC (Research Institute for Symbolic Computation, Johannes Kepler University, Linz, Austria), was designed and directed by the inventor of the Groebner bases theory, Professor Bruno Buchberger, founding chairman of RISC and symbolic computation area leader at RICAM.

#### Goals

The special semester on Groebner bases had the goal of

- bringing together the leading researchers in Gröbner bases and related theories for discussion of the latest developments, joint research, and publication projects,
- intensive training of young researchers, in particular PhD students and PostDocs from all over the world in Groebner bases and related theories and the elaboration of tutorials and other educational material.
- organizing publication projects for the dissemination of in-depth introductions to the various aspects and applications of Groebner bases theory and of recent research results,
- compiling a comprehensive, web-accessible bibliography on the field with links to download-ables, see http://www.ricam.oeaw.ac.at/Groebner-Bases-Bibliography/,
- compiling of a comprehensive, web-accessible data base for current software that implements the Groebner bases method, see http://www.ricam.oeaw.ac.at/specsem/srs/groeb/
- building up of a formal knowledge base for Groebner bases theory.

#### **Activities**

The goals of the special semester were mainly achieved by the organization of workshops that covered the basics and recent advances

• on **Groebner bases theory** (and related theories) and its original application in the area of algebraic geometry and polynomial ideal theory (Workshops A, B1, B2, and C)

• applications of Groebner bases (and related methods) (Workshops D1, D2, D3).

# **Detailed information on the workshops**

# Workshop A, "Groebner Bases Theory and Applications in Algebraic Geometry".

February 06 - February 17.

Chairmen: Gert-Martin Greuel, Gerhard Pfister.

# Workshop B1, "Approximate Commutative Algebra".

February 20 - February 24.

Chairman: Lorenzo Robbiano.

# Workshop B2, "Efficient Computation of Groebner Bases".

February 27 - March 03.

Chairmen: Jean-Charles Faugère, Hans-Gert Gräbe, Viktor Levandovskyy, Quoc-Nam Tran.

# Workshop C, "Formal Groebner Bases Theory".

March 06 - March 10.

Chairman: Bruno Buchberger.

# Workshop D1, "Groebner Bases in Cryptography, Coding Theory, and Algebraic Combinatorics".

April 30 - May 06.

Chairmen: Mikhail Klin, Ludovic Perret, Max Sala.

# Workshop D2, "Groebner Bases in Symbolic Analysis".

May 08 - May 17.

Chairmen: Peter Paule, Dongming Wang, Markus Rosenkranz and Viktor Levandovskyy.

#### Workshop D2a, "Mini-Workshop on Groebner Bases and Theorem Proving in Geometry".

May 13.

Chairmen: Bruno Buchberger, Tetsuo Ida.

# Workshop D3, "Groebner Bases in Control Theory and Signal Processing".

May 18 - May 19.

Chairman: Hyungju Park.

For a complete list of all talks given at the workshop, see the web site

http://www.ricam.oeaw.ac.at/specsem/srs/groeb/

In addition to the workshops, long-term research stays during the special semester were made possible for a couple of PhD and Postdoc students and senior researchers.

#### **Publication output**

The main publication output of the special semester was structured in the form of ten proceedings volumes, whose scope, contents, and responsible guest editors were discussed and defined during the workshops under the direction of Bruno Buchberger. These proceedings volumes will appear with three different publishers:

- Radon Book Series (de Gruyter; series editor: Heinz Engl)
- Journal of Symbolic Computation (Elsevier; journal editor: Hoon Hong),
- and RISC Book Series (Springer; series editor: Peter Paule).

Publication of papers in these volumes is also possible for researchers who did not participate in the special semester, see the call for papers at http://www.ricam.oeaw.ac.at/specsem/srs/groeb/

Details on the proceedings volumes:

Nr. 1, Working Title: "Approximate Commutative Algebra"

Editors: L. Robbiano, J. Abbott Managing Editor: J. Abott

Publisher: Radon Book Series (RICAM)

Nr. 2, Working Title: "Efficient Computation of Groebner Bases" Editors: J.C. Faugère, H.G. Graebe, V. Levandovskyy, Q.N. Tran

Managing Editor: Q. N. Tran Publisher: JSC special issue.

Nr. 3, Working Title: "Polynomial Systems Solving"

Editors: J.C. Faugère, F. Roullier, Managing Editor: J.C. Faugère Publisher: RISC book series.

Nr. 4, Working Title: "Groebner, Coding, and Cryptography"

Editors: T. Mora, L. Perret, S. Sakata, M. Sala, C. Traverso

Managing Editor: M. Sala Publisher: RISC Book Series

Nr. 5, Working Title: "Groebner, Coding, and Cryptography"

Editors: J.C. Faugere, D. Augot, L. Perret

Managing Editor: L. Perret Publisher: JSC special issue

Nr. 6, Working Title: "Algorithmic Algebraic Combinatorics and Groebner Bases"

Editors: G. Jones, A. Jurisic, M. Muzychuk, I. Ponomarenko

Managing Editor: G. Jones (Coordination: M. Klin) Publisher: RISC Book Series.

Nr. 7, Working Title: "Groebner Bases and Symbolic Analysis"

Editors: M. Rosenkranz, D.M. Wang. Managing Editor: M. Rosenkranz Publisher: RICAM Book Series.

Nr. 8, Working Title: "Groebner Bases and Special Functions Identities with Applications in Physics"

Editor: P. Paule

Managing Editor: P. Paule Publisher: RISC Book Series.

Nr. 9, Working Title: "Groebner Bases, Control Theory and Signal Processing"

Editors: H. Park, G. Regensburger

Managing Editor: H. Park Publisher: RICAM Book Series.

Nr. 10, Working Title: "Non-commutative Groebner Bases"

Editors: V. Levandovskyy

Publisher: JSC

# Further publications:

- Wilson Castro, "On methods for the construction of reduction rings". Journal of Symbolic Computation.
- Mingsheng Wang, "Notes on multivariate polynomial matrix factorization problem". Journal of Algebra.
- Roy L. McCasland, Alan Bundy, "MATHsAiD: a Mathematical Theorem Discovery Tool". Proceedings of SYNASC 2006.

#### Web Site

The web site of the special semester, http://www.ricam.oeaw.ac.at/specsem/srs/groeb/, is still active. It contains detailed information on all workshops, information on the participants, the interactive Groebner bases bibliography, and also on the ongoing publication projects, in particular the calls for papers.

The web site, including the Groebner bases on-line bibliography is administered by Alexander Zapletal, scientific assistant of Professor Buchberger.

# Statistics and evaluation

Number of participants: 291

Long-term guests (stay longer than 2 months): 11

Short-term guests: 280

Supported PhD students: 36

Total number of days of participation: 3639

The quality of the activities during the special semester were assessed by the participants in an anonymous evaluation form. The overall assessment ranged from excellent to very good.

# 3.3. SPECIAL SEMESTER ON QUANTITATIVE BIOLOGY ANALYZED BY MATHEMATICAL METHODS, OCTOBER 1, 2007 – JANUARY 27, 2008

This special semester on Quantitative Biology analyzed by Mathematical Methods will take place from October 1, 2007 until January 27, 2008. <a href="http://www.ricam.oeaw.ac.at/ssqbm/">http://www.ricam.oeaw.ac.at/ssqbm/</a>

# **Program Committee**

Robert Anderssen, CSIRO Mathematical and Information Sciences, Canberra, Australia

Martin Burger, University of Münster, Germany

Vincenzo Capasso, University of Milan, Italy

Robert Eisenberg, Rush University and Argonne National Laboratory, Chicago IL, USA

Heinz W. Engl, RICAM & Johannes Kepler University Linz, Austria

Christoph Flamm, University of Vienna, Austria

Philipp Kügler, RICAM & Johannes Kepler University Linz, Austria

Peter Markowich, RICAM & University of Vienna, Austria

Peter Pohl, Johannes Kepler University Linz, Austria

Otmar Scherzer, Leopold Franzens University of Innsbruck, Austria

Christian Schmeiser, RICAM & University of Vienna, Austria

Peter Schuster, University of Vienna, Austria

Heinz Engl is currently chairing the activities.

#### Overview

The goal of the special semester is to provide a stimulating environment for biologists, physicists and mathematicians to jointly address emerging challenges in quantitative biology.

- Problems in the fields of
- Membranes and Channels: Burger, Eisenberg, Engl, Pohl
- Bioimaging: Scherzer
- Systems Biology: Engl, Flamm, Kügler, Schuster
- Pattern Formation and Functional Morphology: Capasso, Anderssen
- Chemotaxis: Markowich, Schmeiser
- Biomechanics of Cells: Schmeiser

These problems will be studied by exploring mathematical methods from the areas of

- Inverse Problems
- PDEs
- Stochastics
- Dynamical Systems

Leading experts, talented post-docs and doctoral students will have the opportunity to collaborate at RICAM in an interdisciplinary atmosphere in order to gain new perspectives and to develop novel approaches.

While the program features tutorials, workshops, social events and a culminating meeting at the University Center Obergurgl in the Austrian Alps, the participants are encouraged to organize additional research activities according to their ideas and needs.

# Main Topics

# Bioimaging - O. Scherzer

The goal of imaging is to make data accessible for efficient visual inspection. Today imaging is a multidisciplinary field, with profound applications in medicine, computer vision, biology, industry, and in general in applied sciences. Imaging is performed on every scale; on the top end is astrophysics where it is used to analyze huge objects such as galaxies. In radiology, cur- rent technological developments aim to improve the detection of disease. Novel measurement devices are developed to enhance resolution and to make imaging techniques applicable for visualization of smaller de- tails with particular applications in the bio sciences.

During the program we study mathematical methods and applications of imaging in the bio sciences. In particular, we focus on mathematical methods for image reconstruction, image filtering, novel applications for data acquisition, visualization and mathematical theory.

#### Biomechanics of Cells - C. Schmeiser

Many fundamental processes in our body depend on the ability of cells to migrate - examples range from embryogenesis and wound healing to the response of our immune system to infections or the generation of new blood vessels. The crawling motion of cells has first systematically been described more than two decades ago and, since then, it has become a field of intensive research. Especially in the last years, the development of new experimental methods and tools has allowed to gain new insights into the biological, chemical and mechanical nature of cell migration.

However, due to the complexity of the processes involved, biologists are still far away from having a complete picture of how cells move. During the special semester we want to use mathematical modelling in an interdisciplinary fashion for getting a deeper under- standing of the observed biological phenomena as well as for providing tools to test different hypotheses and theories formulated by experimentalists. In particular, there will be a focus on the intracellular biomechanical effects and their interplay with the intracellular bio- chemistry and with the mechanical properties of the environment. One emphasis will be on a mechanical description of the dynamics of the cytoskeleton, in particular the growth, decay, and mechanical response of polymer networks. Experiments elucidating the exact structure of the cytoskeleton will be analyzed as well as experiments on the behaviour of living, crawling cells.

## Membranes and Channels - M. Burger, R. Eisenberg, H. W. Engl, P. Pohl

Channels control the flow of many substances into and out of cells and are of enormous importance in health and disease. Channels and transporters make up a large fraction of all the proteins in the human body and are studied experimentally by thousands of molecular biologists. Many of the drugs used by physicians act on channels, and their structure is known with atomic resolution. Ion channels work by switching between open and closed states. In the open state, they have a structure that does not change significantly on a time scale relevant for simulations. Ions move through the open channel by electro-diffusion controlled by the density of permanent and polarization charge on the channel protein, and the shape of the hole in the channel. The driving forces for ion movement are concentration gradients and the electrical potential across the channel protein. The movement of ions through the channel can be described by the Poisson-Nernst-Planck equations. Selectivity of membrane channels is, in part, achieved by size exclusion, in particular in water channels. In the limiting case, pores are so narrow that water molecules and ions cannot pass each other. So far little is known about water mobility in confined pores, and it is an important task to obtain further insight by quantitative mathematical models and simulations.

#### Chemotaxis - P. Markowich, C. Schmeiser

Modelling and simulation of chemotaxis is a success story of Mathematical Biology. On the one hand, prototypical mathematical models like the Keller-Segel model have been investigated thoroughly with many exciting mathematical results. On the other hand, an ongoing modelling effort deals with the incorporation of effects on the individual cell level as well as with alternative transport models for cell ensembles. In the framework of the special semester, the nonlinear inter- action between cells caused by long range (signalling) and short range (adhesion) effects and the consequent mathematical difficulties (e.g. blow-up in finite time) will be investigated. Furthermore, quantitatively accurate models for applications such as immune response, vasculogenesis, embryogenesis will be derived and analyzed. The multiscale (cell vs. ensemble scale) nature will be crucial both from an analysis and from a numerical point of view. We plan to establish an interaction with experimental biologists, leading to experiment-driven modelling and systematic parameter identification by methods for inverse problems.

# Systems Biology - H. W. Engl, C. Flamm, P. Kügler, P. Schuster

Systems biology is heading for a description of the functional relations of all players in an entire cell or an organism by means of chemical reaction kinetics, i.e., complete genetic and metabolic reaction network are the subject of mathematical analysis, modeling, and simulation. Although analysis and modeling of whole cells is still out of reach, modules or semi-autonomous regulation and reaction subnetworks are studied successfully and provide an understanding of important quantities which are characteristic for living systems, e.g., robustness, homeostasis and long term stability of periods. The great challenge of systems biology comes from the large numbers of reactions, often several thousands and more, as well as a similarly large number of parameters, many of which are unknown, leading to high dimensional ODEs.

High-throughput data of cells at the genomic, proteomic and metabolic levels provide an enormous amount of information on the dynamics of functioning cells. During the special semester we focus on mathematical methods to infer the functional network at genomic or metabolic level from such time series data. Problems to be studied include the calcium dynamics during T-cell activation, the analysis of stoichiometric networks and the evolution of metabolic networks.

# Pattern Formation and Functional Morphology - V. Capasso, R. Anderssen

A fundamental question in Biology, Biotechnology and Medicine is how the interplay between the genome and the physical environment drives pattern formation and morphogenesis. As well as experimental observations, the transformation of the genetic information into a spatial- temporal expression pattern is studied by mathematical models together with relevant methods for the analysis of real data, such as geometric statistics and inverse problems. It is our goal to bring together developmental biologists and mathematicians in order to promote a multi-disciplinary approach, by utilizing mathematical modelling, analysis, numerical simulation and visualization in order to validate models based on real experimental data. Major challenges exist in spanning quantitatively the enormous scale gaps that link observational molecular genetics to cell dynamics, cell dynamics to organ function and organ function to organism behaviour. From such perspectives, phyllotaxis is a good model system to investigate. Modelling and simulation related to in vivo and in vitro experiments will have many implications for research in biology and medicine. Final scope of the research would be the development of significant mathematical models suitable for understanding the basic biological issues that may lead to diagnosis, prevention and cure of malfunctioning.

#### Time Schedule

- Tutorial: probably October 1 5, 2007
- Workshop on Ion Channels October 8 12, 2007
- Workshop on Systems Biology November 5 9, 2007
- Workshop on Bioimaging I November 12 16, 2007
- Workshop on Bioimaging II / PDEs November 19 23, 2007
- Workshop on Biomechanics and Chemotaxis December 10 14, 2007
- Workshop on Pattern Formation and Functional Morphology January 7 11, 2008
- Culminating workshop January 22-27, 2008 (in Obergurgl, Tyrol).

# 3.4. <u>Special Semesters – Publications and Outcome</u>

RICAM is now connected to a newly created book series to be published de Gruyter called "Radon Series for Computational and Applied Mathematics". The editorial board consists of:

Hansjörg Albrecher, Heinz W. Engl (Editor-in-Chief), Ronald Hoppe, Karl Kunisch, Ulrich Langer, Harald Niederreiter, Christian Schmeiser

In this book series, we will both publish material originating from the special semesters and research monographs in computational and applied mathematics.

The **Special RICAM Semester** on "Computational Mechanics" was held at RICAM in Linz, October 3 – December 16, 2005. A detailed report on the activities held during this special semester was given in the annual report 2006 and can be found on the homepage of the special semester on "Computational Mechanics" <a href="http://www.ricam.oeaw.ac.at/sscm/">http://www.ricam.oeaw.ac.at/sscm/</a>. However, the main and most valuable results of the special semester are the joint scientific research activities of the participants which were initiated during the special semester and which have resulted in joint publications, in improved or new software packages, in joint presentations at conferences, in joint organizations of conferences, workshops, minisymposia etc., see

- http://www.ricam.oeaw.ac.at/specsem/sscm/publications/ and
- <a href="http://www.ricam.oeaw.ac.at/specsem/sscm/followup/">http://www.ricam.oeaw.ac.at/specsem/sscm/followup/</a>

for publications and follow-up events, respectively.

Some of the lectures and survey talks will be published in the new Radon Series as a kind of proceedings. At least two monographs were initiated during the Special Semester. Both monographs will appear in the new Radon Series for Computational and Applied Mathematics which is published by Walter de Gruyter GmbH & KG. The first monograph written by S. Repin is devoted to his lectures on a posteriori estimates for differential equations which were given during the special semester. The second monograph on "Robust Algebraic Multilevel Methods and Algorithms" is prepared by J. Kraus and S. Margenov. Therefore, this follow-up phase has already indicated the long-term impact of this special semester on the scientific community. The homepage of the special semester on "Computational Mechanics" will be continuously updated with respect to the follow-up phase.