

**AUSTRIAN ACADEMY OF SCIENCES**

# **Annual Report 2005**

Johann Radon Institute for Computational  
and Applied Mathematics

PERIOD: 1.1.2005- 31.12.2005

DIRECTOR: Prof. Heinz W. Engl

ADDRESS: Altenbergerstr. 69  
A-4040 Linz

# Content

|  |           |
|--|-----------|
| <b>1. THE DEVELOPMENT OF THE INSTITUTE IN GENERAL .....</b>                                    | <b>4</b>  |
| <i>Personnel.....</i>  | 4         |
| <i>Office Space.....</i>   | 7         |
| <i>IT Infrastructure.....</i>  | 7         |
| <b>2. THE SCIENTIFIC ACHIEVEMENTS AND PLANS OF THE INSTITUTE.....</b>                          | <b>10</b> |
| 2.1. GROUP “COMPUTATIONAL METHODS FOR DIRECT FIELD PROBLEMS” .....                             | 10        |
| <i>Introduction by Group Leader Prof. Ulrich Langer.....</i>                                   | 10        |
| <i>Almedin Becirovic .....</i>   | 12        |
| <i>Dr. Gergana Bencheva.....</i>   | 13        |
| <i>Dr. Marco Discacciati.....</i>  | 15        |
| <i>Robert Gaisbauer .....</i>  | 17        |
| <i>Dr. Johannes Kraus.....</i>   | 18        |
| <i>David Pusch .....</i>   | 19        |
| <i>Dr. Joachim Schöberl.....</i>   | 21        |
| <i>Dr. Satyendra Tomar.....</i>  | 23        |
| <i>Sabine Zaglmayr.....</i>  | 25        |
| 2.2. GROUP “INVERSE PROBLEMS” .....  | 28        |
| <i>Introduction by Group Leader Prof. Heinz W. Engl.....</i>                                   | 28        |
| <i>PD Dr. Ronny Ramlau.....</i>  | 29        |
| <i>Prof. Dr. Sergei Pereverzyev.....</i>   | 31        |
| <i>Cao Hui .....</i>   | 34        |
| <i>Lu Shuai.....</i>   | 35        |
| <i>Dr. Arnd Rösch.....</i>   | 35        |
| <i>Svetlana Cherednichenko .....</i>   | 38        |
| <i>Nataliya Metla .....</i>  | 39        |
| <i>Klaus Krumbiegel .....</i>  | 40        |
| <i>Andreas Hofinger .....</i>  | 42        |
| <i>Dr. Elena Resmerita .....</i>   | 43        |
| <i>Rainer Stütz .....</i>  | 44        |
| <i>Dr. Herbert Egger .....</i>   | 45        |
| <i>Dr. Stefan Kindermann .....</i>   | 48        |
| <i>Benjamin Hackl .....</i>  | 49        |
| <i>Marie-Therese Wolfram .....</i>   | 50        |
| <i>Inverse Problems in Molecular Biology: A Cooperation with the University of Vienna.....</i> | 51        |
| <i>Dr. Stefan Müller .....</i>   | 52        |
| <i>Dr. James Lu .....</i>  | 54        |
| 2.3. GROUP “SYMBOLIC COMPUTATION” .....  | 56        |
| <i>Overview of the Work of the Symbolic Computation Area in 2005 .....</i>                     | 56        |
| <i>Introduction by Group Leader Prof. Bruno Buchberger .....</i>                               | 57        |
| <i>Research Plan of the Computational Logic Group for 2006 and 2007.....</i>                   | 57        |
| <i>Prof. Dr. Bruno Buchberger .....</i>  | 59        |
| <i>Dr. Martin Giese .....</i>  | 61        |
| <i>Dr. Florina Piroi .....</i>   | 63        |
| <i>Dr. Georg Regensburger .....</i>  | 64        |
| <i>Dr. Markus Rosenkranz .....</i>   | 66        |
| <i>Alexander Zapletal .....</i>  | 67        |
| <i>Overview of the Work of the Computational Algebra Area by Prof. Josef Schicho .....</i>     | 69        |
| <i>Prof. Dr. Josef Schicho.....</i>  | 69        |
| <i>Dr. Willem A. de Graaf .....</i>  | 71        |
| <i>Dr. Oliver Labs .....</i>   | 72        |
| <i>Dr. Pavel Chalmoviansky .....</i>   | 73        |

|  |            |
|--|------------|
| <i>Dr. Ibolya Szilagyi</i> .....                                     | 74         |
| <i>Michael Barton</i> .....  | 75         |
| <i>Tobias Beck</i> .....   | 76         |
| <i>José Manuel García Vallinas</i> .....                             | 77         |
| <i>Janka Pilnikova</i> .....   | 78         |
| <b>2.4. GROUP “FINANCIAL MATHEMATICS” .....</b>                      | <b>80</b>  |
| <i>Introduction by Group Leader Prof. Walter Schayermayer</i> .....  | 80         |
| <i>Univ.-Doz. Dr. Hansjörg Albrecher</i> .....                       | 81         |
| <i>Prof. Walter Schachermayer</i> .....                              | 84         |
| <i>Dr. Jürgen Hartinger</i> .....                                    | 86         |
| <i>Dr. Karel Janeček</i> .....                                       | 87         |
| <i>Dr. Gottlieb Pirsic</i> .....                                     | 89         |
| <i>Dr. Jörn Saß</i> .....  | 90         |
| <i>Dr. Klaus Scheicher</i> .....                                     | 93         |
| <i>Univ.-Doz. Dr. Arne Winterhof</i> .....                           | 94         |
| <i>Nina Brandstätter</i> .....                                       | 98         |
| <i>Markus Hahn</i> .....   | 99         |
| <i>Univ.-Doz. Dr. Wilfried Meidl</i> .....                           | 100        |
| <i>Wolfgang Putschögl</i> .....                                      | 101        |
| <i>Christiaan van de Woestijne</i> .....                             | 102        |
| <b>2.5. GROUP “ANALYSIS OF PARTIAL DIFFERENTIAL EQUATIONS” .....</b> | <b>104</b> |
| <i>Introduction by Group Leader Prof. Peter Markowich</i> .....      | 104        |
| <i>Dr. Shun-Yin Chu</i> .....  | 104        |
| <i>Dr. Marco Di Francesco</i> .....                                  | 105        |
| <i>Dr. Yasmin Dolak-Struß</i> .....                                  | 107        |
| <i>Dr. Arjan Kuijper</i> .....                                       | 109        |
| <i>Dr. Norayr Matevosyan</i> .....                                   | 112        |
| <i>Dr. Lukas Neumann</i> .....                                       | 112        |
| <b>2.6. GROUP “OPTIMIZATION AND OPTIMAL CONTROL” .....</b>           | <b>114</b> |
| <i>Introduction by Group Leader Prof. Karl Kunisch</i> .....         | 114        |
| <i>Dr. Samuel Amstutz</i> .....                                      | 115        |
| <i>Dr. Roland Griesse</i> .....                                      | 116        |
| <i>Nataliya Metla</i> .....  | 120        |
| <i>Dr. Boris Vexler</i> .....  | 120        |
| <b>3. SPECIAL SEMESTER, CONFERENCES, COLLOQUIA .....</b>             | <b>123</b> |
| <b>3.1. OVERVIEW .....</b>   | <b>123</b> |
| <i>Radon Colloquia</i> .....   | 123        |
| <i>Radon Seminars</i> .....  | 127        |
| <i>Group Seminars</i> .....  | 130        |
| <i>Conferences co-organized by RICAM</i> .....                       | 140        |
| <b>3.2. SPECIAL SEMESTER ON COMPUTATIONAL MECHANICS .....</b>        | <b>144</b> |
| <i>Overview by Prof. Ulrich Langer</i> .....                         | 144        |
| <b>3.3. FURTHER PLANS FOR SPECIAL SEMESTERS .....</b>                | <b>147</b> |
| <b>3.4. SPECIAL SEMESTER ON MATHEMATICS IN LIFE SCIENCES .....</b>   | <b>149</b> |
| <b>3.5. SPECIAL SEMESTER – PUBLICATIONS .....</b>                    | <b>150</b> |

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 2005 was a year of major expansion of personnel. On December 31, 2005, RICAM employed 33 scientists with a doctorate and 18 doctoral students; of those, 6 PostDocs and 16 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 2005, RICAM had 51 scientific employees, 22 of them been externally funded. For 2006, our aim is to reach the planned final state of 30 PostDocs funded via basis funds (Academy of Sciences and Upper Austrian Government) and to obtain also more external funds in order to be able to reach our goal of having equal numbers of scientists financed from internal and from external funds.

In the last report, we indicated that we planned to include a further group led by Georg Gottlob (then Vienna). In the meantime, Georg Gottlob has accepted a call by the University of Oxford and moved there, so that these plans cannot be realized.

We currently propose to include a new group (with two internally funded PostDocs) on “Mathematical Imaging” to be led by Prof. Otmar Scherzer (University of Innsbruck). This group will have a scientific overlap with most of the other groups at RICAM (especially Inverse Problems, Analysis of Partial Differential Equations and Symbolic Computation); Otmar Scherzer has already cooperated with several scientists involved in RICAM. A proposal has been sent the Kuratorium. We include a short version here:

#### Mathematical Imaging (by Otmar Scherzer)

In recent years, a great amount of work of the group in Innsbruck (Infmath Imaging) has been devoted to integrating mathematical and numerical methods from Computer Vision into variational regularization theory and to make them suitable for Inverse Problems applications. In particular, we have been developing variational techniques as alternatives to morphological partial differential equations and to discrete filtering.

In the work at the Radon Institute, we are aiming to further developing theory and efficient numerical implementation of non-convex variational methods, in particular, generalization to vector valued data (such as colour data), using concepts of quasi-convexity.

For the calculation of quasi-convex envelopes, we investigate the applicability of symbolic methods. Moreover, we intend to study the combination of non-convex regularization with discontinuous projection operators (which, e.g., appear in level set methods) with methods of Gamma-convergence.

Moreover, the existing joint work with the Radon Institute on image enhancement and the relation to variational regularization theory should be further analyzed and combined with non-convex regularization techniques. This particular subproject has already a strong link to the Industrial Mathematics

Competence Center (IMCC) in Linz, where we are working on enhancing techniques for ultrasound data.

With the addition of this new group, we certainly will have reached a critical mass and would not plan a further extension in the foreseeable future. However, changes in the size, leadership and scientific emphasis of the existing groups should and will always be possible, also based on evaluations and on advice by the Kuratorium. In 2005, a leadership change occurred in the Financial Mathematics Group: Prof. Gerhard Larcher resigned shortly after the visit by the Kuratorium. We were lucky to persuade, after looking at different options, Prof. Dr. Hansjörg Albrecher from the University of Technology in Graz to lead this group together with Walter Schachermayer. Since October 1, 2005, Prof. Albrecher is half-time employed by RICAM and thus spends half of his working time in Linz. Under his and Walter Schachermayer's leadership, the group is in the process of being reorganized scientifically. Results of the process will be available in the next annual report.

The following Scientist left in 2005:

| Name               | Employed until | Left to                       | Position             |
|--------------------|----------------|-------------------------------|----------------------|
| Willem de Graaf    | 28.02.2005     | University of Trento, Italy   | Associate Professor  |
| Norayr Matevosyan  | 28.02.2005     | University of Vienna          | University Assistent |
| Robert Gaisbauer   | 31.05.2005     | VAI                           |                      |
| Karel Janecek      | 30.06.2005     | RSJ Invest, a. s.             | Chief Analyst        |
| Wilfried Meidl     | 31.07.2005     | University of Sabanci; Turkey | Lecturer             |
| Rainer Stütz       | 31.08.2005     | Company in Vienna             |                      |
| Marco Di Francesco | 31.08.2005     | University of L'Aquila, Italy | Research Associate   |
| Ibolya Szilagyi    | 31.08.2005     | EKTF Eger, Hungary            | University Assistent |
| Yasmin Dolak-Struß | 31.12.2005     | University of Vienna          | University Assistent |

In 2005, the following additional PostDocs doctoral and students were hired via RICAM basic funds:

| PostDoc Name               | At RICAM since | Doctorate: year, institution                                | Came to RICAM from  |
|----------------------------|----------------|---|---|
| Satyendra Tomar            | 01.01.2005     | 2001, Indian Institute of Technology Kanpur                 | University of Twente, Netherlands                             |
| Martin Giese               | 01.03.2005     | 2002, University of Karlsruhe                               | Chalmers Institute of Technology, Gothenburg, Sweden          |
| Marco Discacciati          | 01.04.2005     | 2004, Ecole Polytechnique Fédérale de Lausanne, Switzerland | Ecole Polytechnique Fédérale de Lausanne, Switzerland         |
| Gergana Bencheva           | 01.07.2005     | 2005, Bulgarian Academy of Sciences                         | Bulgarian Academy of Sciences                                 |
| Lukas Neumann              | 01.08.2005     | 2005, University of Vienna                                  | University of Vienna, University of the Basque Country Bilbao |
| Samuel Amstutz             | 01.08.2005     | 2003, Laboratoire MIP, Toulouse                             | Fraunhofer Institute, ITWH Kaiserslautern                     |
| Hanna Katriina Pikkarainen | 01.09.2005     | 2005, Helsinki University of Technology                     | Helsinki University of Technology                             |

|  |            |  |  |
|--|------------|--|--|
| Ronny Ramlau                                   | 01.09.2005 | 1997, University of Potsdam                  | University of Bremen                   |
| Oliver Labs                                    | 01.10.2005 | 2005, Johannes Gutenberg University of Mainz | Johannes Gutenberg University of Mainz |
| Jürgen Hartinger                               | 01.10.2005 | 2004, Graz University of Technology          | Graz University of Technology          |
| Hansjörg Albrecher<br>(Group Leader half-time) | 01.10.2005 | 2001, Graz University of Technology          | University of Aarhus (Denmark),        |
| Arjan Kuijper<br>(half-time)                   | 01.11.2005 | 2002, University of Utrecht                  | IT University of Copenhagen, Denmark   |

| Doctoral Student Name: | At RICAM since | Diploma/: year, institution | Came to RICAM from |
|------------------------|----------------|-----------------------------|--------------------|
| David Pusch            | 01.10.2005     | 2003, University of Linz    | University of Linz |

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

| PostDoc Name      | At RICAM since | Doctorate: year, institution                | Came to RICAM from                     |
|-------------------|----------------|---|--|
| James Lu          | 01.08.2005     | 2005, Massachusetts Institute of Technology | MIT Aerospace Computational Design Lab |
| Stefan Kindermann | 01.09.2005     | 2001, University of Linz                    | UCLA                                   |

| Doctoral Student Name       | At RICAM since | Diploma: year, institution             | Project: agency/number/leader   |
|-----------------------------|----------------|--|---------------------------------|
| Markus Hahn                 | 01.02.2005     | 2003, University of Linz               | FWF, P17947, Saß                |
| Wolfgang Putschögl          | 01.03.2005     | 2005, University of Linz               | FWF, P17947, Saß                |
| Svetlana Cherednicheko      | 01.08.2005     | 2005, University of Joensuu            | FWF, P18090-N12, Rösch          |
| Marie-Therese Wolfram       | 01.08.2005     | 2005, University of Linz               | FWF, SFB F1308, Engl            |
| José Manuel Garcia          | 01.08.2005     | 2002, University of Valladolid (Spain) | FWF, SFB F1303, Schicho         |
| Natalyia Metla              | 01.09.2005     | 2005, BTU Cottbus                      | FWF, P18056-N12, Rösch, Griesse |
| Klaus Krumbiegel            | 01.10.2005     | 2005, Technical University of Chemnitz | FWF, P18090-N12, Rösch          |
| Michael Barton              | 01.10.2005     | 2002, Czech Technical University       | FWF, SFB F1315, Schicho         |
| Christiaan van de Woestijne | 01.10.2005     | 1999, University of Leiden             | FWF, S8313, Winterhof           |

Magdalena Fuchs started part-time as secretary in July 2005.

## ***Office Space***

Due to the rapid expansion of the personnel, we had to make additional office space available. In the beginning of 2005, RICAM had a total of 275 square meters of office space. With the help of the University, we were able to rent (currently for a period of four years) four large apartments adjacent to the campus of the University; they were adapted and furnished and equipped with computer infrastructure and now house the groups Financial Mathematics, Symbolic Computation and Analysis of Partial Differential Equations. In addition, there is also a small seminar room and office space for long term visitors there, especially during special semesters.

All together RICAM has now 730 square meters of office space.

Due to the new office space, we were also able to enlarge our main seminar room, which now can hold up to 50 participants. This is not large enough for some events, especially during the special semesters; for such events, we rent a larger lecture hall in the basement of our building from the University.

Of course it would be better if all RICAM scientists could be housed in the same building. The University has very concrete plans to build a Science Park close to the University and has included space for RICAM in these plans. It is expected that in 2008, all of RICAM will be able to move into this new building.

## ***IT Infrastructure***

### 2005

#### Network at the new premises

The new premises were connected to the main RICAM building by a 10Mbit uplink. At the new premises the computers 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 premises mainly used by Special Semester guests is separated from the RICAM internal network by the central firewall at RICAM. The premises were all fitted with wireless lan access points. The wireless lan access points were 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

A central firewall was installed at RICAM. The decision and concept were made together with the Austrian Academy Computer Centre. As vendor, the linux-based PHION firewall was chosen which runs on a standard PC architecture based server. The firewall is integrated into the new centrally managed firewall infrastructure at the Austrian Academy of Sciences. The RICAM systems administration has full access to the central administration interface through a secure VPN connection and manages its firewall completely alone. The firewall divides the RICAM network into 3 different security zones. One for the internal RICAM network where all outgoing connections (and replies from outgoing connections) are allowed, one for the special semester guests where only outgoing connections to essential services like email, web are allowed and one for the servers where also incoming connections to services like email, web are allowed. The firewall also provides VPN service to securely connect from other networks (as example home computers) to the RICAM network via an encrypted tunnel through a standard internet connection.

## Servers

### Print Server

A print server was installed to allow easy access to all RICAM printers. The print server is reachable from the internal RICAM lan, the network segment for Special Semester guests and from the JKU WLAN network. Simple “One-Click installation for all printer”-scripts where written for Windows and Linux clients to allow guests at RICAM printer access without configuration knowledge and help of system administrators. 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. As printing system the free Internet Printing Protocol implementation Cups was chosen.

### Communication server

The server provides the RICAM webpage including database access, email access through pop3 and imap, spam and virus filter for email services, webmail 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 2005 a WikiWiki software was added to let users easily create webpages for internal usage. For the Special Semester, extra webpages and database based scripts for information, registration, program and time schedule where 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 of Linz. 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 2005, no changes where made to the configuration as everything is working well.

### 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 2005, no changes to the configuration where made in 2005 as everything is working well.

### Computing Server

A dedicated dual Processor Computing Server with 8GB af main memory was bought available to all RICAM employees for large calculations. 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.

## Clients

### Laptops

Toshiba Tecra S2 Laptops were bought for the best compromise between mobility and power. Each laptop is equipped with 1GB 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 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 last year. The workstations are able to work in a cluster mode with parallel pro-

grammed 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 were 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 last year. 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 since July 2005)  
Dr. Marco Discacciati (employed since April 2005)  
Dr. Johannes Kraus  
Dipl.-Ing. David Pusch (employed since October 2005)  
Dr. Joachim Schöberl  
Dr. Satyendra Tomar

**Researchers externally funded by the FWF START project Y192 led by Dr. Joachim Schöberl:**

Dipl.-Ing. Almedin Becirovic  
Dipl.-Ing. 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, magnetohydrodynamics, and pharmacy.

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 leads the FWF START project Y192 “hp-FEM” that is also devoted to fast solvers for hp finite element equations. In June 2005, the START project was evaluated very positively by an international jury. The jury prolonged the START project for further three years. M. Discacciati has also contributed to domain decomposition methods. The second group of solvers, developed by J. Kraus and D. Pusch, belong to Algebraic MultiGrid (AMG) methods. AMG methods are very important as black-box solvers for practical applications because they do not require any hierarchical discretization structure.

Recent publications of the group leader have also contributed to these two main research fields in 2005. The publications [3, 6] are devoted to DD techniques, whereas the papers [4, 5] deal with AMG methods for large scale data-sparse boundary element equations. The paper [1] is devoted to the analysis of non-linear eddy current problems with harmonic excitations and their numerical solution via some multiharmonic techniques. The results on multiharmonic techniques and other results obtained in Computational Electromagnetics were presented in an invited talk at the SFB-Abschlusskolloquium of the SFB 393 held in Chemnitz, November 11, 2005, Germany [10]. The new results on Boundary Element Tearing and Interconnecting (BETI) methods were presented in a talk at the Oberwolfach workshop on “Fast Solvers for Partial Differential Equations”, Oberwolfach, Germany, May 22 – 28, 2005, [8], and in a plenary talk at the 5th International Conference on “Large-Scale Scientific Computations” LSSC 2005, Sozopol, Bulgaria, June 6 - 10, 2005, [9]. Our first results on grid computing, where we also use DD techniques for the data distribution, were presented at the 1st Austrian Grid Symposium, Hagenberg, December 1 – 2, 2005, and will be published in the proceedings [7].

- F. Bachinger, U. Langer, J. Schöberl: *Numerical Analysis of Nonlinear Multiharmonic Eddy Current Problems*. Numerische Mathematik, vol. 100, No. 4, 593-616, 2005.
- U. Langer, D. Pusch: *Data-Sparse Algebraic Multigrid Methods for Large Scale Boundary Element Equation*. Applied Numerical Mathematics, vol. 54, No. 3-4, 406-424, 2005.
- U. Langer, G. Of, O. Steinbach, W. Zulehner: *Inexact Fast Data-Sparse Boundary Element Tearing and Interconnecting Methods*. RICAM Report 2005-07, Johann Radon Institute for Computational and Applied Mathematics, Linz, 2005, and submitted.
- 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, June 6 - 10, 2005, Sozopol, Bulgaria, Volume 3743 of Lecture Notes in Computer Science, pp. 130-137, Springer-Verlag, Heidelberg, Berlin, 2006.
- U. Langer, D. Pusch: Convergence Analysis of Geometrical Multigrid Methods for Solving Data-Sparse Boundary Element Equations. Proceedings of the 8<sup>th</sup> European Multigrid Conference on “Multigrid, Multilevel and Multiscale Methods” EMG 2005, Scheveningen, The Netherlands, submitted (an original paper that will be submitted to some journals is in preparation), see also RICAM Report 2005-16, Austrian Academy of Science, 2005.
- 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., Springer, Heidelberg, Berlin, 2006 (accepted for publication).
- U. Langer, H. Yang: *A Parallel Solver for the 3D Incompressible Navier-Stokes Equations on the Austrian Grid*. Proceedings of the 1<sup>st</sup> Austrian Grid Symposium, Hagenberg, December 1 – 2, 2005 (accepted for publication).
- U. Langer, *Inexact Data-Sparse Boundary Element Tearing and Interconnecting Methods*. Talk at the Oberwolfach workshop on “Fast Solvers”, Mathematisches Forschungsinstitut Oberwolfach, Germany, May 22 - 28, 2005.
- U. Langer: Inexact Data-Sparse Boundary and Finite Element Domain Decomposition Methods. Plenary Talk at the 5<sup>th</sup> International Conference on “Large-Scale Scientific Computations”, Sozopol, Bulgaria, June 5 – 10, 2005.
- U. Langer: *Efficient solvers in computational electromagnetics*. Invited Talk at the SFB-Abschlusskolloquium of the SFB 393, TU Chemnitz, November 11, 2005.

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 with the SFB. 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) 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 Hirscheegg, September 25 – 28, 2005.

See home page <http://www.numerik.math.tu-graz.ac.at/tagungen/FastBEM2005.htm> for more information. A special issue of the Springer journal “Computing and Visualization in Science” edited by U. Langer, O. Steinbach and W. Wendland is devoted to this topic. This special issue appeared in December 2005. The Oberwolfach-Workshop “Computational Electromagnetism” held in Oberwolfach (Germany), February 22 – 28, 2004 was organized by Ralf Hiptmair (Zurich), Ronald H.W. Hoppe (Augsburg) and Ulrich Langer (Linz). See home page <http://www.mfo.de/cgi-bin/tagungsdb?type=21&tnr=0409> for more information.

The 17<sup>th</sup> International Conference on Domain Decomposition, that is planned for July 3 – 7, 2006, is chaired by the group leader. See DD17 home page <http://www.RICAM.oeaw.ac.at/dd17> 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 (see Chapter 3.2 for short general

report). The CMG members were especially involved in the work of the special semester. J. Kraus was the program coordinator supported by D. Pusch. J. Schöberl was the co-organizer of the International Workshop on “*Direct and Inverse Field Problems*” that was embedded in the special semester. M. Discacciati, J. Kraus, D. Pusch, J. Schöberl, S. Tomar were local co-organizers of specific topics. They have started joint research works with different participants of the special semester leading to joint publications, talks etc. (see also the individual reports of the CMG members).

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 and J. Schöberl, deals with the development and the grid implementation of distributed mesh generators and distributed finite element solvers. The first results were presented at 1<sup>st</sup> Austrian Grid Symposium, Hagenberg, December 1 – 2, 2005.

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 investigates a non-linear system of coupled diffusion-reaction problems describing the diffusion of ointments through the skin. See the project homepage <http://www.mgnet.org/~douglas/ml-dddas-austria.html> 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 June 2005, R. Blaheta, U. Langer and S. Margenov organized a minisymposium on robust Algebraic Multigrid Methods at the 5<sup>th</sup> International Conference on Large-Scale Scientific Computations, Sozopol, Bulgaria, June 5 – 10, 2005. S. Margenov was one of the long-term visitors of the special semester. He and his PhD student who also participated in the special semester have started joint research work on algebraic multigrid and multilevel methods with J. Kraus, J. Schicho and J. Synka that will lead to at least three papers. Furthermore, joint activities are planned on international conferences.

Last but not least, J. Schöberl received a call a to W2-professorship position in “*Scientific Computing*” at the RWTH Aachen. He accepted the call in December 2005. He will move to Aachen in March 2006.

He will continue to supervise the doctoral students in his Start-Proct until July 31, 2008 under a part-time contract.

### **Almedin Bećirović**

#### **Scientific Achievements 2005**

*Primal-Dual Error Estimator for High Order Finite Elements:* A big challenge in finite element approximation are a posteriori error estimators and adaptivity. Our favourite error estimators works so, that in a first step we solve a primal problem to obtain the finite element approximation. From this, we compute in a post-processing step (second step) the discrete flux. The idea is similar to the standard Zienkiewicz-Zhou error estimator, except that we compute the flux in high order  $H(\text{div})$  finite element space, which seems to be more natural.

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.

*High Order  $H(\text{div})$  Finite Elements:* In order to compute the discrete flux, we need  $H(\text{div})$  finite element space. The elements involve normal components at the boundary, which are set by averaging the normal fluxes.

Therefore we have derived a new basis for a finite element sub-space of  $H(\text{div})$ . A central property of these spaces is the complete sequence property. Presently the following finite elements are implemented: triangular, quadrilateral, tetrahedral and prism.

*High Order EAS Finite Elements for Plates* : Enhanced Assumed Strain (EAS) elements have been introduced to avoid volume and shear locking problems, and are commonly used nowadays. The EAS technique can be considered as a convenient implementation method for realizing selective projection operators. We implemented high order basis functions for quadrilateral and triangular EAS elements for the Reissner Mindlin plate model.

### 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

### Publications 2005

#### Submitted

1. J. Schöberl and A. Becirovic: High Order EAS Elements for plates and 3D structure (submitted to proc of 5th International Conference on Computation of Shell and Spatial Structures, Salzburg 2005)

### **Dr.Gergana Bencheva**

#### Work before joining RICAM

Dr. G. Bencheva joined RICAM in July 2005. Before that she was working as a research scientist at the Department of Scientific Computations, Institute for Parallel Processing, Bulgarian Academy of Sciences.

In the period January – June, 2005 she was mostly involved in the final preparation of her PhD thesis, which was successfully defended on April 4, 2005. The title of the thesis is “Parallel algorithms for separation of variables and sparse matrices factorization”. Her supervisors are Prof. P. S. Vassilevski and Prof. S. Margenov.

The research of Dr. Bencheva before joining RICAM was focussed on development and analysis of parallel direct and iterative methods for numerical solution of elliptic boundary value problems discretized by finite differences or nonconforming finite elements (FE).

A recently introduced parallel preconditioner for the solution of nonconforming FE systems is studied in [A1].

The algorithm is based on the modified incomplete Cholesky factorization MIC(0) applied to a locally constructed approximation of the original stiffness matrix. Its real performance for distributed memory machines is improved by suitable reordering of the computations in the Message Passing Interface (MPI) code which allows overlapping of computations with communications.

In addition, during the summer semester of 2004/2005 academic year, she taught exercises to the course “Parallel Algorithms” in Faculty of Mathematics and Informatics, Sofia University.

She also participated in the local organizing committee of 5<sup>th</sup> International Conference on “Large-Scale Scientific Computations”, Sozopol, June 6<sup>th</sup>-10<sup>th</sup>, 2005.

## Scientific Achievements 2005

After joining RICAM, G. Bencheva started working on coupled time dependent reaction diffusion equations arising in biochemistry.

She also continued her investigations in the area of the parallel algorithms. Theoretical estimates for the parallel speed-up and efficiency coefficients of the algorithm proposed in [A1], are derived in [S1]. Experimental study of Altix 3700 supercluster from the family SGI Altix 3000 is made and qualitative estimates of its communication and computation parameters are derived. The supercluster is available in Johannes Kepler University, Linz. Related numerical results for the algorithm from [A1] are presented in [S1] together with a comparative analysis of the performance on a Beowulf type Linux cluster (Ostrava, Czech Republic) and on a Sun Fire symmetric multiprocessor (Uppsala, Sweden).

Dr. G. Bencheva systematically attended the following lecture series and events of the RICAM special semester:

- Discontinuous Galerkin methods, organized by R. Lazarov (TAMU, USA) and S. Tomar (RICAM, Austria)
- H-matrix techniques, organized by W. Hackbusch (MPI, Leipzig, Germany) and D. Pusch (JKU, Austria)
- Robust parallel algebraic multigrid and multilevel techniques, organized by S. Margenov (BAS, Bulgaria) and J. Kraus (RICAM, Austria)
- Domain Decomposition Methods, organized by S. Nepomnyaschikh (Academy of Science, Novosibirsk, Russia) and S. Beuchler (JKU, Austria)
- Lecture on "Analysis of a finite PML approximation for the three dimensional time-harmonic Maxwell and acoustic scattering problems" by James H. Bramble (Texas A & M University, College Station, USA)
- Block Lectures on "Conversion from imperfection-sensitive into imperfection-insensitive elastic structures" by Herbert Mang (Vienna University of Technology, Austria),
- Computational Mechanics Challenges Day
- International Workshop on "Direct and Inverse Field Computations in Mechanics"
- Public Lecture on "Gottfried Wilhelm Leibniz - far ahead of his time" by Erwin Stein (University of Hannover, Germany)
- Miniworkshop "Domain Decomposition Methods" organized by Sergei Nepomnyaschikh
- Miniworkshop "Miniworkshop on DG methods" organized by Raytcho Lazarov and Satyendra Tomar

## Scientific Cooperations

### Internal

Dr. Marco Discacciati (RICAM)

Dr. Johannes Kraus (RICAM)

### External

Prof. Svetozar Margenov, Ivan Georgiev: Institute for Parallel Processing, Bulgarian Academy of Sciences, Sofia, Bulgaria

Prof. Sergei Nepomnyaschikh: Russian Academy of Sciences, Novosibirsk, Russia (started during the RICAM special semester)

Prof. Maya Neytcheva: Department of Information Technology, Uppsala University, Uppsala, Sweden

Dr. Jirí Starý: Institute of Geonics, Academy of Sciences of Czech Republic, Ostrava, Czech Republic

Justin Clay Harris: Department of Chemistry, Kentucky University, USA

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

- Workshop “Numerical linear algebra: recent advances, experience and applications”, Scientific Computing Division at Department of Information Technology, Uppsala, May 12, 2005
- 5<sup>th</sup> International Conference on “Large-Scale Scientific Computations“, Sozopol, June 6<sup>th</sup>-10<sup>th</sup>, 2005

Scientific Visits

Short term visit at the Department of Information Technology, Uppsala University, Sweden, May 7<sup>th</sup>-14<sup>th</sup>, 2005

Scientific Talks [T]

1. G. Bencheva: Parallel algorithms for separation of variables and sparse matrices factorization. PhD thesis public defence, Sofia, April 4, 2005.
2. G. Bencheva: MPI implementation of a PCG solver for nonconforming FEM problems: overlapping of communications and computations. Workshop “Numerical linear algebra: recent advances, experience and applications”, Uppsala, May 12, 2005.
3. G. Bencheva: Parallel PCG solver for nonconforming FEM problems: overlapping of communications and computations. 5th International Conference on “Large-Scale Scientific Computations“, Sozopol, June 6th-10th, 2005.

**Publications 2005**Appeared[A]

4. G. Bencheva, S. Margenov, J. Starý: Parallel PCG Solver for nonconforming FE problems: overlapping of communications and computations. In: I. Lirkov, S. Margenov, J. Waśniewski (Eds.) LSSC 2005, Springer LNCS 3743, pp. 646-654 (to appear).

Submitted[S]

5. G. Bencheva, S. Margenov, J. Starý: MPI implementation of a PCG Solver for nonconforming FEM problems: overlapping of communications and computations. To be available as Technical Report of Department of Information Technology, Uppsala University, February 2006.

***Dr. Marco Discacciati*****Work before joining RICAM**

I have joined RICAM in April 2005, after finishing my doctoral studies at the Ecole Polytechnique Fédérale de Lausanne, Switzerland, under the supervision of Prof. A. Quarteroni.

My main research interests are the numerical approximation of partial differential equations using finite elements and domain decomposition methods with application to multiphysics problems.

In particular, my doctoral research has focused on the mathematical and numerical analysis of the coupling of surface and porous media flows for environmental applications. A coupled model based on the Navier-Stokes equations and the Darcy equations with appropriate coupling conditions has been studied, and iterative methods based on the domain-decomposition framework have been set up, analysed and validated through several numerical tests.

In January-March 2005 I worked in collaboration with Prof. A. Quarteroni and Dr. S. Deparis (MIT, Boston) on the application of heterogeneous domain decomposition methods to fluid-structure interaction problems. The main results that we have achieved have been published in [A1-A3].

## Scientific Achievements 2005

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., aluminum production, to impose a desired behaviour to the liquid metals.

From the numerical point of view, this problem requires to analyse and implement effective and fast solvers for the coupled Navier-Stokes/Maxwell equations which model the motion of an incompressible conducting fluid subject to magnetic fields. At a first stage, we have considered the coupling of the Maxwell equations together with the Stokes and electric current problems in the fluid region. After proving the well-posedness of this problem, we have considered its conforming finite element discretization adopting Lagrangian, Raviart-Thomas and Nédélec elements. Finally, possible iterative solution methods have been proposed and implemented. The results that we have obtained are presented in the research report [S1].

Numerical approximation of surface-groundwater flows.

This research continues the cooperations established with Prof. A. Quarteroni, Prof. A. Valli, and with Dr. L. Badea. It mainly focuses on the study of the linear and nonlinear Steklov-Poincaré operators associated to the Navier-Stokes/Darcy coupled problem in order to characterize effective preconditioners for its solution using iterative substructuring methods. Two research reports presenting the main results that we have obtained are under completion [S2,S3].

## Scientific Cooperations

### Internal

Dr. Roland Griesse (RICAM)

Dr. Joachim Schöberl (RICAM)

Dr. Johannes Kraus (RICAM)

Dr. Gergana Bencheva (RICAM)

### External

Prof. Alfio Quarteroni, Ecole Polytechnique Fédérale de Lausanne (Switzerland) and MOX-Politecnico di Milano (Italy)

Prof. Alberto Valli, Department of Mathematics, University of Trento (Italy)

Dr. Lori Badea, Institute of Mathematics of the Romanian Academy, Bucharest (Romania)

Dr. Simone Deparis, Department of Mechanical Engineering, MIT - Massachusetts Institute of Technology, Boston (USA)

Heiko Berninger, PhD student in the group of Prof. Ralf Kornhuber, Institut für Mathematik II, Freie Universität Berlin (Germany)

## Participation at Conferences, Scientific Visits and Talk

### Conferences

16<sup>th</sup> International Conference on Domain Decomposition Methods, New York, January, 12<sup>th</sup>-15<sup>th</sup>, 2005

### Scientific Talks

- M. Discacciati: *Domain Decomposition Methods for Multiphysics Problems*. Miniworkshop on Domain Decomposition Methods – Special Radon Semester on Computational Mechanics, RICAM, Linz, November 18<sup>th</sup>, 2005.
- M. Discacciati: An introduction to magneto-hydrodynamic problems and Filtration of fluids through porous media. Lecture series held in the framework of the course Numerical Simulation of Coupled Fields organised by Dr. M. Kaltenbacher (University of Erlangen, Germany). Special Ra-

don Semester on Computational Mechanics, RICAM, Linz, November 30<sup>th</sup> and December 1<sup>st</sup>, 7<sup>th</sup>, 2005.

## Publications 2005

### Appeared [A]

1. S. Deparis, M. Discacciati and A. Quarteroni: A domain decomposition framework for fluid-structure interaction problems. In Proceedings of the 3rd International Conference on Computational Fluid Dynamics, Toronto 2004. Springer, New York. To appear (2005).
2. S. Deparis, M. Discacciati, G. Fourestey and A. Quarteroni: Fluid-structure algorithms based on Steklov-Poincaré operators. To appear in Comput. Methods Appl. Mech. Eng. (2005)
3. S. Deparis, M. Discacciati, G. Fourestey and A. Quarteroni: Heterogeneous domain decomposition methods for fluid-structure interaction problems. Accepted in Proceedings of the 17th International Conference on Domain Decomposition Methods, New York, 2005.

### Submitted [S]

4. M. Discacciati: Mathematical and numerical analysis of a Stokes magneto-hydrodynamic problem. To be available as RICAM report, January 2006.
5. M. Discacciati, A. Quarteroni and A. Valli: Robin-Robin methods for the Stokes-Darcy coupling. To be submitted and to be available as RICAM Report, January 2006
6. L. Badea, M. Discacciati and A. Quarteroni: Mathematical and numerical methods for coupling Navier-Stokes and Darcy equations. To be submitted and to be available as RICAM Report.

## ***Robert Gaisbauer***

### Scientific Achievements 2005

Robert Gaisbauer was working for RICAM and the Start Projekt “hp – Finite Elements” until May 31, 2005, and has left for industry. He was working on the implementation of finite element mesh generation and mesh adaption algorithm for the software package NGSolve.

### Scientific Cooperations

#### Internal

Roman Stainko, SFB 013: Mesh generation for optimization

#### External

- Paul Carrico, Auxitrol Aerospace Equipment: Integration of opensource geoemtry kernel OpenCascade into Netgen.
- Prof. Leszek Demkowicz, UT Austin: hp mesh refinement algorithms.

### Participation at Conferences, Scientific Visits and Talk

none in 2005

**Dr. Johannes Kraus****Scientific Achievements 2005**

*Agglomeration techniques in three-dimensional space:* This work provides a basis for various element-based algebraic multigrid and multilevel preconditioning methods. Its focus is on generating hierarchies of topological relations for unstructured three-dimensional finite element meshes. We provide practical definitions and propose efficient procedures, for the set-up of a multilevel topology concept. These techniques are useful in building element-based (or edge-based) algebraic multigrid methods.

*Multilevel preconditioning using local Schur complements:* A new construction of multiplicative two-level preconditioners for symmetric positive definite matrices has been proposed and analyzed. Avoiding hierarchical basis representations the case of non-M matrices deserves closer attention. Our approach is based on element agglomeration and assumes access to the individual element stiffness matrices. The coarse-grid element matrices are simply Schur complements computed from local neighborhood matrices, i.e., small collections of element matrices. The combination of this type of approximation with certain incomplete factorization techniques (in the framework of algebraic multilevel iteration) yields a new class of robust and efficient linear solvers.

*Algebraic multigrid based on computational molecules:* Based on disassembling symmetric positive semidefinite (SPSD) element matrices into SPSD edge matrices a new concept of “strong” and “weak” connections (edges) has been developed, which provides a basis for selecting the coarse-grid nodes in algebraic multigrid methods. In particular, we have examined the utilization of computational molecules (small collections of edge matrices) for deriving interpolation rules. The reproduction of edge matrices on coarse levels offers the opportunity to combine classical coarsening algorithms with effective (energy minimizing) interpolation principles yielding a flexible and robust new variant of AMG that can be applied to scalar problems as well as problems governed by systems of elliptic partial differential equations.

*Multilevel preconditioning of non-conforming finite element problems:* We have investigated and studied algebraic two-level and multilevel preconditioning algorithms for second order elliptic boundary value problems, where the discretization has been done using Rannacher-Turek non-conforming rotated bilinear finite elements on quadrilaterals. 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.

**Scientific Cooperations**Internal

Prof. Dr. Josef Schicho (RICAM)

Dr. Gergana Bencheva (RICAM)

Dr. Marco Discacciati (RICAM)

Dr. Satyendra Tomar (RICAM)

Dr. Josef Synka (Institute for Industrial Mathematics, Johannes Kepler University Linz)

External

Prof. Dr. R. Falgout, Prof. Dr. V. E. Henson, Prof. Dr. P. Vassilevski: CASC, Lawrence Livermore National Laboratory, CA, USA

Prof. Dr. L. Zikatanov: Department of Mathematics, Pennsylvania State University, PA, USA

Prof. Dr. S. Margenov, Dr. Ivan Georgiev: Institute for Parallel Processing, BAS, Sofia, Bulgaria

Prof. Dr. R. Hiptmair: Department of Mathematics, Swiss Fed. Inst. of Technology, ETH Zürich, Switzerland

Prof. Dr. G. Haase: Institute for Mathematics, University of Graz, Austria

Dr. Dalibor Lucas: University of Ostrava, Czech Republic

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

#### Conferences

21<sup>st</sup> GAMM-Seminar, Max-Planck-Institute for Mathematics in the Sciences, Leipzig, January, 26<sup>th</sup>-28<sup>th</sup>, 2005

5<sup>th</sup> International Conference on “Large-Scale Scientific Computations“, Sozopol, June 6<sup>th</sup>-10<sup>th</sup>, 2005

#### Scientific Visits

Guest Scientist at Lawrence Livermore National Laboratory, August 1<sup>st</sup>-31<sup>st</sup>, 2005

#### Scientific Talks [T]

- J.K. Kraus: *Algebraic Multigrid based on Computational Molecules, 1: Scalar Elliptic Partial Differential Equations.* 21<sup>st</sup> GAMM-Seminar, Max-Planck-Institute for Mathematics in the Sciences, Leipzig, January, 26<sup>th</sup>-28<sup>th</sup>, 2005.
- J.K. Kraus: *Algebraic Multigrid based on Computational Molecules, 2: Systems of Elliptic Partial Differential Equations.* 5<sup>th</sup> International Conference on “Large-Scale Scientific Computations“, Sozopol, June 6<sup>th</sup>-10<sup>th</sup>, 2005.
- J.K. Kraus: *An Edge-Based Algebraic Multigrid Method for Finite-Element Elasticity Problems.* Lawrence Livermore National Laboratory, Livermore CA, USA, August 16<sup>th</sup>, 2005.
- J.K. Kraus: *Algebraic Multilevel Preconditioning using Local Schur Complements.* Special Radon Semester on Computational Mechanics, RICAM, Linz, November 29<sup>th</sup>, 2005.
- J.K. Kraus: *Multilevel Preconditioning of Rotated Bilinear Non-conforming FEM Problems.* Special Radon Semester on Computational Mechanics, RICAM, Linz, December 13<sup>th</sup>, 2005.

### **Publications 2005**

#### Appeared [A]

1. J.K. Kraus: Computing interpolation weights in AMG based on multilevel Schur complements. *Computing* 74, 319-335 (2005).
2. J.K. Kraus: Algebraic multilevel preconditioning of finite element matrices using local Schur complements. *Num. Lin. Alg. Appl.* 12, 1-19 (2005).
3. J.K. Kraus, J. Schicho: Algebraic multigrid based on computational molecules, I: scalar elliptic problems. Accepted for publication in *Computing*, 2005.
4. J.K. Kraus: On the utilization of edge matrices in algebraic multigrid. Accepted for publication in *Lecture Notes in Computer Science*, Springer, 2005.

#### Submitted [S]

5. J.K. Kraus, J. Synka: An agglomeration-based multilevel-topology concept with application to algebraic multigrid. Submitted to *Comput. Visual. Sci.*, 2005.
6. J.K. Kraus: Algebraic multigrid based on computational molecules, II: systems of elliptic partial differential equations. Submitted to *SIAM J. Sci. Comput.*, 2005.
7. I. Georgiev, J.K. Kraus, S. Margenov: Multilevel preconditioning of rotated bilinear non-conforming FEM problems. To be submitted and to be available as RICAM Report, January 2006.

### **David Pusch**

#### **Work before joining RICAM**

From April 2003 since September 2005 I was working in the FWF-research project P14953 “Robust Algebraic Multigrid Methods and their Parallelization”. Therein, my main research field was con-

structing efficient multigrid solvers and multigrid preconditioners for system matrices arising from the boundary element method. Since these matrices are fully populated provided by standard techniques, the efficiency of iterative solving procedures are always bounded by the matrix times vector multiplication of order  $O(n^2)$ . Therefore approximation methods for the dense matrices have to be considered. In particular we are concerned with hierarchical matrices (e.g. W. Hackbusch. A sparse arithmetic based on H-matrices. Computing 62(2): 89-108, 1999) which in our case were constructed by the adaptive-cross-approximation (ACA) technique (e.g. M. Bebendorf, S. Rjasanow: Adaptive low-rank approximation of collocation matrices. Computing 70(1): 1-24, 2003).

Consequently, the ingredients within the multigrid algorithm have to be adapted properly to the underlying data-sparse system matrices. Moreover, we have taken into account that a typical operator arising in the boundary element method, the single layer potential operator, is a pseudo-differential operator of order minus one. That means, the spectral behaviour of the eigenvalues and eigenvectors act conversely compared to classical finite element matrices. In this case the usual smoothers (e.g. damped Jacobi, Gauss-Seidel) are not an appropriate choice. Our numerical methods were tested for the interior Dirichlet problem for the Laplace equation. The results are including solutions for the geometric multigrid in 2D and 3D as well as for the algebraic multigrid variants.

## Scientific Achievements 2005

*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](http://www.hlib.org)). Moreover, we discussed several ideas to perform an efficient strategy to construct a matrix hierarchy consisting of H-matrices on each level. Since the number of unknowns is reduced on each level, one can also try to reduce the number of block matrices, obtained by an appropriate clusterpair-tree on the finest grid. Merging a set of blocks to one single block can improve the performance as well as modifying a low-rank block into a full block.

*Convergence Results:* Bramble, Leyk and Pasciak showed a nice convergence result for the multigrid V-cycle applied on the discrete single layer potential operator. In many practically important cases, the full regularity and approximation condition can not be ensured. However, they could show the uniform V-cycle convergence under weaker assumptions on the bilinear form and a special multigrid smoother for the single layer potential operator. Based on their result we investigated the convergence behaviour for the H-matrix approximation of the discrete single layer potential. Confirming perturbation arguments for the bilinear form we could show the necessary assumptions for the theory. Furthermore, conditions on the smoother can be shown in order to ensure the smoothing assumptions.

## Scientific Cooperations

### Internal

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

Dipl. Ing. C. Pechstein: Institute of Computational Mathematics, Johannes Kepler University Linz, Austria

### External

Prof. Dr. W. Hackbusch, Dr. S. Börm, Dr. L. Grasedyck: Max-Planck-Institute for Mathematics in Science, Leipzig, Germany

Dipl. Math. G. Of: Institut für Angewandte Analysis und Numerische Simulation, University of Stuttgart, Germany

## Participation at Conferences, Scientific Visits and Talk

### Conferences

5<sup>th</sup> International Conference on Large-Scale Scientific Computations, Sozopol, Bulgaria, June 6<sup>th</sup>-10<sup>th</sup>, 2005

8<sup>th</sup> European Multigrid Conference on Multigrid, Multilevel and Multiscale Methods, Scheveningen, The Hague, The Netherlands, September 27<sup>th</sup>-30<sup>th</sup>, 2005

#### Scientific Talks

- D. Pusch: "Data-sparse Algebraic and Geometric Multigrid Methods for Boundary Element Equations", 5<sup>th</sup> International Conference on Large-Scale Scientific Computations, Sozopol, Bulgaria, June 6<sup>th</sup>-10<sup>th</sup>, 2005.
- D. Pusch: "Multigrid Preconditioners for Data-sparse Boundary Element Matrices", 8<sup>th</sup> European Multigrid Conference on Multigrid, Multilevel and Multiscale Methods, Scheveningen, The Hague, The Netherlands, September 27<sup>th</sup>-30<sup>th</sup>, 2005.
- D. Pusch: "Multigrid Methods for Data-sparse Boundary Element Matrices", Special Radon Semester on Computational Mechanics, RICAM Linz, November 22<sup>nd</sup>, 2005.

#### **Publications 2005**

##### Appeared

1. U. Langer, D. Pusch. *Algebraic Multigrid Preconditioners for Adaptive Cross Approximated Boundary Element Matrices*, Lecture Notes of IMAMM 03, Proceedings of the Industrial Mathematics and Mathematical Modelling, 2005.
2. U. Langer, D. Pusch. *Data-sparse Algebraic Multigrid Methods for Large Scale Boundary Element Equations*. Applied Numerical Mathematics, Vol. 54, Issues 3-4, 406-424, 2005.
3. U. Langer, D. Pusch. Convergence Analysis of Geometric Multigrid Methods for Solving Data-Sparse Boundary Element Equations, RICAM Report, 2005-16.
4. 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, June 6-10, 2005, Sozopol, Bulgaria, Volume 3743 of Lecture Notes in Computer Science, pp. 130-137, Springer-Verlag, Heidelberg, Berlin, 2006.

##### Submitted

6. U. Langer, D. Pusch. Convergence Analysis of Geometric Multigrid Methods for Solving Data-Sparse Boundary Element Equations. to be submitted.

#### ***Dr. Joachim Schöberl***

#### **Scientific Achievements 2005**

J. Schöberl's Start project "hp-Finite Elements" of the Austrian Science Foundation FWF succeeded its evaluation in June 2005, and was continued for three more years. The main results obtained by J. Schöberl and his co-workers in the Start project are:

Fast integration methods for high order finite elements on tetrahedral meshes

High order EAS finite element methods for plate and shell structures (with A. Bećirović)

High order finite elements for electromagnetic field problems (with S. Zaglmayr)

New a posteriori error estimates for Maxwell's equation have been obtained. The first class are residual type estimates based on the quasi-interpolation operator introduced by J. Schöberl in 2001. A new estimate for these operators allows to prove the reliability of the residual error estimator in very general cases. Another class of a posteriori error estimators are so called equilibrated residual error estimators, which provide a guaranteed upper bound for the error. Together with Prof. Braess such methods have been developed for Maxwell's equations.

A new mixed formulation for elasticity has been developed and introduced during the RICAM special semester. This method puts some continuity constraints to the displacement, and some continuity on the stress variables. It is free of volume and shear locking, and allows the construction of relatively simple elements. First numerical tests in 3D are very promising.

### **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. M. Ainsworth, Prof. D. Arnold, Prof. T Apel, Prof. D. Boffi, Prof. D. Braess, Prof. C. Carstensen, Prof. L. Demkowicz, Prof. R. Falk, Prof. J. Gopalagrishnan, Prof. R. Lazarov, Prof. J. Pasciak, Prof. R. Stenberg, Prof. R. Winther, Prof. J. Xu,

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

#### Conferences

- Domain Decomposition 16, New York, Jan 12.-18., plenary talk “Schwarz Methods for High Order Finite Elements”
- Oberwolfach meeting on Mixed and Nonstandard Finite Element Methods, Jan 30. – Feb 5., talk “High order finite elements for plates and shells”
- Computation of Shell & Spatial Structures, June 1. - 4., Salzburg, talk “High order EAS Finite Elements”
- US National Conference on Computational Mechanics, July 20.-28., Austin, TX, organization of MS “High Order FEM”, and talk on “Mixed Methods in Elasticity”
- CMA workshop on Compatible Discretization, Sept 26.-28., Oslo, invited talk “Commuting Interpolation Operators for Mixed Finite Elements”
- European Multigrid Conference, Sept. 28.-30., Den Haag, plenary talk “Additive Schwarz Methods for Maxwell Equations”
- OMG/DMV Annual meeting, Sept 19.-23., Klagenfurt, talk “High Order Finite Element Methods for Maxwell Equations”
- International Workshop at RICAM Special Semester, Nov. 7-11., talk “Mixed Finite Element Methods in Elasticity”

#### Scientific Visits

- University of Illinois at Chicago, Jan. 18.-22., Prof. Shabana and Dr. Gerstmayr, Multibody Systems
- Bundeswehruniversität München, Mar 16.-18., Prof. T. Apel, Finite Element Analysis
- ARC Seibersdorf, April 26, Dr. N. Finger, Simulation of Laser Devices
- Konrad Zuse Zentrum Berlin, June 5.-9., Dr. A. Schädle, Electromagnetic field simulation

#### Scientific Talks

see above

**Publications 2005**Appeared

1. Z. Dostal and J. Schöberl: Minimizing quadratic functions over non-negative cone with the rate of convergence and finite termination. Computational Optimization and Applications 30, pp 23-44 (2005)
2. S. Beuchler and J. Schöberl: Optimal extensions on tensor-product meshes. Applied Numerical Mathematics 54(3-4), 391-405 (2005)
3. F. Bachinger, U. Langer, and J. Schöberl: Numerical Analysis of Nonlinear Multiharmonic Eddy Current Problems. Numerische Mathematik. 100(4), 593 – 616 (2005)
4. J. Schöberl and S. Zaglmayr: High order Nedelec elements with local complete sequence properties. International Journal for Computation and Mathematics in Electrical and Electronic Engineering (COMPEL) 24(2), 374-384 (2005)
5. D. Boffi, F. Kikuchi, and J. Schöberl: Edge element computation of Maxwell's eigenvalues on general quadrilateral meshes. Mathematical Models and Methods in Applied Sciences, to appear
6. C. Carstensen, J. Schöberl: Residual-Based A Posteriori Error Estimate for a Mixed Reißner-Mindlin Plate Finite Element Method, Numerische Mathematik, to appear
7. S. Hain, W. Koch and J. Schöberl: Acoustic Resonances in a 2D Slate Cove and 3D Open Cavity. Proc to 11th AIAA/CEAS Aeroacoustics Conference 2005, Monterey CA, AIAA Paper 2005-2867
8. J. Schöberl, J. Melenk, C. Pechstein, and S. Zaglmayr: Schwarz Preconditioning for High Order Simplicial Finite Elements proceedings to DD16, New York 2005
9. A. Becirovic, and J. Schöberl: High order EAS elements for plates and 3D structures (proc of 5th International Conference on Computation of Shell and Spatial Structures, Salzburg, 2005)
10. S. Zaglmayr, J. Schöberl, and U. Langer: Eigenvalue Problems in Surface Acoustic Wave Filter Simulation (proc of European Conf on Math in Industry (ECMI), Eindhoven, 2004)

Submitted

11. J. Schöberl: A posteriori error estimates for Maxwell Equations. submitted to Math Comp
12. J. Schöberl, J. Melenk, C. Pechstein, and S. Zaglmayr: Additive Schwarz Preconditioning for p-Version Triangular and Tetrahedral Finite Elements. Submitted to IMAJNA
13. S. Beuchler and J. Schöberl: New shape functions for triangular p-FEM using integrated Jacobi polynomials. Submitted to Numer. Math.
14. F. Bachinger, U. Langer, and J. Schöberl: Efficient Solvers for Nonlinear Time-Periodic Eddy Current Problems. Submitted to Computing and Visualization in Science

***Dr. Satyendra Tomar*****Work before joining RICAM**

Before joining RICAM I was working as a post-doctoral research fellow in the Department of Applied Mathematics, University of Twente (UT), Netherlands. I did my Ph.D. from Indian Institute of Technology (IIT) Kanpur, India. My research interests are in high order discretization methods for partial differential equations, their application in real life problems arising in computational mechanics and computational fluid dynamics, linear algebra solution techniques, parallel computing and scientific software development.

**Work at UT-Netherlands:** **Discontinuous Galerkin (DG) method for free-surface gravity waves.** As part of a large project from Maritime Research Institute and the University of Twente Netherlands I was involved in the development of a stable and efficient numerical scheme for the simulation of water waves in a model basin. We developed a numerical method which is unconditionally stable and does not require additional smoothing or artificial viscosity terms in the free surface boundary condi-

tions to prevent numerical instabilities caused by the non-uniform mesh, which is inevitable for the fully nonlinear water wave simulation.

**Work at IIT Kanpur: Parallel  $h$ - $p$  spectral element method for elliptic problems on non-smooth domains.** We developed a parallel  $h$ - $p$  spectral element method to solve elliptic boundary value problems with mixed Neumann and Dirichlet boundary conditions on non-smooth domains. The method is exponentially accurate and asymptotically faster than the standard  $h$ - $p$  finite element method.

## Scientific Achievements 2005

*Discontinuous Galerkin method for free-surface gravity waves with high order explicit time discretization scheme:* The previous implicit approach, though unconditionally stable on non-uniform mesh, was low order accurate in time, and hence, a very small time-step was required to have an accurate simulation over a long period of time. In this work we studied high order explicit time-discretization scheme (Runge-Kutta) with DG method for free-surface gravity waves. Though the explicit approach is conditionally stable and it is required to add dissipative terms to circumvent the computational instabilities arising from the asymmetric spatial discretization, however, it is shown that using super convergent gradient recovery techniques a negligibly small dissipative term is sufficient to guarantee the stability. This allows a larger time step and thus results in overall reduction of simulation time. Stability analysis of the semi and fully discrete scheme has been conducted and the scheme has been tested on a number of problems.

## Scientific Cooperations

### Internal

Prof. U. Langer (RICAM)  
 Dr. Johannes Kraus (RICAM)  
 Dr. Marco Discacciati (RICAM)  
 Dr. Jan Valdman (SFB013, JKU)

### External

Prof. J.J.W. van der Vegt (University of Twente, Netherlands)  
 Prof. Raytcho Lazarov (Texas A&M, College Station, Texas, USA)  
 Prof. Sergei Repin (St. Petersburg, Russia)

## Participation at Conferences, Scientific Visits and Talk

### Conferences

6<sup>th</sup> European Conference on Numerical Mathematics and Advanced Applications (ENUMATH), Universidade de Santiago de Compostela, Santiago de Compostela, Spain, July 18-22, 2005.

### Scientific Talks/Lectures

- S.K. Tomar: A study of discontinuous Galerkin methods for water waves simulation. RICAM, Linz, July 14<sup>th</sup>, 2005.
- S.K. Tomar (with J.J.W. van der Vegt): A new discontinuous Galerkin finite element method for free surface flow simulation. 6<sup>th</sup> ENUMATH Conference, Santiago de Compostela, Spain, July 18-22, 2005.
- S.K. Tomar (with R. Lazarov and S. Repin): Discontinuous Galerkin methods for elliptic problems: An overview and error analysis. Miniworkshop on discontinuous Galerkin methods, Special Radon Semester on Computational Mechanics, RICAM, Linz, November 29<sup>th</sup>, 2005.
- S.K. Tomar: Unified analysis of discontinuous Galerkin methods for elliptic problems: I. Special Radon Semester on Computational Mechanics, RICAM, Linz, December 6<sup>th</sup>, 2005.

- S.K. Tomar: Unified analysis of discontinuous Galerkin methods for elliptic problems: II – Stability and error estimates. Special Radon Semester on Computational Mechanics, RICAM, Linz, December 13<sup>th</sup>, 2005.

## Publications 2005

### Appeared

1. J.J.W. van der Vegt and S.K. Tomar: Discontinuous Galerkin method for linear free-surface gravity waves. Journal of Scientific Computing 22-23, 531-567, June 2005.

### Submitted/In-Progress

2. S.K. Tomar: Parallel h-p spectral element method for elliptic problems on non-smooth domains, submitted.
3. S.K. Tomar and J.J.W. van der Vegt: A discontinuous Galerkin method for linear free-surface gravity waves with explicit time discretization, submitted.
4. J.J.W. van der Vegt, S.K. Tomar and R.H.M. Huijsmans: Numerical simulation of nonlinear water waves using discontinuous Galerkin method (to be submitted soon).
5. R. Lazarov, S. Repin and S.K. Tomar: A posteriori error estimates for discontinuous Galerkin method (work in progress).

## Sabine Zaglmayr

### Scientific Achievements 2005

#### High order elements for Maxwell problems:

The variational formulation of Maxwell problems involves the function space  $H(\text{curl})$ . In contrast to standard finite elements (for  $H^1$  problems)  $H(\text{curl})$ -conforming finite elements require tangential continuity over element interfaces, while the normal components can jump. We state a new approach for a general strategy of constructing  $H(\text{curl})$ -conforming hierarchical finite elements of variable polynomial order for hybrid meshes (involving tetrahedral, prismatic, and hexahedral elements). Our strategy uses the complete sequence property (DeRham Complex) in a more local sense. By this we gain several advantages: We can use arbitrary polynomial order varying over the mesh without any constraints on the order distribution, which will be important for p-adaptivity in Maxwell problems. Already cheap ASM-block preconditioners are sufficient. In magneto-static problems and non-conduction regions of Eddy-current problems we can use a reduced base approach, which saves degrees of freedom and moreover, leads to better conditioned system matrices.

#### Maxwell Eigenvalue solvers for closed cavities:

The main problem in solving Maxwell eigenvalue problems lies in the large null-space of the curl-curl system matrix. Our goal is to construct efficient eigenvalue solvers which exploits the a-priori knowledge of the null-space, namely the gradient functions of  $H^1$ . The first suggestion is a preconditioned inverse iteration with inexact projection into the complement of the kernel. The solver involves Maxwell and Poisson preconditioners as well as discrete gradient operators, where we can benefit from using  $H^1$  and  $H(\text{curl})$ -conforming elements fulfilling the localized complete sequence property. We improved the eigenvalue iteration by simultaneous concepts and by applying locally optimal block preconditioned conjugate gradient methods.

#### Geometric mesh refinement and anisotropic finite elements:

Corners and edges, which are usual in geometries involved in practical applications, cause a loss of regularity in the solution. Here the advantages of hp-methods can be only exploited if we use special geometric refinement strategies towards corners and edges. The resolution of skin effects, which is relevant in Eddy-current simulation of Maxwell equations, calls for special refinement towards faces.

An anisotropic geometric refinement tool which refines towards a-priori marked vertices, edges, and/or faces

was implemented into the software package Netgen/NgSolve. By this we achieve hybrid meshes with elements of the required high-aspect ratio. This required finite elements providing anisotropic polynomial order distribution and anisotropic smoothing operators for achieving aspect-ratio-independent condition numbers.

## **Scientific Cooperations**

### Internal

DI Clemens Pechstein, Institut für Numerische Mathematik

Dr. DI Joachim Schöberl, RICAM Linz

### External

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

Prof. Dr. B. Wohlmuth, Institut für Angewandte Analysis und Numerische Simulation, Universität Stuttgart, Germany

Prof. Dr. U. van Rienen, Dr. U. Schreiber, Dr. G. Pöplau, Dipl.-Math. S. Schulze, Institut für Allgemeine Elektrotechnik, Universität Rostock, Germany

Dr. N. Finger, Dr. W. Boxleitner, Dr. C. Pacher, Smart-Systems, ARC Seibersdorf Research, Vienna, A

Dr. F. Schmidt, Dr. A. Schädle, Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB), Germany

Prof. Dr. A. Knyazev, Department of Mathematics, Colorado University at Denver, USA

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

### Conferences

- 16<sup>th</sup> International Conference on Domain Decomposition Methods (DD16), New York City, USA, January 12. - 15., 2005.
- 8<sup>th</sup> US National Congress on Computational Mechanics, Austin, Texas, 24.-27. 08. 2005
- International Union of Radio Science (URSI) Jahrestagung, Kleinheubacher Tagung 2005, Miltenberg, Germany, 26.-30.9. 2005

### Scientific Visits

- Prof. Dr. C. Wieners, Prof. Dr. W. Dörfler, Institute for Scientific Computing and Mathematical Modelling, University Karlsruhe, Germany 4.-5.4.2005
- Prof. Dr. B. Wohlmuth, Institut für Angewandte Analysis und Numerische Simulations, Universität Stuttgart, 20.-22. 04. 2005
- Dr. Norman Finger, Smart Systems – Optoelectronic Engineering, ARC Seibersdorf Research, 26.04.2005
- Dr. A. Schädle , Konrad-Zuse-Zentrum für Informationstechnik Berlin (ZIB), 05.-08.07.2005
- Prof. Dr. U. van Rienen, Dr. U. Schreiber, Institut für Allgemeine Elektrotechnik, University Rostock, 17.-19.11. 2005.

### Scientific Talks

- S. Zaglmayr: *ASM-Preconditioning for High Order Nedelec Elements*, Minisymposium "Computational Electromagnetics", 16th International Conference on Domain Decomposition Methods (DD16), New York City, USA, January 12. - 15. , 2005.
- S. Zaglmayr: *High Order Nedelec Elements and Maxwell Eigenvalue Problems*, Institute for Scientific Computing and Mathematical Modelling, University Karlsruhe, Germany 5.4.2005
- S. Zaglmayr: Maxwell Eigenvalue Problems with High Order Nedelec Elements,
- Institut für Angewandte Analysis und Numerische Simulations, Universität Stuttgart, 21. 04. 2005

- S. Zaglmayr: *Eigenvalue solvers exploiting a-priori known nullspace*, Mini-Workshop " Laser Resonators", RICAM Linz,
- S. Zaglmayr: *Maxwell Eigenvalue Problmes with High Order Nedelec Elemlnts*. Symposium "Aspects of hp-FEM: Singularities, Solvers and Thin Structures", 8<sup>th</sup> US National Congress on Computational Mechanics, Austin, Texas, 24.-27. 08. 2005
- S. Zaglmayr: *A new approach to High Order Nedelec Elements*, Symposia "Numerische Methoden zur Berechnung elektromagnetischer Felder und Wellen", International Union of Radio Science (URSI) Jahrestagung, Kleinheubacher Tagung 2005, Miltenberg, Germany, 26.-30.9. 2005
- S. Zaglmayr: *Eigenvalue Problems in Surface Acoustic Wave Filters Simulations*, Mini-Workshop " Direct and inverse problems in piezoelectricity", Special Radon Semester 2005, RICAM Linz, 06.-07.09.2005
- S. Zaglmayr: *Maxwell Eigenvalue Problems with High Order Nedelec Elements*, Institut für Allgemeine Elektrotechnik, University Rostock, 19.11. 2005
- S. Zaglmayr: *High Order Nedelec Elements: Construction, Preconditioning and Maxwell Eigenvalue Problems*, Mini-Workshop "High Order Finite Elements", Special Radon Semester 2005, RICAM Linz, 19.10.2005

**Publications 2005**Appeared

1. S. Zaglmayr, J. Schöberl, and U. Langer: *Eigenvalue Problems in Surface Acoustic Wave Filter Simulation*, Progress in Industrial Mathematics at ECMI 2004; Buccianico, Mattheij, Peletier(Eds); Springer Verlag 2005
2. J. Schöberl, S. Zaglmayr: *High order Nedelec elements with local complete sequence properties*. International Journal for Computation and Mathematics in Electrical and Electronic Engineering (COMPEL), Vol. 24., No. 2., 2005
3. J. Schröberl, J. Melenk, C. Pechstein, S. Zaglmayr :*Schwarz Preconditioning for High Order Simplicial Finite Elements*, proceedings to DD16, New York 2005

Submitted

4. J. Schöberl, J. Melenk, C. Pechstein, S. Zaglmayr,: Additive Schwarz Preconditioning for p-Version Triangular and TetrahedralFinite 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:**

MSc Hui Cao  
MSc Svetlana Cherednichenko  
Dr. Herbert Egger  
DI Benjamin Hackl  
DI Andreas Hofinger  
Dr. Stefan Kindermann  
DI Klaus Krumbiegel  
Dr. James Lu  
MSc Shuai Lu  
Mag. Svetlana Metla  
Dr. Hanna Katriina Pikkarainen  
DI Marie-Therese Wolfram

In addition, Doz. Dr.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***

The group has grown considerably; more than two thirds of its staff is externally funded. It deals with several groups of topics in the field of inverse problems:

- Development and (convergence) analysis of iterative regularization methods for nonlinear inverse problems in a functional analytic setting
- Level set and related methods for (geometric) inverse problems
- Efficient and implementable parameter choice rule for variational regularization methods
- Non-quadratic regularization methods, e.g., maximum entropy and related methods, bounded variation regularization and its dual
- Relations between inverse problems and optimal control
- Attempts to develop a convergence theory for inverse problems with stochastic noise concepts and with randomness in the data and models, relations to both deterministic and Bayesian approaches
- Applications to finance, geophysics, mechanics, semiconductor models, and biology.

The group leader is personally involved in some, but not all topics: A subgroup structure has already developed via FWF projects led by Drs.Pereverzyev and Rösch.

In late 2005, the FWF decided to fund a doctoral college “Molecular Biophysics: Transport through membranes”. This and ongoing cooperations with Peter Schuster (Vienna) and R.S. Eisenberg (Chicago) will lead to even more emphasis on inverse problems in the life sciences in the coming years.

The group has scientific cooperations with all other groups at RICAM and, of course, numerous outside cooperations.

### ***PD Dr. Ronny Ramlau***

#### **Work before joining RICAM**

Dr. Ramlau joined RICAM in September 2005. During the last 6 years he has been working at the Center for Industrial Mathematics, University of Bremen, Germany, where he did his habilitation in 2003. The focus of his work is mainly on theory and applications on the field of Inverse and Ill – Posed Problems. In particular, he has studied nonlinear operator equations and their efficient regularization. Additionally, he works on a number of industrial applications. They include cooperations with Rolls – Royce (Balancing of airplane engines), Siemens (Model updates for generators), FIELAX GmbH ( Monitoring of Wind Power Plants) and ThermoElectron (Signal Processing in mass spectrometry).

#### **Scientific Achievements 2005**

##### **Research (partly before having joined RICAM)**

Tikhonov – Regularization for nonlinear Ill – Posed Problems: Dr. Ramlau has worked on different aspects of the regularization of nonlinear ill posed operator equations by Tikhonov regularization. His main focus in 2005 was the development of efficient methods for the computation of a global minimizer of the Tikhonov functional. He investigated a fast fixed point method and introduced so called *Surrogate functionals* for nonlinear Tikhonov regularization (with G. Teschke). They allow the approximate computation of a global minimizer by minimizing the strict convex surrogate functionals. A main achievement in 2005 was the generalization of this method to non – Hilbert – Space penalty terms, that allow e.g. sparse reconstructions.

Simultaneous reconstruction and segmentation for CT: Together with Dr. Ring, Dr. Ramlau has developed an algorithm that allows the simultaneous reconstruction and segmentation of a density distribution directly from tomography data. They use a Mumford – Shah like functional, that has to be optimized for geometrical variables (the shape) and functional variables (the density distribution). Previously, the Mumford – Shah approach in connection with operator equations was mostly used to obtain geometrical information only.

Two step regularization methods (w. E. Klann): In this project, regularization methods for linear operator equations were developed that combine a nonlinear estimation of the data and an approximate inversion of the operator equation. The resulting method is nonlinear and thus better adapted to the data structure. The introduced reduced *methods* prevent the typical oversmoothing of the reconstructed solution and allow thus better reconstruction of edges in images.

Blind Deconvolution (w. L. Justen): A non – iterative algorithm was developed that allows a rapid reconstruction of the convolved image and the convolution kernel. The basis of the algorithm is an exact inversion formula for the problem. Regularization of the problem is achieved by smoothing the data into the range of the nonlinear operator.

Imbalance reconstructions in rotor dynamics (w. J. Niebsch, K. Arning): Models, inversion methods as well as regularization schemes have been developed for different problems in rotor dynamics. For Rolls – Royce, positions of missing blades were computed. For wind power plants a model describing the oscillation of the plant caused by an imbalance was created. Based on the model, an algorithm for

the detection of the imbalances was designed. Both the model and the reconstruction were verified with real data. For Siemens, existing models of generators have been adapted in order to achieve optimal description of the oscillations as well as to allow good reconstruction of imbalances.

Improved signal processing for mass spectroscopy (F. Knicker): During the last years, new signal processing methods have been developed for an improved accuracy in mass spectroscopy. In this year, the methods were adapted in order to allow for an inclusion of the developed code into the company software.

### **Scientific Cooperations**

#### Internal

Prof. Dr. Sergei Pereverzev

DI Shuai Lu

Dr. Martin Burger

Dr. Stefan Kindermann

DI Marie – Therese Wolfram

#### External

Prof. Wolfgang Ring, University of Graz, Austria

Prof P. Maaß, University of Bremen, Germany

Dr. Esther Klann, University of Bremen, Germany

Dr. Michael Wolff, University of Bremen, Germany

Dipl. Math. Lutz Justen, University of Bremen, Germany

Dipl. Math. Florian Knicker, University of Bremen, Germany

Cand. Math. Katrin Arning, University of Bremen, Germany

Dr. Holger Raffel, Institut für elektrische Antriebe, Leistungselektronik und Bauelemente, University of Bremen, Germany

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

Dipl. Math. Maria Zhary, Konrad – Zuse – Institute, Berlin, Germany

Prof. Bernd Hofmann, TU Chemnitz, Germany

Dr. Henning Voss, Medical Imaging Center, Cornell University, New York, USA

Dr. Kevin Bowman, NASA JPL, Pasadena, USA

Dr. Jenny Niebsch, FIELAX GmbH, Germany

Dr. Regina Usbek, FIELAX GmbH, Germany

Dipl. – Ing. Michael Melsheimer, Deutsche Windguard Dynamics GmbH, Germany

Dipl. – Ing. Jan Liersch, Deutsche Windguard Dynamics GmbH, Germany

Holger Fritsch, μ-Sen GmbH, Germany

Dr. Bernard Staples, Rolls – Royce Derby, UK

Dr. Horst Kümmlee, Siemens, Germany

Dr. Ingo Menz, Siemens, Germany

Dipl. – Ing. Martin Regener, Siemens, Germany

Dr. Hans – Jürgen Schlüter, ThermoElectron GmbH, Germany

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

#### Conferences

Inverse Problems Reunion Conference, Lake Arrowhead, California, USA

Applied Inverse Problems, Cirencester, UK

Chemnitz Minisymposium on Inverse Problems

#### Scientific Visits

Dr. Henning Voss, Medical Imaging Center, Cornell University, New York, USA

Prof. Dr. Bernd Hofmann, Technical University Chemnitz, Germany

Dr. Peter Mathe, Weierstrass – Institute, Berlin, Germany

### Scientific Talks

University of Hamburg ( May )  
 Technical University Chemnitz ( September)  
 Weierstrass – Institute Berlin (November)

### **Publications 2005**

#### Appeared

1. V. Dicken, P. Maass, R. Ramlau, C. Streller and A. Rienäcker.  
 Inverse Imbalance Reconstruction in Rotordynamics.  
 To appear in ZAMM.
2. R. Ramlau and G. Teschke  
 Tikhonov Replacement Functionals for Iteratively Solving Nonlinear Operator Equations  
*Inverse Problems*, Vol. 21, No. 5 (2005), 1571--1592.
3. V. Dicken, I. Menz, P. Maaß , J. Niebsch, and R. Ramlau.  
 Inverse imbalance reconstruction for nonlinearly damped systems.  
*Inverse Problems in Science and Engineering*, Vol. 13, No. 5 (2005), 507--543.
4. R. Ramlau.  
 On the use of fixed point iterations for the regularization of nonlinear ill-posed problems.  
*Journal for Inverse and Ill-Posed Problems*, Vol.13, No. 2 (2005),175--200.

#### Submitted

5. L. Justen and R. Ramlau  
 A non-iterative regularization approach to blind deconvolution
6. R. Ramlau and W. Ring.  
 A Mumford-Shah approach for contour tomography.
7. R. Ramlau and G. Teschke.  
 A Tresholding Iteration for Nonlinear Operator Equations with Sparsity Constraints.
8. E. Klann, P. Maass and R. Ramlau.  
 Tikhonov regularization with Wavelet shrinkage for linear inverse problems.

### ***Prof. Dr. Sergei Pereverzyev***

### **Scientific Achievements 2005**

In the year 2005 the realization of the FWF-Project P17251-N12 “Fixed point regularization schemes for nonlinear ill-posed problems and their discretization” has been continued. The team of this project consists of Mag. Shuai Lu and Mag. Cao Hui. Within the project scientific supervision for both of them has been provided by Dr. Perverzyev.

During the year 2005, which is the second Project year, the main research activity has been aimed at developing an adaptive strategy for the choice of weights in general penalty methods. The penalty methods have in common that they converge as a penalty parameter goes to zero, and the data are assumed to be given without noise, or/and the problem in penalty formulation is assumed to be solved exactly, without discretization. Of course, in reality the data are noisy and discretization is indispensable. Then the accuracy of any penalty method depends on the interplay between its ideal convergence rate and its robustness measured by a *degree of stability* (a non-positive quantity which quantifies stability in such a way that the higher this degree, the “more” stability). Thus, in reality a penalty parameter should not go to zero, but its choice should provide the balance between error components related with stability and convergence. In the existing literature the choice of penalty parameter is usually made on the base of *a priori* estimates of the stability terms, because for standard penalty

methods such as Phillips-Tikhonov or Lavrentiev, the degree of stability is known and problem independent. At the same time, for problem oriented penalty techniques, such as *penalty methods for PDE*, *regularization by projection* or *method of lines* developed by Eldén for inverse heat conduction problems, there is no general stability theory that can be used for selecting an appropriate level of penalty parameter. Moreover, in *natural linearization* technique, introduced recently in the paper by Heinz Engl, Peter Fusek and Sergei Pereverzev (Journ. Inv. Ill-posed Problems) as an alternative to an optimal control approach to parameter identification, the stability in the last linearization step also cannot be known, because the data error in this step is nothing but a solution error of ill-posed problem from the previous step, and as such, it cannot be estimated *a posteriori*. The goal of the project team was to fill the above mentioned gap in the analysis of an important class of numerical methods. As a result, a new adaptive strategy, named *balancing principle*, has been proposed which automatically chooses the best possible approximation for the *degree of stability* from any finite set. It is shown that under natural assumptions the accuracy provided by the *balancing principle* is worse only by a constant factor than one could achieve in the case of known stability and convergence rates. In the joint research with Prof. Lazarov ( Texas A&M University) and project team member Mag. Shuai Lu a *balancing principle* has been successfully applied for the choice of a weight in *interior penalty discontinuous Galerkin approximation* on non-matching grids, and for *self-regularization* of Volterra-type severely ill-posed problems, such as a sideway heat equation with non-constant coefficients. (RICAM Report 2005-25). Moreover, in joint research with a project team member Mag. Cao Hui the same idea has been realized in *natural linearization* of parameter identification for parabolic systems. Numerical experiments on a series of model problems support the theoretical results.

## 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 TIGRA - algorithm for regularizing non-linear ill-posed problems.

### External

Group of Geomathematics headed by Prof. Dr. Willy Freeden, Department of Mathematics, University of Kaiserslautern.

Joint organization of the Workshop “Inverse Problems” in Trippstadt (Germany), 24.11.2005 – 25.11.2005.

PD. Dr. Peter Mathé (Weierstrass-Institute, Berlin).

Joint research on the discretized discrepancy principle under general source conditions. As a result, a joint article has been submitted to “Journal of Complexity”.

Prof. Dr. Ullrich Tautenhahn (University of Applied Sciences Zittau/Görlitz) and Prof. Dr. Thamban Nair (Indian Institute of Technology, Madras).

Joint research on regularization in Hilbert scales under general smoothing conditions. As a result, a joint article has been submitted to “Inverse Problems”.

Dr. Frank Bauer (University of Göttingen)

Joint research on the utilization of a rough approximation of a noise covariance within the framework of multi-parameter regularization.. As a result, a joint article has been submitted to “**International Journal of Tomography & Statistics**” (Preprint 2005-38, Institute for Numerical and Applied Mathematics, University of Göttingen)

## Participation at Conferences, Scientific Visits and Talk

### Conferences

Workshop “Inverse Problems” 11-13.04.2005 in Obergurgl

Scientific talk with the title “Regularization of ill-posed problems with random noisy data”.

Workshop “Inverse Problems” in Trippstadt (Germany), 24.11.2005 – 25.11.2005.

Invited talk with the title “An utilization of a rough approximation of a noise covariance within the framework of multi-parameter regularization”.

International Conference “Topics in Functional & Numerical Analysis” in Bombay (India), 07.12.2005 - 09.12.2005.

Invited plenary talk “On the balancing principle for some problems of Numerical Analysis”.

Indian National Symposium on Mathematical Methods and Applications in Madras, 22.12.2005. To commemorate the birthday of Srinivasa Ramanujan.

Invited plenary talk “Regularization of some linear ill-posed problems with discretized random noisy data”.

#### Scientific Visits

May, 2005 –Visit of WIAS-Berlin within the framework of cooperation between RICAM and WIAS.

Scientific talk in Forschungsseminar Mathematische Statistik with the title “Regularization in Hilbert scales under general smoothing conditions”.

Joint article with PD. Dr. Peter Mathé and Dr. Frank Bauer **“Local Solutions to Inverse Problems in Geodesy: The Impact of the Noise Covariance Structure upon the Accuracy of Estimation”**, has been prepared for the submission during the visit (Preprint 2005-14, Institute for Numerical and Applied Mathematics, University of Göttingen).

December, 11 – December, 14, 2005 – Visit of Mathematical Department, Goa University (India).

Delivering “Professor D.B. Wagh endowment lecture 2005” with the title “Numerical differentiation from the view point of regularization theory”.

December, 14 – December, 17, 2005 – Visit of Indian Institute of Sciences and Tata-Institute of Fundamental Research, Bangalore (India).

Scientific talk in the seminar of Mathematical Department of IIS with the title “Natural linearization technique for non-linear parameter identification problems”.

December, 17 – December, 21, 2005 – Visit of Mathematical Department, Indian Institute of Technology, Madras.

Scientific talk in the seminar of Mathematical Department of IIT-Madras with the title “Natural linearization technique for non-linear parameter identification problems”.

#### **Publications 2005**

##### Appeared

1. S. Pereverzev, E. Schock, On the adaptive selection of the parameter in regularization of ill-posed problems, SIAM J. Numer. Analysis , v.43, N 5, 2005, pp. 2060 – 2076..
2. T. Nair, S. Pereverzev, U. Tautenhahn, Regularization in Hilbert scales under general smoothing conditions, Inverse Problems, v.21, N.6, 2005, pp. 1851 – 1871.
3. F. Bauer, S. Pereverzev, Regularization without preliminary knowledge of smoothness and error behaviour, European Journal of Applied Mathematics, v. 16, 2005, pp. 303 – 317.
4. H. W. Engl, P. Fusek, S.V. Pereverzev, Natural linearization for the identification of nonlinear heat transfer laws, Journal of Inverse and Ill-Posed Problems, 2005, v. 13, N6, pp. 567 - 582.
5. P. Mathe, S. Pereverzev, Regularization of some linear ill-posed problems with discretized random noisy data, Mathematics of Computations, accepted.
6. Lu Shuai; S Pereverzev, .Numerical differentiation from a view point of regularization theory, Mathematics of Computations, accepted.

7. P. Mathe, S. Pereverzev, The discretized discrepancy principle under general source conditions, *Journal of Complexity*, accepted.

#### Submitted

8. R. Lazarov, S. Lu, S. Pereverzev, On the balancing principle for some problems of Numerical Analysis, submitted (RICAM Report 2005-25)

9. F. Bauer, P. Mathe, S. Pereverzev, **Local Solutions to Inverse Problems in Geodesy: The Impact of the Noise Covariance Structure upon the Accuracy of Estimation**, submitted (Preprint 2005-14, Institute for Numerical and Applied Mathematics, University of Göttingen).

10. F. Bauer, S. Pereverzev, **An utilization of a rough approximation of a noise covariance within the framework of multi-parameter regularization** (Preprint 2005-38, Institute for Numerical and Applied Mathematics, University of Göttingen).

#### **Cao Hui**

The year 2005 is the second year which I work as a research scientist in the group of Inverse Problem of Johann Radon Institute for Computational and Applied Mathematics (RICAM). I am a team member of FWF-Project P17271-N12 “Fixed point regularization schemes for nonlinear ill-posed problems and their discretization”. The main topic for my research is “Natural linearization for parameter identification problems” which can be considered as a part of the project mentioned above.

#### **Scientific achievements 2005**

During this year I have finished the paper of “Discretized Tikhonov-Phillips regularization for a naturally linearized parameter identification problem”. In this article, natural linearization approach, originally proposed by H.Engl, P.Fusek, and S.Pereverzev for identifying an unknown nonlinearity in the boundary conditions, has been extended to the identification of diffusion coefficients in elliptic type systems. The main advantages of natural linearization here can be seen as follows: the original non-linear problem is reduced to two linear problems and each of them can be effectively regularized using an adaptive strategy for the choice of regularization parameter. No a priori information concerning the smoothness or monotone behaviour of the unknown coefficients is used. In particular, it is not assumed that the initial problem is strongly elliptic, i.e. we allow the diffusion coefficient to vanish at some points, and the location of these points may also be unknown.

#### **Participation of Workshop**

I attend the Workshop “Inverse Problem” in Obergurgl in April 2005, and gave the talk “Discretized Tikhonov-Phillips regularization linearized parameter identification problems in partial differential equations”.

#### **Publications 2005**

1. Discretized Tikhonov-Phillips regularization for naturally linearized parameter identification problem, *January of Complexity*, 2005 21/6 864-877

#### **PhD program**

As a registered PhD student in JKU, I have taken the following courses:

- Stochastic differential equation (Passed with excellent mark)
- Inverse problem (Passed with excellent mark)
- Statistical method (examination is scheduled for January 2006)
- Mathematical methods of continuum mechanics (examination is scheduled for March 2006)

- Seminars at the Institute of Industrial Mathematics

During the Special Radon Semester 2005 I have participated in two lecture courses such as “Parameter Identification in Partial Differential Equations” held by Barbara Kaltenbacher and “Discontinuous Galerkin Methods” held by Raytcho Lazarov.

### ***Lu Shuai***

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 2005**

Balancing principle for some problems of Numerical Analysis (Joint research with Prof. R. Lazarov and Prof. Perverzyev):

We discuss a choice of weight in penalization methods. The motivation for the use of penalization in Computational Mathematics is to improve the conditioning of the numerical solution. One possibility for such an improvement is regularization, where penalization substitutes an ill-posed problem by a well-posed one. In modern numerical methods for PDE a penalization is used, for example, to enforce continuity of approximate solution on non-matching grids. A choice of penalty weight should provide a balance between error components related with convergence and stability, which are usually unknown. We propose and analyze a simple adaptive strategy for the choice of the penalty weight which does not rely on a priori estimates of above mentioned components, but nevertheless it provides order optimal accuracy under rather natural assumptions. This whole approach amounts to transfer of expertise from the theory of ill-posed problems (regularization) to a well-posed, but ill-conditioned problem.

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

#### Scientific Talks

Inverse Problems Workshop, Obergurdl, April 2005: presentation with the title of “Regularization by discretization for some severely ill-posed problems”.

#### **Publications 2005**

##### Accepted

1. S. Lu, S. Pereverzev, Numerical Differentiation from a view point of Regularization Theory, accepted by Mathematics of Computation.

##### Submitted

2. R. Lazarov, S. Lu, S. Pereverzev, On the balancing principle for some problems of Numerical Analysis, submitted (RICAM Report 2005-25)

### ***Dr. Arnd Rösch***

#### **Introduction**

Dr. Rösch' main research areas are optimal control and inverse problems governed by partial differential equations. The research interests include theoretical and numerical aspects of these areas.

## Scientific Achievements 2005

The research in 2005 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. The existence of regular Lagrange multipliers is shown in a joint paper with F. Tröltzsch (TU Berlin). The optimal regularity of mixed constrained optimal control problems was studied together with D. Wachsmuth (TU Berlin). It was shown that the optimal control is Lipschitz continuous. Mixed constrained optimal control problems occur as regularized state constrained problems. General results for sufficient optimality conditions were worked out in a joint work with F. Tröltzsch (TU Berlin).

### 2. Approximation of linear least squares problems

The approximation of linear least squares problems is a field of active research. Linear-quadratic optimal control problems with control constraints can be interpreted as least squares problems in infinite dimensional function spaces with additional inequality constraints. Such problems have to be discretized for numerical reasons. In a joint paper with R. Simon (JKU Linz) we investigated piecewise linear, but discontinuous controls. Error estimates in different norms are shown. The superconvergence approach was extended in two directions, to the Stokes equations and to general classes of finite elements; this was established in a joint work with B. Vexler (RICAM Linz). The generalization to non-convex domains and non-uniform meshes was investigated together with T. Apel and G. Winkler (both UniBw Munich).

## Scientific Cooperations

### Internal Cooperations with

Roland Griesse (Group Optimisation and Control)

Boris Vexler (Group Optimisation and Control)

Herbert Egger (Group Inverse Problems)

### External Cooperations with

Prof. F. Tröltzsch (TU Berlin)

Prof. W. Alt (FSU Jena)

Prof. M. Mateos (Oviedo)

Dipl.-Math. D. Wachsmuth (TU Berlin)

Dipl.-Ing. C. Meyer (TU Berlin)

Dipl.-Math. R. Simon (SFB 013 Linz)

Prof. T. Apel (Universität der Bundeswehr München)

Dipl.-Math. G. Winkler (Universität der Bundeswehr München)

Dipl.-Math. U. Prüfert (TU Berlin)

## Participation at conferences

- Annual meeting of the GAMM, Luxemburg, from 05/03/28 to 05/01/04
- Workshop “Inverse Problems”, Obergurgl, from 05/04/11 to 05/04/13
- Conference “Optimal Control of Coupled Systems of PDEs”, Oberwolfach from 05/04/17 to 05/04/23
- SIAM Optimisation Conference SIAM OP05, Stockholm, from 05/05/15 to 05/05/19
- AMS-DMV-ÖMG joint meeting, Mainz, from 05/06/16 to 05/06/19
- IFIP Conference 2005-TC 7, Torino, from 05/07/18 to 05/07/22
- International Scientific Conference Operations Research, Bremen, from 05/09/07 to 05/09/09

- Mini-Symposium on inverse problems, Chemnitz, 05/09/15
- 18th Chemnitz FEM Symposium, Schöneck, from 05/09/19 to 05/09/21
- Participation on several workshops during the special semester in Linz

## Publications

### Appeared

1. A. Rösch and D. Wachsmuth. Regularity of the adjoint state of the instationary Navier-Stokes equations. *Zeitschrift für Analysis und ihre Anwendungen*, 24(1): 103-116, 2005.
2. C. Meyer, A. Rösch, and F. Tröltzsch. Optimal Control of PDEs with regularized pointwise state constraints. Accepted for publication in *Computational Optimization and Applications*.
3. A. Rösch. Error estimates for linear-quadratic control problems with control constraints. Accepted for publication in *Optimization Methods and Software*.
4. C. Meyer and A. Rösch.  $L^\infty$ -Estimates for approximated optimal control problems, *SIAM Journal Control and Optimization*, 44(5):1636-1649, 2005.
5. A. Rösch and F. Tröltzsch. Existence of regular Lagrange multipliers for a nonlinear elliptic optimal control problem with pointwise control-state constraints. Accepted for publication in *SIAM Journal Control and Optimization*.
6. A. Rösch and D. Wachsmuth. Regularity of solutions for an optimal control problem with mixed control-state constraints. Accepted for publication in TOP (TOP is published by the Spanish Statistical and Operations Research Society (SEIO)).
7. A. Rösch and R. Simon. Linear and discontinuous approximations for optimal control problems. *Numerical Functional Analysis and Optimization*, 26(3): 427-448, 2005.

### Submitted

8. A. Rösch and Boris Vexler. Superconvergence in Finite Element Methods for the optimal control of the Stokes equations.
9. T. Apel, A. Rösch, and G. Winkler. Optimal control in nonconvex domains: a priori discretization error estimates.
10. A. Rösch and F. Tröltzsch. Sufficient second-order optimality conditions for an elliptic optimal control problem with pointwise control-state constraints.
11. T. Apel, A. Rösch and G. Winkler. Discretization error estimates for an optimal control problem in a nonconvex domain.

## Talks

- On piecewise linear discretizations for optimal control problems governed by PDEs, Annual meeting of the GAMM, Luxemburg, from 05/03/28 to 05/01/04
- Numerical analysis for optimization problems with PDE constraints. Workshop “Inverse Problems”, Obergurgl, from 05/04/11 to 05/04/13
- Sufficient second-order optimality conditions for mixed constrained optimal control problems. Conference “Optimal Control of Coupled Systems of PDEs”, Oberwolfach from 05/04/17 to 05/04/23
- Elliptic optimal control problems in nonconvex domains. SIAM Optimisation Conference SIAM OP05, Stockholm, from 05/05/15 to 05/05/19
- Optimal control problems with pointwise state constraints. AMS-DMV-ÖMG joint meeting, Mainz, from 05/06/16 to 05/06/19
- Sufficient second-order optimality conditions for optimal control problems with pointwise control-state constraints. IFIP Conference 2005-TC 7, Torino, from 05/07/18 to 05/07/22
- On the numerical verification of optimality conditions for optimal control problems. International Scientific Conference Operations Research, Bremen, from 05/09/07 to 05/09/09
- Lavrentiev regularization for state constrained optimal control problems. Mini-Symposium on inverse problems, Chemnitz, 05/09/15

- On the numerical verification of optimality conditions for optimal control problems. 18th Chemnitz FEM Symposium, Schöneck, from 05/09/19 to 05/09/21
- On the quality of numerical solutions for semilinear optimal control problems. Workshop "Efficient methods for time-dependent optimal control: preconditioning, reduced ordermodelling and feedback control", Linz, from 05/11/21 to 05/11/24
- Wie gut sind numerische Lösungen für Optimierungsprobleme bei partiellen Differentialgleichungen? Cottbus, 05/12/13
- Herausforderungen und Perspektiven bei der optimalen Steuerung partieller Differentialgleichungen. Stuttgart, 05/12/16

## Projects

- FWF-Project P18056-N12 SSC and SQP for mixed constrained optimal control problems (joint project with Roland Griesse), positions: Nataliya Metla (1PhD)
- FWF-Project P 18090-N12 Approximation of optimal control problems governed by PDEs, positions: Svetlana Cherednichenko, Klaus Krumbiegel (2PhDs)

## *Svetlana Cherednichenko*

### Work before joining RICAM

I graduated from the Faculty of Applied Mathematics and Control Processes at the State University in St. Petersburg (Russia). My recent field of research was mainly in the sphere of computer science. In the early part of the year, I have received a master's degree in Computer Science Department at University of Joensuu (Finland). After that I was working on the basis of my thesis topic. We have obtained new results for the extended version of the thesis.

### Scientific Achievements 2005

In my work, I studied optimal control problems governed by partial differential equations. I established a new technique for estimation of the regularization error for optimal control problems with pointwise state constraints using a Lavrentiev type regularization. Moreover, I investigated stability properties of such problems with respect to perturbations in the data.

### Scientific Cooperations

#### Internal

DI. K. Krumbiegel (Group Inverse Problems)  
 MSc. N. Metla (Group Inverse Problems)  
 Dr. Arnd Röscher (Group Inverse Problems)

### Participation at Conferences, Scientific Visits and Talk

#### Conferences

Scandinavian Conference on Image Analysis at June 2005 in Joensuu, Finland: "Improving K-Means by Outlier Removal", poster.

Participation on several workshops during the special semester at RICAM.

#### Scientific Talks

"Outlier detection in clustering" in group seminar, Linz, 05/06/14.

"Lavrentiev regularization for state constrained optimal control problems" in industrial mathematics seminar, Linz, 05/11/30.

## Publications 2005

Master's thesis "Outlier detection in clustering" at University of Joensuu.

### Submitted

1. "Improving K-Means by Outlier Removal": V. Hautamäki, S. Cherednichenko, I. Kärkkäinen, T. Kinnunen and P. Fränti. SCIA 2005: 978-987, June 2005, Joensuu, Finland.

## **Nataliya Metla**

### Work before joining RICAM

I graduated from Faculty of Mathematic, Science and Informatics at the Brandenburg University of Technology of Cottbus (Germany). I finished my study in August 2005. In my diploma thesis I was dealing with linear time-optimal control problems, in which initial state values depend on a parameter, and with the investigation of the solution structure for small perturbations of the parameter.

#### Scientific Achievements 2005

From September 2005 I work on the nonlinear optimal control problems with pointwise mixed control-state constraints, in particular on elliptic optimal control problem with linear inequality constraints. I started with the investigation of the Lipschitz stability of optimal solutions with respect to perturbations for such type of problems.

### Scientific Cooperations

#### Internal

MSc. Cherednichenko (Group Inverse Problems)

DI. Krumbiegel (Group Inverse Problems)

Dr. Rösch (Group Inverse Problems)

Dr. Griesse (Group Optimisation and Control)

### Participation at Conferences

Workshop on non-linear PDEs and Financial Mathematics at the University of Halmstad (May 5-7th 2005, Sweden)

Participation at several workshops during the special semester

### Talks

- "Newton's method for inverse scattering meets the method of least squares" (5th of December 2005, RICAM, Seminar industrial mathematics, Linz)
- "Time-optimal control problem with initial state of values depending on a parameter" (July 5th 2005).

## Publications 2005

1. "Time-optimal linear control problem with initial values depending on a parameter" 20th August 2005, BTU Cottbus, diploma thesis, advisor: Prof. S. Pickenhain

## ***Klaus Krumbiegel***

### **Work before joining RICAM**

In September 2005 I obtained my diploma from the Technical University of Chemnitz. My general field during my studies was applied mathematics and numerics. In my diploma thesis I dealt with inverse problems and the theme was “The influence of approximated source conditions on the accuracy and convergence rates of regularized solutions”.

### **Scientific Achievements 2005**

I studied in [1] approximate source conditions concerning to the accuracy and convergence rates of the regularized solution analytically and numerically. The regularized solutions were determined by Tikhonov regularization. I also compared the analytical results to numerical results with respect to different regularization parameter choice methods.

In [2] we presented some new ideas and results for finding convergence rates in Tikhonov regularization for ill-posed linear inverse problems with compact and non-compact forward operators based on the consideration of approximate source conditions and corresponding distance functions. For the case of compact operators we could show that there is a one-to-one correspondence between the maximal power type decay rates for the distance functions and maximal exponents of Hölder rates in Tikhonov regularization linked by the specific singular value expansion of the solution element. Some numerical studies on simple integration illustrated the compact operator case and the specific situation of discretized problems.

In joint work with Prof. B. Hofmann we exploited the decay rates of the distance functions at a numerical example on the simple integration operator. In particular we showed the correspondence between the decay rate of distance functions and the convergence rates of regularized solutions in Tikhonov regularization in the case of compact operators.

### **Scientific Cooperations**

#### Internal

S. Cherednichenko, Group Inverse Problems

Dr. B. Vexler, Group Optimization and Optimal Control

Dr. R. Griesse, Group Optimization and Optimal Control

#### External

Prof. B. Hofmann, TU Chemnitz, Faculty of Mathematics, Group Inverse Problems

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

#### Conferences

05/09/15 TU Chemnitz, Inverse Day

Workshops and lectures at the Special Radon Semester 2005 RICAM Linz

#### Scientific Talks

05/06/01 RICAM Linz, Approximate source conditions and resulted convergence rates

05/10/26 Industrial Mathematical Seminar RICAM Linz, Approximate source conditions in regularization

### **Publications 2005**

1. Klaus Krumbiegel, The influence of approximated source conditions on the accuracy and convergence rates of regularized solutions, diploma thesis at the Technical University of Chemnitz

2. B. Hofmann, D. Düvelmeyer, K. Krumbiegel, Approximate source conditions – Some new analytical and numerical studies, submitted to Mathematical Modelling and Analysis

### ***Dr. Hanna Katriina Pikkarainen***

#### **Work before joining RICAM (those who joined RICAM 2005)**

Dr. Pikkarainen received the degree of Doctor of Science in Technology from Helsinki University of Technology, Finland, in June 2005. Her doctoral dissertation has the title “A Mathematical Model for Electrical Impedance Process Tomography”. In Dr. Pikkarainen’s thesis, a process tomography problem of the following kind is considered: based on electromagnetic measurements on the surface of a pipe, describe the concentration distribution of a given substance in a fluid moving in the pipeline. The problem is viewed as a state estimation problem. The concentration distribution is treated as a stochastic process satisfying a stochastic partial differential equation referred to as the state evolution equation. The measurements are described in terms of an observation equation containing measurement noise. Since the motive is to monitor the flow in the pipeline in real time, a filtering problem in which the estimator is based on the current history of the measurement process is studied. There have been used various branches of mathematics in Dr. Pikkarainen’s thesis, among others functional analysis, measure and probability theory, the theory of PDE’s, complex analysis and statistical inversion theory.

Dr. Pikkarainen organised with Dr. Nuutti Hyvönen (Helsinki University of Technology, Finland) two minisymposia at the conference “Applied Inverse Problems 2005” held in Royal Agricultural College, Cirencester, United Kingdom. The titles of the minisymposia were “Statistical methods in EIT and X-ray tomography” and “Inverse problems arising from scattering phenomena“.

Dr. Pikkarainen had a position as a teaching assistant at the Institute of Mathematics in Helsinki University of Technology until August 2005. In the spring term 2005 she gave tutorials in the course “Foundations of the Modern Analysis”. Dr. Pikkarainen started to work at RICAM in September 2005.

#### **Scientific Achievements 2005**

In the autumn term 2005 Dr. Pikkarainen wrote an article in which the results presented in her doctoral dissertation concerning electrical impedance process tomography were extended to a certain class of linear nonstationary inverse problems. The novel contribution of the article is the analysis of the space discretization of the corresponding infinite dimensional state estimation system. The preprint was published in “RICAM Reports” series. The article was submitted to the journal “Inverse Problems” and was accepted for publication in December 2005.

Numerical implementation of the method introduced in Dr. Pikkarainen’s dissertation could not be included to the thesis. However, a possible one dimensional model case was presented. The implementation of the model case is done in collaboration with Ph. Lic. Janne Huttunen (University of Kuopio, Finland). The effectiveness of the method introduced will be presented in the forthcoming article.

#### **Scientific Cooperations**

##### External

Prof. Erkki Somersalo, Institute of Mathematics, Helsinki University of Technology, Finland  
Ph. Lic. Janne Huttunen, Department of Applied Physics, University of Kuopio, Finland

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

“Statistical approach to electrical impedance process tomography” (talk), Applied Inverse Problems 2005, Cirencester, Great Britain, June 26-30 2005.

“State estimation approach to nonstationary inverse problems: discretization error and filtering problem” (talk), The Eleventh Inverse Days, Helsinki, Finland, December 14-16 2005

**Scientific Visits**

RICAM, Linz, Austria, June 22-25 2005

Institute of Mathematics, Helsinki University of Technology, Finland, December 19-23 2005

**Scientific Talks**

“A mathematical model for electrical impedance process tomography”, Radon Seminar, RICAM, Linz, June 23 2005

“Stochastical approach to inverse problems in infinite dimensional spaces”, Industrial Mathematics Seminar, JKU, Linz, December 7 2005

**Publications 2005****Appeared**

1. Hanna Katriina Pikkarainen. *A Mathematical Model for Electrical Impedance Process Tomography*. Doctoral dissertation, Helsinki University of Technology, Espoo, Finland, 2005. ISBN 951-22-7651-8.
2. Hanna Katriina Pikkarainen. State estimation approach to nonstationary inverse problems: discretization error and filtering problem. *Inverse Problems* (in press).

***Andreas Hofinger*****Scientific Achievements 2005**

The research Andreas Hofinger did during 2005 can be divided into the following topics:

**Stochastic Inverse Problems:**

Here the goal to extend results from the deterministic theory of inverse problems to a stochastic setting. The chosen approach utilizes the Prokhorov-metric to quantify speed of convergence in the new framework.

**Inverse Problem of Endocrinology:**

In this context a model problem is studied, which is related to a new method for diagnosing heart diseases. The resulting equations describe an inverse, time-dependent Cauchy-problem, which is well-known to be severely ill-posed.

**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.

**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 is a cooperation with Stefan Kindermann and Heinz W. Engl.

External

Topic (ii) is investigated together with Ricardo Celorrio, Departamento de Matemática Aplicada, Zaragoza.

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

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

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

April 11<sup>th</sup>-14<sup>th</sup>, Workshop "Inverse Problems", Obergurgl.

June 6<sup>th</sup> – 10<sup>th</sup>, Inverse problems reunion conference, Lake Arrowhead, USA.

Scientific Visits

Related to (ii), Andreas Hofinger was guest at the University of Zaragoza (July, 25<sup>th</sup> – August 8<sup>th</sup>).

Scientific Talks

Hofinger, A real-time solution for an inverse Cauchy problem in cardiology, Workshop "Inverse Problems", Obergurgl, April 2005.

Hofinger, R. Celorrio, A real-time solution for an inverse Cauchy problem in cardiology, Lake Arrowhead, June 2005.

**Publications 2005**Appeared

1. M. Burger, A. Hofinger, Regularized Greedy Algorithms for Network Training with Data Noise, Computing, 74 (1), 1—22., 2005

2. H.W. Engl, A. Hofinger, S. Kindermann, Convergence Rates in the Prokhorov Metric for Assessing Uncertainty in Ill-Posed Problems, Inverse Problems, 21:399-412, 2005.

Submitted

3. R. Celorrio, A. Hofinger, A real-time solution for an inverse Cauchy problem in cardiology.

nA. Hofinger, F. Pillichshammer, Learning a Function from Noisy Samples at a Finite Sparse Set of Points.

***Dr. Elena Resmerita*****Scientific Achievements 2005**

The research work of E. Resmerita in 2005 concerns qualitative and quantitative aspects of variational and iterative regularization methods for ill-posed problems. In this respect, error estimates have been established for convex variational regularization of linear problems [1], as well as of nonlinear problems [3] - in cooperation with Prof. Otmar Scherzer.

In order to solve a subclass of inverse problems which have positive solutions and positive data, the same non-quadratic functional, i.e., the Kullback-Leibler divergence, has been used in [4] both for the residual term and the regularizer; this work is being pursued together with Dr. Robert Anderssen.

Partial results on iterative methods for image denoising in BV (Bounded Variation) spaces have been obtained in cooperation with Dr. Martin Burger.

The work on a mathematical theory of the EM method, which is widely used in practice, has been continued, but with only partial results so far.

### **Scientific Cooperations**

#### Internal

Dr. Martin Burger - J. Kepler University of Linz and RICAM

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

#### External

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

Prof. Dan Butnariu - University of Haifa, Israel

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

Prof. Otmar Scherzer - University of Innsbruck, Austria

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

*Regularization of ill-posed problems in Banach space: convergence rates*, April 2005. Talk at the Workshop "Inverse Problems", Obergurgl, Austria.

*Regularization of ill-posed problems in Banach spaces*, June 2005. Invited talk at the conference "Inverse Problems", Lake Arrowhead - UCLA Conference Center, California, USA.

### **Publications 2005**

#### Appeared

1. E. Resmerita: Regularization of ill-posed problems in Banach spaces: convergence rates, *Inverse Problems* 21 (2005) 1303-1314.

#### Accepted

2. D. Butnariu and E. Resmerita: Bregman distances, totally convex functions and a method for solving operator equations, *Abstract and Applied Analysis*, to appear, 2006.

#### Submitted

3. E. Resmerita and O. Scherzer: Error estimates for non-quadratic regularization and the relation to enhancing, 2005.

#### Preprint

4. E. Resmerita and R.S. Anderssen: Joint additive Kullback-Leibler residual minimization and regularization for linear inverse problems, 2005.

### **Rainer Stütz**

#### **Introduction**

DI Stütz joined RICAM in February 2005 immediately after finishing his diploma studies at the University of Linz. His diploma thesis was written in the framework of the former Subproject F1317 of the special research program SFB F013. At RICAM he was working in the Subproject F1308 "Computational Inverse Problems and Applications". Rainer Stütz left RICAM in August 2005.

Inverse and ill-posed problems with discontinuous solutions were the main research area of Rainer Stütz. Such problems arise in many practical applications, e.g., in signal and image processing or in parameter identification problems. It has been observed that many existing standard regularization schemes in Hilbert spaces do not yield satisfactory results for such problems due to the lack of smoothness. An interesting alternative approach to standard regularization methods is regularization for curve and surface representations, which has been developed by Prof. Neubauer (Linz) et al.

The basic idea of this approach is to treat a continuous parameterization of the graph of the solution as an unknown instead of the unknown discontinuous solution. In the case of a general two-dimensional surface parameterization this approach leads to a nonlinear optimization problem with nonconvex constraints, which is too much involved for a numerical realization. Therefore, a regularization algorithm was developed to approximate a surface representation using an r-adaptive mesh, the so-called Moving Grid Method.

### **Research at RICAM**

The aim of the work of Rainer Stütz was to investigate BV-type regularization methods and regularization for curve/surface representations. Furthermore, it was an objective to develop new regularization algorithms and efficient numerical implementations using h-adaptive Finite Element discretizations and mesh dependent regularization norms to approximate curve/surface representations for linear and nonlinear problems. A prototype mesh refiner and solver for parameter identification problems has been implemented using Matlab.

### **Scientific Talks**

Estimation of Discontinuous Solutions of Ill-posed Problems, SFB Statusseminar, Strobl, Austria, March 2005.

Estimation of Discontinuous Solutions of Ill-posed Problems via the Moving Grid Approach, Workshop Inverse Problems, Obergurgl, Austria, April 2005.

### **Scientific Cooperations**

#### Internal Cooperations:

Permanent exchange with Andreas Neubauer, Industrial Mathematics Institute, University of Linz.  
Cooperation with Stefan Müller in spring 2005: Bifurcation analysis of a discrete dynamical system from Systems Biology.

### ***Dr. Herbert Egger***

#### **Introduction**

Dr. Herbert Egger is working in the Subproject F1308, “Computational Inverse Problems and Applications” of the SFB013, “Numerical and Symbolic Scientific Computing” and until September 2005 as PhD. student in the group “Inverse Problems” at RICAM. Since September 2005, he is employed as PostDoc in the same projects. Dr. Egger’s main topics of research are the development and analysis of fast, mainly iterative, numerical algorithms for inverse and ill-posed problems and applications.

#### **Scientific Achievements 2005**

During the year 2005 Dr. Egger has carried out research in several directions:

Inverse problems in finance, in particular parameter identification problems:

Volatility is one of the key parameters in many stochastic models in mathematical finance. Earlier research on volatility identification in extended Black-Scholes models has been pursued [2]. In cooperation with Prof. B. Hofmann (TU Chemnitz), a new approach to volatility identification has been considered: if a special (non-parametric) structure of the local volatility surface is assumed, the parameter identification problem can be shown to decompose into two separate subproblems, whose solution is computationally much faster and more stable. A joint publication has been submitted [5]. A second line of research within this area started cooperation with the Dr. J. Sass from the group “Financial Mathematics” at RICAM, is devoted to parameter identification in Levy-processes from observations of a state trajectory.

Preconditioning iterative regularization methods:

Especially for nonlinear and even large scale linear inverse problems, iterative regularization methods are an attractive, widely used alternative to classical regularization methods, like Tikhonov regularization. One of the drawbacks of iterative regularization algorithms, especially of simple methods like Landweber iteration, is that usually many iterations are needed in order to obtain optimal results. While for well-posed problems, preconditioning is very well understood and successfully used to accelerate iterative methods, the question of (optimal) preconditioning of iterative methods for ill-posed equations has not been analysed in detail so far. In joint publication with Prof. A. Neubauer (Uni Linz), Dr. Egger proposed a preconditioning strategy for Landweber iteration for inverse problems [3]. In his PhD. thesis [6] on “Preconditioning Iterative regularization in Hilbert Scales”, Dr. Egger investigated the construction of efficient preconditioners for large classes of linear and nonlinear ill-posed problems and for several iterative regularization methods under relatively mild assumptions. In a subsequent publication [4], the acceleration of semiiterative regularization methods has been investigated. In recent research, so called Y-scale regularization methods are considered: while in standard regularization in Hilbert scales, scales of spaces over the domain of the operator under consideration are used to either extend the range of optimal convergence of regularization methods or to accelerate iterative methods, scales of spaces over the range space of the operator are considered in Y-scale regularization. This allows to apply the idea of Hilbert scale regularization to new classes of problems.

Convergence analysis of iterative regularization methods for nonlinear inverse problems: One of the drawbacks of iterative regularization methods is a saturation effect when the iteration is stopped by a discrepancy principle. As shown in [3,4,6], saturation can be partially overcome, i.e., better convergence rates can be achieved, if a more sophisticated a-posteriori stopping rule is considered. In a joint work with G. Regensburger (F1322/RICAM), the use of polynomial identities involving non commutative operators for convergence rates proofs of certain Newton-type regularization methods is investigated. The possible improvement of convergence results by applying new a-posteriori stopping rules has been considered in [7].

Stability analysis of parameter identification problems for nonlinear parabolic equations:

A cooperation with M. Klibanov (UNCC Charlotte) has been continued and led to a joint publication [1].

## Scientific Cooperations

### Internal

on “Decomposition of non commutative polynomials in the convergence analysis of iterative regularization methods”, with G. Regensburger (F1322/RICAM)  
 on “Preconditioning Landweber iteration in Hilbert scales”, with A. Neubauer (Universität Linz).  
 on “Identifying model parameters in Levy processes from observations of a price trajectory”, with J. Sass (Financial Mathematics group/RICAM).

**External**

on “Decoupling of smile and 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:

**Conferences**

GAMM Conference, “76. Jahrestagung der Gesellschaft für Angewandte Mathematik und Mechanik e.V.”, Luxembourg. Invited minisymposium talk on “Preconditioning iterative regularization methods in Hilbert scales”.

“Applied Inverse Problems” conference, AIP2005, Cirencester, UK. Invited minisymposium talk on “Inverse problems techniques for curve fitting, model calibration and parameter identification in computational finance applications”.

**Scientific Talks**

“Some aspects in iterative regularization” at the workshop on “Symmetries, Inverse Problems and Image Processing”, RICAM, Linz, January 2005.

“Preconditioning iterative regularization in Hilbert scales” at the workshop on “Inverse Problems”, Obergurgl, Austria, April 2005.

“Some aspects of parameter identification problems in computational finance” at the workshop on “Inverse Problems and Financial Mathematics”, RICAM, Linz, December 2005.

**Publications 2005****Articles in Journals:**

1. H. Egger, H. W. Engl and M. V. Klibanov, Global Uniqueness and Hölder stability for recovering a nonlinear source term in a parabolic equation, *Inverse Problems* 21, 271-290, 2005.
2. H. Egger and H. W. Engl, Tikhonov regularization applied to the inverse problem of option pricing: convergence analysis and rates, *Inverse Problems* 21, 1027-1045, 2005.
3. H. Egger and A. Neubauer, Preconditioning Landweber iteration in Hilbert scales, *Numerische Mathematik* 101, 643-662, 2005.
4. H. Egger, Semiiterative regularization in Hilbert scales, *SIAM J. Numer. Anal.*, 2005, accepted.

**Submitted**

5. H. Egger, T. Hein and B. Hofmann, “On decoupling of the volatility smile and term structure in inverse option pricing”, 2005, submitted.

**Thesis:**

6. H. Egger, Preconditioning iterative regularization methods in Hilbert scales, PhD. thesis, J. Kepler University, August 2005.

**Preprints:**

7. H. Egger, Accelerated Newton-Landweber iterations for regularizing nonlinear inverse problems, SFB-Report 03-05, January 2005.

**Dr. Stefan Kindermann**

Stefan Kindermann started working as a Research Scientist for the Group "Inverse Problems" at RICAM in September 2005. His main research interest is in the fields of parameter identification problems, level set method and PDE methods for image processing.

**Work before joining RICAM**

Dr. Kindermann finished his Ph.D. thesis at the Industrial Mathematics Institute in Linz in 2001, and worked there for several years within the SFB013 "Numerical and Symbolic Scientific Computing" in the Project F1317. From April 2004 to June 2005 he had a position as a CAM-assistant professor at the University of California, Los Angeles.

**Scientific Achievements 2005**

In 2005 the main focus of research was on using variational methods for image processing, in particular using the bounded variation norm. This work was mainly done before joining the RICAM collaborating with researchers at the UCLA. Several publications resulted from this work.

In [2] a joint work with S. Osher (UCLA) and P. Jones (Yale) investigated the use of nonlocal functionals for image processing problems. Inspired by a work of Buades, Coll and Morel on nonlocal mean filters the authors introduced nonlocal functionals for a variational approach to the denoising problem. Convergence for the corresponding algorithm were proved and numerical results were given in [2].

In another cooperation with S. Osher and J. Xu (UCLA) the so-called G-norm was used for the denoising. The G-norm can be roughly seen as dual of the bounded variation norm and was introduced by Y. Meyer as a suitable norm for highly oscillatory signals. It turned out, that it is natural to use it for bounded variation regularization problems. It has been shown in [2] that it can be computed by the level-set method and that it leads to new noise filters for highly degraded images.

Furthermore, in a cooperation with C. Navasca (UCLA) the use of control theoretic methods for regularization of inverse problems were analysed ([4]). This is a continuation of a joint work with A. Leitao (Florianopolis, formerly at RICAM) on dynamic programming for dynamic inverse problems. In [4] a regularization based on linear quadratic control problems has been introduced and its convergence has been proved.

**Scientific Cooperations**Internal

with Ronny Ramlau on the use of surrogate functionals and thresholding for interface problems in inverse problems (just started).

with Andreas Hofinger on the Prokhorov metric for stochastic inverse problems

External

Stanley Osher, Jinjin Xu (UCLA) and Peter Jones (Yale) on image processing

Carmeliza Navasca (UCLA) on control theory and inverse problems.

with Antonio Leitao (Florianopolis) on an improvement of level set method by using splitting indicators and topological derivatives.

with Maicon Alves (Ph.D-Student of A. Leitao, visiting Linz from October to November): supervising his work on level set methods for elliptic Cauchy problems.

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

April 2005, "Denoising by BV-Duality", Contributed Talk, Inverse Problems Reunion Conference, Lake Arrowhead, California

September 2005, "Denoising by BV-Duality", Contributed Talk, Workshop on Level Set Method for Direct and Inverse Problems, University Linz

October 2005, "Convergence Rates in the Prokhorov Metric for ill-posed Problems", Workshop on Inverse Problems, Toulouse

**Scientific Visits**

April 2005, Universidade Federal de Santa Catarina, Florianopolis, Brazil (Antonio Leitao).

**Publications 2005****Appeared**

1. H. Engl, A. Hofinger, S. Kindermann, "Convergence Rates in the Prokhorov metric for assessing uncertainty in ill-posed problems", Inv. Probl, 21, 399-412, 2005
2. S. Kindermann, S. Osher, P. Jones, "Deblurring and Denoising of Images by Nonlocal Functionals", SIAM J. on Multiscale Modelling and Simulation, Vol. 4, Nr. 4, pp 1091—115, 2005

**Submitted**

3. Kindermann, S. Osher, J. Xu, "Denoising by BV-Duality", to appear in J. Sci. Comp.
4. Kindermann, C. Navasca, "Optimal Control Method for Ill-posed Problems", to appear in J. Inv. Ill. Probl.

***Benjamin Hackl*****Scientific Achievements 2005**

Geometric inverse problems governed by partial differential equations were the main research area of Mr. Hackl.

Besides the ill-posed character of geometric inverse problems, a crucial problem is the numerical solution of them. To deal with the ill-posed character, perimeter regularization is usually used, while level set methods are widely used for the numerical realization. Even when level set methods are supposed to allow topological changes, theory and practice show that these topological changes might not happen. To force nonetheless topological changes, the concept of topological gradients were incorporated into the level set methods. Topological gradients indicate where to force a topological change but do not provide information about the global influence of this change to the objective function. Furthermore the widely used perimeter regularization is not topologically differentiable.

Hence Mr. Hackl together with Dr. M. Burger (Linz) developed, for a small class of geometric inverse problems,

first and a second order methods, that estimates the change of the objective function with respect to the topology change. These methods can deal also with perimeter regularizations and provide global information about the influence of the topology change to the objective function. The first order estimate is in principle very similar to the topological gradient, while the second order estimate is based on a minimization problem governed by another partial differential equation. While the first order method is very cheap and simple to implement, the second order method provides better estimates when already close to the solution. Both methods were incorporated into the level set methods and numerically tested. The results were presented at several conferences [2,3,4]. The report is in preparation.

Besides level set methods, also phase field methods are used for the numerical treatment of geometric problems and perimeter regularization. In the context of geometric inverse problems these methods are not well studied. A numerical exploration to the same class of problems considered before, together with Dr. M. Burger (Linz), showed a good performance of these methods. Results were presented at [3,4] and a report is in preparation. The results give rise to a further numerical and especially theoretical study of these methods in the context of geometric inverse problems.

In the context of geometric inverse problems Mr. Hackl considered, together with Dr. H. Ben Ameur (Tunis) and Dr. M. Burger (Linz), the problem of cavity identification for elastic and thermoelastic materials from boundary measurements. Local stability estimates in the Hausdorff distance were established and numerical tests for the thermoelastic case, using level set methods, were performed [6].

## **Scientific Cooperations**

### Internal

Dr. Martin Burger, Industrial Mathematics Institute, JK University Linz, Austria and Scientific Adviser at RICAM, Group “Inverse Problems”. Level set methods and topological derivatives for geometric inverse problems [6, in preparation], Phasefield methods in inverse problems [in preparation].

### External

Dr. Hend Ben Ameur, Laboratoire de Modelisation Mathematique et Numerique, Ecole Nationale d'Ingenieurs de Tunis. Level set methods for geometric inverse problems [6].

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

### Conferences

1. Inverse Problems Workshop, Obergurgl, Austria, April 2005, “Level set methods for geometric inverse problems”
2. SIAM Annual Meeting, New Orleans, USA, July 2005, “Topological derivative and the level set method for geometric inverse problems”
3. Workshop on “Level Set Methods for Direct and Inverse Problems”, Linz, Austria, September 2005, “Level sets, phase field and topological gradients in inverse problems”

### Scientific Talks

4. SFB Meeting, Strobl, April 2005, “First attempt to interface prediction in plasticity via level set methods”
5. SFB Meeting, Linz , December 2005, “Level sets, phase field and topological gradients in inverse problems”

## **Publications 2005**

### Submitted

6. Hend Ben Ameur, Martin Burger, Benjamin Hackl, “Cavity identification in linear elasticity and thermoelasticity”, Mathematical Methods in the Applied Sciences.

## ***Marie-Therese Wolfram***

### **Work before joining RICAM**

Before joining RICAM, I was studying technical mathematics at the Johannes Kepler University in Linz. My diploma thesis “Semiconductor Inverse Dopant Profiling from Transient Measurements”

was supervised by Martin Burger and I finished my studies in August 2005. At the beginning of October 2005 I started to work at RICAM.

## Scientific Achievements 2005

During the last year I worked on inverse problems which arise, when identifying doping profiles in semiconductor devices from transient indirect measurements. In my master thesis I considered the case of one-dimensional semiconductor devices, where I discussed the underlying analysis and presented numerical examples. Furthermore I showed that in case of bipolar diodes multiple regularized solutions exist.

When starting at RICAM I extended my computational framework to two dimensional identification problems for unipolar devices. Additionally I considered different regularization methods for bipolar diodes to avoid multiple regularized solutions. Due to numerical difficulties in the FEMLAB solver we started to consider different implementation techniques. This is joint work with Ronny Ramlau, who provides knowledge of global convergent Tikhonov type regularization methods and wavelet analysis.

## Scientific Cooperations

### Internal

Ronny Ramlau  
Martin Burger

## Participation at Conferences, Scientific Visits and Talk

### Conferences

April 11<sup>th</sup>-14<sup>th</sup>, Workshop "Inverse Problems", Obergurgl  
June 6<sup>th</sup>-10<sup>th</sup>, Inverse problems reunion conference, Lake Arrowhead, USA

### Talks

M.-T. Wolfram, Semiconductor Inverse Dopant Profiling From Transient Measurements, Lake Arrowhead, June 2005

## Publications 2005

### In preparation

SFB-report "Semiconductor Inverse Dopant Profiling from Transient Measurements"

## **Inverse Problems in Molecular Biology: A Cooperation with the University of Vienna**

The work to be described below by Drs. Müller and Lu is in the framework of a cooperation project with the University of Vienna (Profs. Schuster and Köhler) funded by WWTF whose abstract is as follows:

"Genetic and metabolic reaction networks of cells are modeled by multidimensional nonlinear ODEs using a purpose oriented software package "MiniCellSim" developed in house. This conventional (forward) analysis of biologically relevant dynamical systems will be complemented by usage of existing and design of novel methods to solve inverse problems. Two classes of problems will be addressed:

(i) Unknown or inaccurately accessible parameters will be reconstructed from equilibrium data and recorded solution curves (Level I)

and

(ii) the qualitative behavior of the dynamical systems will be engineered through introduction of calculated changes into system parameters (Level II).

Reverse engineering techniques will be developed, implemented, and tested first on small simulated biological regulatory networks. Second, we plan applications to experimentally accessible chemical reaction networks containing autocatalytic terms, which lead to typical nonlinear phenomena like multistability, chemical hysteresis, or oscillations, and to engineer modifications in the dynamical patterns by means of predicted changes in the external conditions that are transferred to the system parameters through known physical relations, for example Arrhenius' law. Third, the algorithms will be scaled up to the size of small modules of cellular metabolism in order to be ready for applications to real biological problems. A typical mathematically interesting and biologically relevant engineering task is, for example, to keep the domain that leads to oscillations small in parameter space and to construct a wide range of bistability in case the module has to act as a genetic switch, whereas the opposite is required for a pacemaker like the circadian clock.“

The RICAM part of this project is led by Heinz W. Engl and Dr.Philipp Kögler (Industrial Mathematics Institute, Univ.Linz).

### ***Dr. Stefan Müller***

#### **Scientific Achievements 2005**

Stefan Müller continued his work on the dynamics of cellular networks using both forward and inverse methods. His studies included parameter identification in biochemical reaction networks, bifurcation analysis in gene regulatory networks, and bifurcation optimization. Moreover, he contributed to the development of the SBML ODE Solver Library (SOSlib).

##### Parameter identification:

Stefan Müller started to adapt and test (in MATLAB) the iterative regularization techniques developed and used in the Inverse Problems Group. Inverse simulations have been run for small standard biochemical systems, and these results now serve as a benchmark for the implementation of inverse methods based on the SBML ODE Solver library (SOSlib).

##### Bifurcation analysis:

Stefan Müller started with the bifurcation analysis of simple gene regulatory systems: (i) two gene systems with all kinds of cross regulation and (ii) n gene systems with cyclic repression and auto-activation. A detailed mathematical analysis of the dynamical behavior was provided for both systems. In system (i), he found one-dimensional bifurcations (saddle-node, hysteresis, pitchfork) in the case of rep-rep or act-act regulation and Hopf bifurcations in the case of rep-act regulation. In system (ii), he found pitchfork and highly degenerate bifurcations for n even and Hopf bifurcations and heteroclinic bifurcations for n odd.

##### Bifurcation optimization:

In cooperation with James Lu, Stefan Müller started to optimize the bifurcation patterns of simple biochemical systems. He designed the location, the size and the shapes of bifurcation sets for simple biochemical systems. In particular he obtained desired thresholds of gene switches and robustness of certain qualitative dynamical behavior. The problem formulation required optimality criteria and constraints on the parameter range. The method involved the calculation of the closest bifurcation point for certain co-dimension 1 bifurcations (saddle node, Hopf).

## Software development:

The SBML ODE Solver Library (SOSlib) is a programming library for symbolic and numerical analysis of chemical reaction network models encoded in the Systems Biology Markup Language (SBML). It is written in ISO C and distributed under the open source LGPL license. The package employs libSBML structures to construct a system of ordinary differential equations (ODEs) for a chemical reaction network. SUNDIALS' CVODES is incorporated for numerical integration and sensitivity analysis. Optional modules based on XMGrace and Graphviz allow quick inspection of structure and dynamics. Among other things, Stefan Müller implemented functions for formula simplification and symbolic differentiation (to provide the ODE solver with the Jacobian matrix and other derivatives).

## Scientific Cooperations

### Internal

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

Cooperation with Yasmin Dolak (Analysis Group) on a continuum model of cell movement, cell division and mutation

### External

Cooperation with Prof. Peter Schuster (Institute for Theoretical Chemistry, University of Vienna) and Prof. Josef Hofbauer (Department of Mathematics, University College London) on bifurcation analysis in gene regulatory networks

Cooperation with Dr. Christoph Flamm and Mag. Rainer Machne (Institute for Theoretical Chemistry, University of Vienna) on the development of the SBML ODE Solver Library (SOSlib)

## Participation at Conferences, Scientific Visits and Talks

### Scientific Visits

Work on cyclic gene regulatory systems (cooperation with Josef Hofbauer), March 14-17, Department of Mathematics, University College London

Course on "Bifurcation Theory", October 24-28, Department of Mathematics, Imperial College London

### Talks

"Modeling the Dynamics of Cellular Networks using Inverse Methods", March 30, SFB Status Seminar, Strobl, Austria

"MiniCellSim: Genotype-Phenotype Maps of Minimal Cells", July 12, Wissenschafts-Kolleg Differential Equations, Weissensee, Austria

## Publications

### Submitted

1. S Müller, J Hofbauer, C Flamm, L Endler, S Widder, P Schuster, "A Generalized Model of the Repressilator"
2. R Machne, A Finney, S Müller, J Lu, S Widder, C Flamm, "The SBML ODE Solver Library: a native API for symbolic and fast numerical analysis of reaction networks"

**Dr. James Lu**

James Lu joined the Johann Radon Institute for Computational and Applied Mathematics in August 2005. He studied Mathematics and Aerospace Engineering at the Massachusetts Institute of Technology. His research in computational mathematics includes applying adjoint method/control theory to finite element solution of compressible Navier-Stoke equations. Currently, he is involved in developing methods of Inverse Problems and Optimization to differential equation models of gene regulatory networks.

**Scientific Achievements 2005**Research 2005 before RICAM

James Lu completed his PhD at the Aerospace Computational Design Lab at MIT. His research was concerned with the development of adjoint solution method and error estimation for functional output, in the context of compressible Navier-Stokes equations. In particular, using a discontinuous Galerkin discretization, he demonstrated an efficient multilevel, concurrent flow-adjoint solution method in an adaptive precision optimization framework. The discretization and iterative error estimates are based on discrete and continuous formulations of the Lagrangian, as allowed by taking care in the dual-consistency of the discretization treatment.

Research 2005 at RICAM

The regulatory networks of cells are highly complex systems that respond to information from ever-changing environmental conditions and regulates the cellular processes in order to ensure survival. The molecular species of the regulatory system form a network of interactions, where the presence of one species may either up- or down-regulate the production of the others. These complex molecular interactions lead to the triggering of a wide array of responses.

Given the current understanding of the molecular mechanisms underlying gene regulatory networks (GRNs), the underlying biological goal is to derive the general principles underlying the design of biological control systems, and understand how the control systems may be "engineered" to perform a desired function.

Mathematically, the questions may be formulated as Inverse Problems. At the first level, from observations of the physiological properties of the cellular mechanisms, one would like to infer both the underlying topology as well as the reaction rates and binding functions of the biochemical reaction network. The questions that need to be addressed include that of Model Identification. In particular, one would like to find the "core" molecular mechanism that give rise to the observations, while at the same time preserving certain structural properties in the observed behavior. The mathematical issues that have to be resolved may include a theory for the  $L_p$  regularization of the interaction graph, as well as how to infer combinatorial features of the network [1] from "robust" features in the observations.

At the second level, one would like to understand how the desired bifurcation diagrams may be engineered through parameter variations or network topology. The shape optimization of bifurcations may give insights into whether physiological properties of gene networks arise out of "tuning" of parameters or topology optimization of the reaction network.

A strategy for bringing about changes to the bifurcation diagram via parameter variation has been developed and verified for simple gene model systems. Motivated by problems of biological relevance, the maximization of bistability and oscillatory regimes have been demonstrated.

For the computational aspect of this research, methods for efficiently calculating the forward and adjoint ODE system have to be developed in the context of cell biology. Furthermore, these have to be coupled with methods for forward and inverse bifurcation analyses. These are currently underway. In particular, extensions to the SBML OdeSolver based on the forward and adjoint capabilities of CVODES are being developed.

[1] "Nonlinear Dynamics of Networks: the Groupoid Formalism", M. Golubitsky and I. Stewart, Bulletin of AMS, to appear.

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

#### Conferences

"Adaptive precision optimization based on a posteriori error estimates", presentation.  
IPAM Inverse Problems Conference 6-10 June 2005, Lake Arrowhead, California (USA)

#### Scientific Visits

London Dynamical Systems Group, 24-28 October 2005  
RICAM Special Semester: Discontinuous Galerkin Course

### **Scientific Cooperations**

#### Internal

Internal Cooperations with Prof. Heinz Engl, Dr. Stefan Müller, Dr. Philipp Kuegler

#### External

External Cooperations with Prof. Peter Schuster, Lukas Endler, Rainer Machne, Institute for Theoretical Chemistry, University of Vienna

### **Publications**

#### Submitted

1. "The SBML ODE Solver Library: a native API for symbolic and fast numerical analysis of reaction networks", R. Machne, A. Finney, S. Müller, J. Lu, S. Widder, C. Flamm. Bioinformatics.
2. "A posteriori discretization and iterative error control framework for adaptive precision optimization", J. Lu and D. L. Darmofal. SIAM Journal on Control and Optimization.
3. "Dual-consistency analysis and error estimation for discontinuous Galerkin discretization: application to first-order conservation laws", J. Lu and D. L Darmofal. IMA Journal on Numerical Analysis.

### **2.3. 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 (employment at RICAM since March 2005)

Dr. Willem de Graaf (till February 2005)

Dr. Oliver Labs (since October 2005)

Dr. Florina Piroi (employment at RICAM since October 2004)

Dr. Markus Rosenkranz (employment at RICAM since July 2004)

Ao.Univ.-Prof. Dr. Josef Schicho

Mag. Alexander Zapletal (PhD student, employment at RICAM since October 2004)

**Researchers externally funded:**

Msc. Michael Barton (SFB 1315, since December 2005)

Dipl.Inf. Tobias Beck (SFB 1303)

Dr. Pavel Chalmoviansky (SFB 1315)

Msc. Jose-Manuel Garcia-Vallinas (SFB 1303, since August 2005)

Msc. Jana Pilnikova (SFB 1303)

Dr. Georg Regensburger (paid by SFB 1322 since November 2004)

Dr. Ibolya Szilagyi (SFB 1303, till September 2005)

***Overview of the Work of the Symbolic Computation Area in 2005***

In accordance with the initial proposal for the area “Symbolic Computation” within RICAM, the strategic long-term research lines of the area did not change, see Annual Report 2004 for more details:

- I. Research on Groebner bases and other algorithmic algebraic theories like cylindrical algebraic decomposition as a basis for exact non-linear mathematics.
- II. Research on the **automation of mathematical theory exploration** and implementation of relevant methods in a coherent mathematical software system (“Theorema”).
- III. Application of the above two research lines to the numerical research lines in the other areas of RICAM.

The RICAM Working Group on Computational Algebra concentrates more on I and III, whereas the RICAM Working Group on Computational Logic concentrates more on II and III. However, the strong interaction between algebra and logic in both working groups is a strength of the Symbolic Computation Area at RICAM as a whole and corresponds to the overall view on Symbolic Computation as expressed already in 1985 in the editorial of the Journal of Symbolic Computation by the founding editor B. Buchberger, which gradually starts to materialize in recent years.

***Introduction by Group Leader Prof. Bruno Buchberger*****Research Line I (Groebner Bases Theory and Related Subjects)**

The main achievements in 2004 were:

- Detailed scientific design and preparation of a **special semester on Groebner bases theory** in 2006, which will involve the world's key researchers in Groebner bases theory and its applications. (Buchberger, Zapletal.)
- The further development of **symbolic techniques for boundary value problems** based on Groebner bases techniques. (Rosenkranz, Regensburger.)
- First sketches of a **formal knowledge base** on Groebner bases theory and the reasoning techniques for working with the knowledge base. (Buchberger, Zapletal.)

**Research Line II (Algorithm-Supported Mathematical Theory Exploration)**

This research line is intimately connected with the work of the Theorema Group at RISC (led by B. Buchberger; partly supported by SFB 1302 and partly supported by other, e.g. EU projects). Here we report only on the achievements in research line II within the RICAM Working Group:

- Implementation of the automated reasoning techniques necessary for a **fully automated synthesis of verified critical-pair completion algorithms**. (Buchberger with RISC PhD student Adrian Craciun.)
- Implementation of **organizational tools for handling large knowledge bases**, in particular label management techniques. (Piroi – Buchberger.)
- Advance in the logical and software-technological analysis of the logic language features necessary for enabling the **correctness proofs of formal reasoners** for various special theories (expressed in predicate logic) within predicate logic itself. (Buchberger – Giese.)

**Research Line III (Applications of I and II to Other RICAM Areas)**

- Starting from 2001, a main focus of the application of our research in computational algebra (notably Groebner bases) for other RICAM areas was on new symbolic techniques for the symbolic solution of differential equations. In the past years, research concentrated on linear boundary value problems. In 2005, the main focus was on **extending the new techniques to other classes of differential equations and to more general boundaries**. (Rosenkranz, Buchberger, Engl)
- **Comparisons** were made between Groebner based techniques for differential equations and similar techniques for solving symbolic recurrences and inventing and verifying combinatorial identities. (Seminar organized by Buchberger and Rosenkranz.)
- G. Regensburger continued his study on using algebraic techniques (including Groebner bases) for the optimal construction of **wavelets**.
- G. Regensburger, in close cooperation with M. Burger (SFB 1308) and M. Rosenkranz initiated a new research line on **nonlinear differential equations and semirings**. The appropriate algebraic setting is the max-plus semiring. Within this framework he developed a symbolic method to compute generalized solutions for nonlinear first-order ordinary boundary value problems.

***Research Plan of the Computational Logic Group for 2006 and 2007*****1. Semi-Automated Mathematical Theory Exploration**

The various research lines pursued in the Computational Logic Group,

- organizational tools for handling large formal mathematical knowledge bases
- quotation and reflection constructs in logic languages for expressing and proving the correctness of reasoners in logic itself,
- the use of schemes and automated analysis of failing proofs for the automated generation of conjectures
- special efficient reasoners for certain logic theories based on computer algebra algorithms,

will be integrated more and more in order to semi-automate mathematical research in two important areas of mathematics, Groebner bases theory and functional analysis, which are themselves of high relevance for the research pursued in all RICAM groups. Under the direction of B. Buchberger, all the members of the Computational Logic Group will contribute in their specific way to this overall goal.

## 2. Symbolic Functional Analysis

The two methodologies, Groebner bases and rewriting based symbolic operator calculations and max-plus rings based theory for nonlinear differential equations, will be systematically expanded for developing symbolic methods for more and more general classes of differential equations and boundary classes. M. Rosenkranz and G. Regensburger, under the guidance of B. Buchberger and H. Engl, will be the two people mainly involved in this research. As a new direction, we will study the possibilities of the “proof mining” techniques by U. Kohlenbach (U. Darmstadt) and others by which proofs in functional analysis, by highly sophisticated methods from proof theory, are automatically analysed for their algorithmic content and very precise estimates for convergence rates etc. are automatically generated, which sometimes are numerically much better than what is known in the literature. We also expect exciting insights by combining these techniques, which so far had no interaction with neither automated theorem proving nor computer algebra, with our computer algebra and automated theorem proving based approaches developed in the RICAM Computational Logic Group. Some preliminary ideas on this have been presented by B. Buchberger in a first meeting with the group of U. Ohlenbach in the frame of the MAP 06 Meeting.

### **Scientific Cooperations of the Computational Logic Group**

We list here all those cooperations of the Computational Logic Group that are central to the whole group; in the succeeding individual reports we will only mention specific cooperations beyond those mentioned here.

#### Internal Cooperations

- Group of H.W. Engl: Expanding the range of applicability of the Groebner bases (operator rewriting approach) to solving differential equations.
- Group of P. Markowich: Discussion of possible applications of the symbolic operator simplification methods for special classes of partial differential equations.
- Group of J. Schicho: Groebner bases theory and other methods for non-linear algebra.
- M. Burger: Max-plus ring theory for the symbolic solution of nonlinear differential equations.

#### External Cooperations

- Project F1302 “THEOREMA: Proving, Solving, and Computing in the Theory of Hilbert Spaces” in SFB F013 of the FWF.
- Project F1303 “Proving and Solving over the Reals” in SFB F013 of the FWF (Principal investigator: J. Schicho). The interaction of Groebner bases techniques with quantifier elimination techniques.
- Project F1308 “Computational Inverse Problems and Applications” in SFB F013 of the FWF (Principal investigator: H.W. Engl).
- Project F1322 „Computer Algebra for Pure and Applied Functional Analysis“, in SFB F013 of the FWF. Principal investigators: B. Buchberger, H.W. Engl.
- *Theorema* project of the Research Institute for Symbolic Computation, Johannes Kepler University of Linz (group leader B. Buchberger).
- EU MKM (Mathematical Knowledge Management) Thematic Network (ongoing).
- European Network on “Mathematics, Algorithms, and Proofs” (French, German, and Austrian math institutes).
- Symbolic Computation groups at the following Japanese universitites: U. of Tsukuba (Prof. T. Ida), U. of Kyoto (Prof. M. Sato), Rikkyo U. in Tokyo (Prof. Yokoyama), Kobe U. (Prof. Takahashi).

***Prof. Dr. Bruno Buchberger*****Organizational Work for RICAM**

Leading RICAM Working Group “Computational Logic”.

Coordination with RICAM Working Group “Computational Algebra”.

Hiring postdoc Dr. Giese (screening 25 applicants, interviewing 2, selection, preparation of employment).

Preparation of Special Semester on “Groebner Bases 2006”, Feb. – July 2006 (see 3.3)

Organization of building up a web-accessible papers data base on Groebner bases theory with downloadable papers and powerful search facilities (currently, more than 700 papers are already entered and accessible)

Organizing monthly joint seminar with SFB and RISC on “Symbolic Methods for DE”. Organizing the interaction with numeric groups and group on applied mathematics (Engl, Langer, Markowich).

Organizing one-day workshop with group of Prof Blatt (Academy Institute on Quantum Optics in Innsbruck) on possible cooperation and project proposal in quantum computing algorithms (Feb 22, 2005, in Salzburg).

Organizing one-day workshop with group of Prof Fensel (U Innsbruck) on possible cooperation and project proposal in mathematical knowledge management and semantic web (Feb 25, 2005, in Salzburg).

Organizing 4 talks by visitors (Dr. Guidi / Bologna; Dr. Giese / Chalmers, Sweden; Dr. Urban / Munich; A. Damiano / George Mason U, USA; Dr. J. Blümlein / DESY Berlin).

Preparation of a collaboration with the DESY Institute in Berlin-Zeuthen on the use of Groebner-bases methods in various new algebraic domains.

Co-organizer (together with S. Oishi / Waseda Univ, Japan; M. Plum / U. of Karlsruhe; S. Rump / TU Hamburg-Harburg) of the Workshop “Algebraic and Numeric Algorithms and Computer-assisted Proofs”, Research Center Schloss Dagstuhl, Germany, Sep 26-30, 2005

Supervising RICAM Postdocs and Docs: Dr. Markus Rosenkranz, Dr. Florina Piroi, Dr. Georg Regensburger (paid by SFB 1300), Dr. Martin Giese, Mag. Alexander Zapletal

**Scientific Achievements 2005**

- New logical design of the Theorema system.
- Case studies in formal mathematical theory exploration.
- Strategies and research directions for the future of symbolic computation.
- Automated synthesis of critical pair-completion algorithms.

**Participation at Conferences, Scientific Visits and Talk**Invited talks at conferences

B. Buchberger

Algorithmic Algorithm Synthesis: Case Study Groebner Bases

East Coast Computer Algebra Day, March 12, 2005, University of Ohio, Ashland, USA.

B. Buchberger

Introduction to Groebner Bases

Conference on Algorithms and Information Theory

University of Vaasa, Finland, May 16-18, 2005.

B. Buchberger

Algorithmic Algorithm Invention in the Theorema Project

Conference on Algorithms and Information Theory

University of Vaasa, Finland, May 16-18, 2005.

B. Buchberger

Symbolic Computation: Current Trends

International Workshop on Advanced Computing and Analysis Techniques in Physics Research

Research Institute DESY, Zeuthen (Berlin), Germany, May 22-27, 2005.

B. Buchberger.

A Historic Introduction to Groebner Bases.

Summer School on Groebner Bases and Applications, IASBS (Institute for Advanced Studies in Basic Sciences) , Zanjan, Iran, July 9-22, 2005.

B. Buchberger.

From Groebner Bases to Automated Theorem Proving and Back (3 lectures).

Summer School on Groebner Bases and Applications, IASBS (Institute for Advanced Studies in Basic Sciences) , Zanjan, Iran, July 9-22, 2005.

B. Buchberger.

A View on the Future of Symbolic Computation.

ISSAC 2005 (International Symposium on Symbolic and Algebraic Computation), Beijing, July 25-27.

B. Buchberger.

Formal Mathematical Theory Exploration in Theorema (4 lectures).

Summer School on Theoretical Computer Science, Marktoberdorf, August 3-13, 2005, organized by U. of Munich.

Invited talks at universities and research institutes

B. Buchberger

Theorema: A System for Formal Mathematics

North Carolina State University, Dept of Computer Science, March 15, 2005

B. Buchberger

Algorithmische Beweisverfahren: Das Ende der Mathematik?

Kepler Symposium, Universität Linz, April 20, 2005.

B. Buchberger

Mathematik: Die Kunst des effektiven Handelns

MathSpace, Wien, May 12, 2005.

B. Buchberger

Algorithm Synthesis in Theorema: Case Study Groebner Bases

University of Edinburgh, School of Informatics, June 23, 2005.

B. Buchberger.

Lazy Thinking: A New Method for Algorithm Synthesis.

Workshop “Algebraic and Numeric Algorithms and Computer-Assisted Proofs”. Research Center Schloss Dagstuhl, Germany, Sep. 26-30, 2005 East Coast Computer Algebra Day, March 12, 2005, University of Ohio, Ashland, USA.

## Publications 2005

### Appeared or Accepted

B. Buchberger. Towards the Automated Synthesis of a Groebner Bases Algorithm. RACSAM (Reviews of the Spanish Royal Academy of Science), Vol. 98/1, pp. 65-75.

W. Windsteiger, B. Buchberger, T. Jebelean, M. Rosenkranz. The Proof of the Irrationality of  $\sqrt{2}$  in Theorema. To appear in the special issue of LN Computer Science (ed. F. Wiedijk), “The World’s Leading Theorem Provers”), Springer.

B. Buchberger, T. Jebelean, F. Piroi, M. Rosenkranz, W. Windsteiger. Theorema: Towards Systematic Mathematical Theory Exploration. To appear in Journal of Applied Logic.

### Technical Report

F. Piroi, B. Buchberger "Label Management in Mathematical Theories". RICAM Report Series, 2004-16, 2004.

## ***Dr. Martin Giese***

### Work before joining RICAM

Before joining RICAM in March 2005, M. Giese was employed for 2 years as a post-doc researcher at Chalmers University of Technology in Gothenburg, Sweden. From 1998 to 2005 he was a member of the KeY project on formal software development, and as such has been working on various aspects of automated theorem proving, in particular for first-order logic, as well as software specification and verification.

## Scientific Achievements 2005

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 centre 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.

M. Giese has been participating in a research effort initiated and led by B. Buchberger to develop an understanding of the reflection principles necessary to put such meta-mathematical reasoning on a sound formal basis. In particular, the goal is to make the use of meta-mathematical techniques possible within the Theorema system that is being developed at RISC. M. Giese has explored various alternatives for the formal foundation and evaluated their respective merits for use in a realistic system. In the course of this research, he has analysed the relevant capabilities of existing systems, like ACL2. He has also implemented a prototypical reflective system that illustrates the basic principles, and that can be used to evaluate their practicality. M. Giese has presented his findings in this area at two international workshops [2,3], as well as numerous internal seminars.

Furthermore, M. Giese has been investigating logical calculi for classical first-order logic with subtyping. The notion of subtyping arises naturally, for instance, in the formal treatment of modern computer programming languages, but also in the formalization of certain mathematical domains. Although it has been known for some time how to define such a logic, previous research has only unsatisfactorily covered *reasoning* for logics with subtyping. M. Giese has developed an analytic calculus that formalizes reasoning about subtypes, and has shown it to be sound and complete for first-order logic with subtypes. These results have been published and presented at the leading international conference on tableaux and related calculi [5].

Finally, M. Giese has completed previous research on the mechanical simplification of expressions of the OCL language, a logic-based language used to express constraints on the behaviour of object-oriented programs. The results have been published and presented at an international conference on software engineering [6].

## **Scientific Cooperations**

### Internal

Cooperation with M. Rosenkranz, concerning the reflection mechanism.

### External

Cooperation with B. Buchberger and T. Kutsia at RISC, concerning the reflection mechanism.

Cooperation with D. Larsson and R. Hähnle at Chalmers University in Gothenburg, Sweden, B. Beckert at the University of Koblenz, Germany, P. H. Schmitt at the University of Karlsruhe, Germany, and other members of the KeY project on the questions of OCL simplification and the calculus for logic with subtyping.

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

### Conferences

1. SFB Status Seminar, 31<sup>st</sup> March to 2<sup>nd</sup> April 2005, Strobl, Österreich.
2. The 4<sup>th</sup> KeY Symposium, 8<sup>th</sup> June to 10<sup>th</sup> June 2005, Lökeberg, Sweden. Talk on “Verified Provers”.
- Automated Reasoning with Analytic Tableaux and Related Methods, Tableaux 2005, 14<sup>th</sup> Sept. to 17<sup>th</sup> Sept. 2005, Koblenz, Sweden. Talk on “A Calculus for Type Predicates and Type Coercions”.
3. Theorema-Ultra-Omega Workshop, 14<sup>th</sup> Nov. to 15<sup>th</sup> Nov. 2005, Saarbrücken, Germany. Talk “Towards an effective Reflection Mechanism in Theorema”.

## Publications 2005

### Appeared

4. W. Ahrendt, T. Baar, B. Beckert, R. Bubel, M. Giese, R. Hähnle, W. Menzel, W. Mostowski, A. Roth, S. Schlager, and P. H. Schmitt. The KeY Tool, *Software and Systems Modeling* 4(1), 2005.
5. M. Giese. A Calculus for Type Predicates and Type Coercions. In B. Beckert, editor, *Automated Reasoning with Analytic Tableaux and Related Methods*, vol. 3702 of LNAI, pp. 123–137. Springer, 2005.
6. M. Giese and D. Larsson. Simplifying Transformations of OCL Constraints. In L. Briand and C. Williams, editors, *Model Driven Engineering Languages and Systems (MoDELS) Conference 2005, Montego Bay, Jamaica*, vol. 3713 of LNCS, pp. 309–323. Springer, 2005.

## **Dr. Florina Piroi**

### Scientific Achievements 2005

Among the research goals of the “Computational Logic” group stated in the last year's annual report, the systematic, computer-supported exploration of theories was also listed. F. Piroi's role in this research goal is the development of tools for the logical and organizational management of large formal knowledge bases. In the past year she has optimized and improved these tools. In collaboration with T. Jebelean and C. Rosenkranz (RISC), she has worked towards a systematic development of a library of formal knowledge and towards developing tools for searching within the library and theory exploration.

Ongoing research in automated reasoning has underlined the importance of the user interaction with the automated reasoners (which are computer programs). In the specific literature about interfaces for automated theorem provers several design principles have been formulated. In collaboration with T. Kutsia (RISC) F. Piroi has improved the Theorema environment for interactive proof development by identifying the user actions corresponding to these principles [4].

In further cooperation with T. Kutsia and T. Jebelean (RISC), F. Piroi has concentrated on efficient ways of representing reasoning objects (e.g., proofs) and on techniques of representing and combining inference rules.

Finally, F. Piroi has done some research in the area of quantum algorithms, and in cooperation with A. Winterhof (Financial Mathematics group) have investigated their implications in the subject of period recovery for periodic binary sequences.

### Scientific Cooperations

#### Internal

Cooperation with A. Winterhof (Financial Mathematics group) on existence of quantum algorithms for computing periods of binary sequences.

#### External

Cooperation with C. Rosenkranz and T. Jebelean (RISC), concerning retrieval of mathematical knowledge from a (large) repository of mathematical knowledge.

Cooperation with T. Jebelean and T. Kutsia (RISC) on the design of an efficient inferencing mechanism for a theorem prover (Theorema).

Cooperation with T. Kutsia (RISC) on improvements to Theorema's environment for interactive proof development.

## Participation at Conferences, Scientific Visits and Talk

### Conferences

1. SFB Statusseminar, Strobl, Austria. March 2005.
2. 4<sup>th</sup> International Conference on Mathematical Knowledge Management, Bremen, Germany. July 2005. Talk on “Label Management in Theorema”.
3. Theorema-Ultra-Omega Workshop, Saarland University, Germany. November 2005.
4. 12<sup>th</sup> International Conference on Logic for Programming, Artificial Intelligence and Reasoning, Montego Bay, Jamaica. December 2005. Talk on “The Theorema Environment for Interactive Proof Development”.

## Publications 2005

### Appeared

5. F. Piroi, B. Buchberger. Label Management in Theorema. In M. Kohlhase, editor, informal proceedings of the 4<sup>th</sup> International Conference on Mathematical Knowledge Management, Bremen, Germany. July 2005.
6. F. Piroi, T. Kutsia. The Theorema Environment for Interactive Proof Development. In: G. Sutcliffe and A. Voronkov, editors, *Logic in Programming, Artificial Intelligence and Reasoning. Proceedings of the 12th International Conference LPAR'05*. December 2-6, 2005. Montego Bay, Jamaica. Volume 3835 of Lecture Notes in Artificial Intelligence. Springer Verlag, 2005. 261-275.

### Submitted

7. 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*. 2005. ISSN 1570-8683. To appear.
8. F. Piroi, A. Winterhof. Quantum Periodic Reconstruction of Binary Sequences. In M. Fossorier, H. Imai, S. Lin, A. Poli, editors, *Applied Algebra, Algebraic algorithms and Error-Correcting Codes*. Proceedings of the 16<sup>th</sup> International Symposium, AAECC-16, Las Vegas, NV, USA, February 20-24, 2006. Volume 3857 of Lecture Notes in Computer Science. Springer Verlag, 2006. To appear (submitted in 2005).

## ***Dr. Georg Regensburger***

### Scientific Achievements 2005

A main focus of G. Regensburger's work was on nonlinear differential equations and semirings. He surveyed the relevant literature on idempotent and pseudo analysis in connection with differential equations [2,6]. The max-plus semiring, where the addition is replaced by the maximum and the multiplication by the sum, showed to be particularly useful for symbolic computation. G. Regensburger developed based on max-plus linear algebra a symbolic method to compute generalized solutions for nonlinear first-order ordinary boundary value problems. An implementation for max-plus linear systems and the method for the computer algebra system Maple is already available.

He also successfully continued his work on symbolic computation and wavelets and extended results on parametrized wavelets based on joint work with Prof. O. Scherzer [8] in several directions [1,3,4,7]. See in particular [11] where new parametrizations of filter coefficients of scaling functions and wavelets are obtained using Groebner bases which were introduced by Prof. B. Buchberger.

In June he received his doctorate “sub auspiciis Praesidentis rei publicae” (with highest distinction) from the University of Innsbruck.

## Scientific Cooperations

### Internal

G. Regensburger works and cooperates closely with Dr. M. Rosenkranz in the SFB project F1322 “Computer Algebra for Pure and Applied Functional Analysis” led by Prof. B. Buchberger and Prof. H. W. Engl. He cooperated with Prof. M. Burger who first suggested studying idempotent and pseudo analysis and Dr. H. Egger, see [5], both from the research group “Inverse Problems”. He worked with Prof. J. Schicho on parametrized wavelets and a new cooperation on symbolic computation for Witt rings has just started.

### External

The discussions on differential equations and semirings [6] within the framework of the series of seminars on differential equations organized by Prof. B. Buchberger and Dr. M. Rosenkranz were very fruitful.

G. Regensburger also worked

- With Prof. O. Scherzer (Univ. of Innsbruck) [8].
- With Dr. A. Matt [10] and the paper “Policy Iteration for Several Environments” is in preparation.
- With Prof. H. Hauser (Univ. of Innsbruck) [9].

## Participation at Conferences, Scientific Visits and Talks

### Conferences

1. Workshop on Resolution of Algebraic Varieties, Brandenberg, Austria, September 19–22  
Talk: “Parametrized wavelets and algebraic curves”.
2. Workshop on “Level Set Methods for Direct and Inverse Problems”, Special Session on Symbolic Computation and PDEs, RICAM Linz, Austria, September 14–16.  
“Semirings, Idempotent Analysis and Differential Equations”.
3. ACA 2005, Conference on Applications of Computer Algebra, Nara, Japan, July 31 – August 3.  
“Construction of Parameterized Wavelets Using Groebner Bases”.
4. Workshop on Inverse Problems, Obergurgl, Austria, April 11–13.  
“Construction and Applications of Parametrized Wavelets”.
5. SFB Statusseminar, Strobl, Austria, March 31 – April 2.  
with H. Egger: “Decomposition of noncommutative polynomials in the convergence analysis of iterative regularization methods”.

### Scientific Talks

6. “Semirings, Idempotent and Pseudo Analysis”, within a series of seminars on differential equations organized by Prof. B. Buchberger and Dr. M. Rosenkranz, RICAM, June 21.
7. “Parametrized Wavelets”, Radon Seminar, RICAM, February 1.

## Publications 2005

### Appeared

8. G. Regensburger, O. Scherzer, “Symbolic Computation for Moments and Filter Coefficients of Scaling Functions”, Annals of Combinatorics, 9(2), 223-243, July 2005.
9. H. Hauser, G. Regensburger, “Explizite Auflösung von ebenen Kurvensingularitäten in beliebiger Charakteristik”, Enseign. Math. (2), 50(3-4), 305-353, December 2004.
10. Matt, G. Regensburger, “An Adaptive Clustering Method for Model-free Reinforcement Learning”, Proceedings IEEE-INMIC 2004 (8th International Multitopic Conference), 362-367, Lahore, Pakistan, December 24-26, 2004.

### Submitted

11. G. Regensburger, “Parametrizing compactly supported orthonormal wavelets by discrete moments”, preprint, 2005.

***Dr. Markus Rosenkranz*****Scientific Achievements 2005**

Markus Rosenkranz has extended the methodology of **Symbolic Functional Analysis**, developed in his PhD thesis (“A Polynomial Approach to Boundary Value Problems”, available as RISC Technical Report 2003-05) and published as [11], in various directions [1,2]:

1. The structure of “analytic polynomials” has been generalized in the frame of **integro-differential rings**, introduced in [7] and presented in [3]. Its logical significance is explained in [4].
2. An analytic solution has been established in [6] for the **Riccati equation** with homogeneous initial condition and symbolic right-hand side (a kind of “non-linear boundary value problem”).
3. The Green’s algebra, crucial for the solution method of two-point BVPs presented in [8,11], has been connected with the **Mikusiński calculus**; see the preliminary survey in [12].

**Scientific Cooperations**Internal

The subject matter of Symbolic Functional Analysis is situated at the interface between computer algebra and functional analysis. It profits from discussions with the group on **Inverse Problems**, in particular with Prof. Martin Burger. Research is carried out in the frame of a Special Research area of the FWF in project F1322, whose joint initiators and principal investigators are Prof. Buchberger and Prof. Engl.

External

Under the auspices of Prof. Bruno Buchberger, Markus Rosenkranz has organized a series of 10 **seminars on differential equations**, covering various topics mostly from symbolic computation (like holonomic method, Lie groups, factorization of differential operators, Green’s algebra, differential algebra) but also other areas (like genetic networks).

The implementation of the solution method for linear two-point BVPs, also described in [11], is integrated into the **Theorema system**, developed by the Theorema group under the supervision of Prof. Buchberger. The continuous updating of this implementation along the current modifications of the Theorema system – in particular also the ongoing discussions on a complete redesign of the system – is done in close contact to the Theorema group of RISC.

Markus Rosenkranz has participated in a (still ongoing) series of seminars on **logical reflexion** in the Theorema system, conducted by Prof. Buchberger and Martin Giese. The idea of reflexion – shifting knowledge between the object level and meta level of a mathematical theory – plays a prominent role in the formation of generalized polynomials of all kinds, in particular also for the Green’s polynomials of [11]; see the outline in [4].

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

1. M. Rosenkranz, “New Symbolic Computation Methods for the Exact Solution of Two-Point Boundary Value Problems”, Invited Conference Talk, Algorithmic Information Theory (AIT’05), Vaasa, Finland, May 2005.
2. M. Rosenkranz, “An Operator Calculus for the Symbolic Solution of Linear Two-Point BVPs”, Invited Conference Talk, Algebraic and Numerical Algorithms and Computer-assisted Proofs, Dagstuhl, Germany, September 2005.

3. M. Rosenkranz, "Linear Two-Point Boundary Value Problems in Symbolic Computation: A New Approach", Contributed Conference Talk, Foundations of Computational Mathematics (FoCM'05), Santander, Spain, July 2005.
4. M. Rosenkranz, "Using Polynomial Structures in Reasoning with Reflexion", Theorema-Ultra-Omega Workshop, Saarbruecken, Germany, December 2005.
5. M. Rosenkranz, "Linear Two-Point Boundary Value Problems", Workshop on Level Set Methods for Direct and Inverse Problems, Special Session on Symbolic Computation and PDEs, September 2005.
6. M. Rosenkranz, "Symbolic Solution of Nonlinear BVPs? - First Steps and Considerations", Workshop on Inverse Problems, Obergurgl, April 2005.
7. M. Rosenkranz, "Integro-Differential Rings and Operators", SFB Statusseminar, Strobl, April 2005.
8. M. Rosenkranz, "Symbolic Methods for Differential Equations", SFB Statusseminar, Strobl, April 2005.

**Scientific Talks**

9. M. Rosenkranz, "Using Mathematica's Rewriting Machinery for the Symbolic Solution of Linear Two-Point BVPs", Murmansk Technical University, Murmansk, Russia, May 2005.
10. M. Rosenkranz, "Proving and Computing in Theorema: A Tutorial", Rovaniemi Polytechnic, Rovaniemi, Finland, May 2005.

**Publications 2005****Appeared**

11. M. Rosenkranz, "New Symbolic Method for Solving Linear Two-Point Boundary Value Problems on the Level of Operators", Journal of Symbolic Computation, 39(2):171-199, February 2005.
12. M. Rosenkranz, "Symbolic Computation Methods for Functional Analysis", Lecture Notes, 2005.

**Submitted**

13. 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, to appear.

***Alexander Zapletal*****Work before joining RICAM (those who joined RICAM 2005)**

A. Zapletal completed his diploma in Computer Science in April 2004 and is studying Mathematics at the Technical University of Vienna. The topic of his diploma thesis is "Algorithmen in der Computer-algebra für Polynomideale und -moduln".

**Scientific Achievements 2005**

A. Zapletal's main topic of research is to build up of a formal knowledge base for Groebner bases. This is done within the Theorema software, which is developed at RISC under the direction of B. Buchberger with contributions from the members of the computational logic group at RICAM.

Additionally, A. Zapletal is the scientific assistant of Professor Buchberger in the organization of the "Special Semester on Groebner Bases and Related Methods 2006". It will bring together the leading researchers in Groebner Bases and related theories for intensive joint research.

In the frame of preparing the special semester a database of papers on Groebner bases was built up. This bibliography was initiated by B. Buchberger and is being built up under his direction. The managing editor of the bibliography and the developer of the web-interface (<http://www.RICAM.oeaw.ac.at/Groebner-Bases-Bibliography/>) is his scientific assistant A. Zapletal.

## **Scientific Cooperations**

### External

With the Research Institute for Symbolic Computation (RISC), Johannes Kepler University of Linz, *Theorema* group. Since the formal knowledge base developed by A. Zapletal is implemented within the *Theorema* system, there is a close cooperation with this research group.

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

### Conferences

“*Theorema-Ultra-Omega'05 Workshop*”, November 14<sup>th</sup> -15<sup>th</sup> 2005, Saarland University, Germany.

### ***Overview of the Work of the Computational Algebra Area by Prof. Josef Schicho***

The second group is involved in the two SFB subprojects 1303 (Solving over the Reals) and 1315 (Algebraic spline surfaces); these projects also support several PhD studies. Ibolya Szilagyi finished her PhD study in September 2005, Tobias Beck and Jana Pilnikova will probably finish within 2006.

In SFB 1303, special emphasis has been given to questions of numerical analysis of problems/algorithms that are traditionally connected with symbolic/exact methods, such as the implicitization problem and the parametrization problem. This was also the topic of the PhD thesis of Szilagyi.

SFB 1315 is dealing with topics in the main interest of Prof. Dr. Bert Jüttler (Univ. Linz), namely applied geometry, and has lead to several co-productions between members of RICAM and members of the Institute of Applied Geometry.

Even though Willem de Graaf left the institute after 5 months, he was (and still is) cooperating in the very successfull development of the Lie algebra method for solving certain types of Diophantine equations, together with Pilnikova and Schicho. His successor was Oliver Labs, who finished his PhD in computational algebraic geometry in October 2005. Labs has applied for a postdoctoral fellowship at the special year on applications of algebraic geometry in the IMA (Minnesota) and has good chances to get this position (beginning with October 2006); it is planned that Tobias Beck, who will finish his PhD study around that time, will replace him. His PhD topics are algebraic power series and their applications in singularity analysis and parametrization, but he also achieved results on sparse parametrization (together with Schicho).

### ***Prof. Dr. Josef Schicho***

#### **Scientific Achievements 2005**

##### **Parametric Degree:**

The degree of a parametric curve is also the degree of any of its parametrizations. For parametric surfaces, the situation is more complicated: for the same surface, there are parametrizations of different degree, even arbitrary large degree. The parametric degree is the degree of the smallest possible parametrization. This concept has its subtleties, for instance it depends on the choice of the field: for a fixed real algebraic surface, we may have a complex parametric degree and a real parameteric degree. S. discovered some relations to known numerical invariants (nefness value) that explain the relation between implicit and parametric degree.

##### **The Lie algebra method:**

Already in 2004, S. introduced a new method for solving certain types of Diophantine equations, together with W. de Graaf, M. Harrison, and J. Pilnikova. In 2005, the Lie algebra method was extended and developed further, so that it applies to a wider class of equation systems.

A central topic of SFB 1303, where S. is the principal investigator, ia the numerical study of classical symbolic algorithms. In 2005, S. could clarify stability questions for the implicitization problem from an algebraic and from a geometric viewpoint, together with B. Jüttler, M. Aigner, and A. Szilagyi.

He also continued his joint research with J. Kraus in the development of algebraic multigrid methods, and could make contributions in research on molecular biology (by P. Schuster and S. Widder).

## Scientific Cooperations

### Internal

Johannes Kraus: 1 joint paper, 1 planned.

Willem de Graaf: 1 joint paper (together with Harrison and Pilnikova), 1 submitted (together with Pilnikova).

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

### External

- Bert Jüttler, Linz: 2 joint papers. He is co-investigator in the FWF-funded special research area SFB 13, subproject 15. Together with him, S. submitted another project to FWF.
- Herwig Hauser, Innbruck: 1 joint FWF project (not running under RICAM because it started 2002), plus another FWF project submitted. 3rd joint seminar of a series alternating in Tirol and Upper Austria.
- Rafael Sendra, Madrid: 1 joint paper submitted, 1 special issue in a journal jointly edited (in preparation).
- Mike Harrison, Sydney: 1 joint paper accepted, 1 paper in preparation.
- Peter Schuster and Stephanie Widder: 1 paper in preparation.
- Günter Landsmann (Linz) and Peter Mayr (Linz): 1 joint paper, plus 1 joint paper submitted.
- Christian Haase (Berlin): 1 joint paper submitted.

## Participation at Conferences, Scientific Visits and Talk

### Conferences

- Algorithmic Algebra and Logic (A3L, Passau 2005): “A topological criterion for polynomiality”, contributed talk.
- Effective Methods in Algebraic Geometry (MEGA, Alghero 2005):
  - co-organization, together with 6 colleagues from Italy, France, Spain, Argentina
  - “The parametric degree of rational surfaces”, contributed talk.
- Algebraic Geometry and Group Theory (Magma workshop, Warwick 2005): “Computation of adjoints and the parametrization problem”, invited talk.
- Computational Methods for Algebraic Spline Surfaces (COMPASS, Oslo 2005): “Sparse parametrization of algebraic curves and surfaces”, invited talk.

### Scientific Visits

- SFB status seminar (Strobl 2005): project meeting.
- MEGA conference organisation (Pisa 2005): meeting of executive committee
- Joint Seminar Innsbruck-Linz (Brandenberg 2005): workshop in algebraic geometry and singularities together with colleagues from Linz, Innsbruck, Trento, Valladolid.

## Publications 2005

### Appeared or accepted:

#### Journal papers:

1. J. Schicho, I. Szilagyi: Numerical stability of surface implicitization. *J. Symb. Comp.* 40/6 (2005), pp 1291-1301.
2. B. Jüttler, J. Schicho, I. Szilagyi: Local parametrization of cubic surfaces. *J. Symb. Comp.* de Graaf, M. Harrison, J. Pilnikova, J. Schicho: A Lie algebra method for the parametrization of Severi-Brauer surfaces. *J. Symb. Comp.*
3. J. Kraus, J. Schicho: Algebraic multigrid based on computational molecules, I: scalar elliptic problems. *Computing.*
4. J. Schicho: The parametric degree of rational surfaces. *Math. Zeitschr.*

**Proceedings:**

5. G. Landsmann, P. Mayr, J. Schicho: A topological criterion for polynomiality. Proc A3L, Norderstest 2005, pp 155-158.
6. M. Aigner, B. Jüttler, J. Schicho, I. Szilagyi: Implicitization and distance bounds. Proc AGGM 2004, Springer.n
7. W.A. de Graaf, M. Harrison, J. Pilnikova, J. Schicho: A Lie algebra method for rational parametrization of Severi-Brauer surfaces (extended abstract). Proc MEGA 2005,
8. J. Schicho: The parametric degree of rational surfaces (extended abstract). Proc. MEGA 2005.

**Submitted**

9. J. G. Alcazar, J. Schicho, J. R. Sendra: Computation of the topological types of the level curves of an algebraic surface.
10. T. Beck and J. Schicho: Approximate roots in graded rings.
11. G. Landsmann, P. Mayr, J. Schicho: A topological criterion for polynomial functions on  $GL(2, \mathbb{R})$ .

***Dr. Willem A. de Graaf*****Introduction**

He won the competition for a “Ricercatore” at the University of Trento, Italy, which he entered upon in March 2005. Even though he was employed at RICAM only for a short time (5 months altogether), he could achieve a substantial contribution to the research of RICAM. His joint cooperations with RICAM are still continuing, in particular with J. Pilnikova and J. Schicho.

**Scientific Achievements 2005****Parametrizing varieties using Lie algebras.**

The Lie algebra of a variety is the Lie algebra of the group of automorphisms of the variety. If the two varieties are isomorphic, also their Lie algebras are isomorphic and using the isomorphism of varieties we can find an isomorphism of their Lie algebras. In many interesting cases also the other implication is valid: Using an isomorphism of the Lie algebras of two varieties one can construct an isomorphism of the varieties and consequently parametrize the given variety. This idea was used to solve the cases of Del Pezzo surfaces of degree 9 and 8. This was joint research with J. Pilnikova and J. Schicho, and partially with M. Harrison from the University of Sydney.

De Graaf also devised a practical method for constructing homomorphisms between Verma modules, during the time he was at RICAM.

**Scientific Cooperations****Internal**

J. Schicho, J. Pilnikova: 1 joint paper, 1 joint paper in preparation

**External**

M. Harrison (Sydney): 2 joint papers (together with Pilnikova and Schicho)

**Participation at Conferences, Scientific Visits and Talk****Scientific Visits and Talks**

W. A. de Graaf participated in the workshop on algebraic geometry and singularities in Brandenberg, Tirol, jointly organized by RICAM and the University of Linz.

**Publications 2005****Accepted**

1. W.A. de Graaf, M. Harrison, J. Pilnikova and J. Schicho. A Lie algebra method for rational parametrization of Severi-Brauer surfaces. *Journal of Algebra*, to appear.
2. W.A. de Graaf, M. Harrison, J. Pilnikova and J. Schicho: A Lie algebra method for parametrization of Severi-Brauer surfaces (extended abstract). *Proc. MEGA 2005*
3. W.A. de Graaf: Constructing homomorphisms between Verma modules. *J. Lie Theory* 15/2 (2005), pp 415-428.

***Dr. Oliver Labs***

He joined RICAM as a PostDoc in October 15, 2005.

**Work before joining RICAM**

He received my Ph.D. on October 14, 2005. The topic of my thesis was “Hypersurfaces with Many Singularities – History, Constructions, Algorithms, Visualization”. My main results improved many of the best known lower bounds for the classical problem of determining the maximum number  $\mu(d)$  of singularities on hypersurfaces of given degree  $d$ .

The result which attracted the most interest in the algebraic geometry community was my construction of a surface of degree 7 (also called septic) in three-space with 99 real singularities. E.g., G.-M. Greuel chose it as the logo of the conference which took place in 2004 at Kaiserslautern at the occasion of his 60<sup>th</sup> birthday because I used the computer algebra program Singular for the construction.

After this discovery, he found several other constructions. But the result which has the greatest potential to be applied in other areas of mathematics and science is an algorithm for locating interesting varieties within families. In his Ph.D. thesis, he only applied it to find hypersurfaces with many singularities: all previous constructions of low degree  $d \leq 10$  which reach the currently best known lower bounds for  $\mu(d)$  can be found by simply applying my algorithm.

**Scientific Achievements 2005 (after joining RICAM)**

As already remarked in the previous section, my algorithm for locating interesting varieties within families has the potential of being applied in many situations. So, my aim during the first months at RICAM was the improvement of this algorithm and the search for applications.

In November, he completed the implementation of a parallel version of it which works quite well: in all examples which I tested, the speed-up is by a factor which comes close to the number of processors used. E.g., the construction of the 99-nodal septic mentioned above takes less than a minute when using 25 of the workstations at RICAM instead of one minute when only using one of them.

**Scientific Cooperations**

For more details, see also the section on plans for 2006.

**Internal**

Prof. Josef Schicho

External

Prof. Duco van Straten (Mainz, Germany),  
 Stephan Holzer (Mainz, Germany),  
 Frederic Bihan (Univ. Savoie, France).

**Participation at Conferences, Scientific Visits and Talk (after joining RICAM)**Conferences

Workshop “Topology of Real Algebraic Varieties”, Institut Henri Poincare, Paris (France).

Scientific Visits

One day: Invited by Frank-Olaf Schreyer, Saarbrücken (Germany).

Scientific Talks

- Invited talk: “Flächen mit vielen reellen Singularitäten”, at the Algebraic Geometry Seminar at Saarbrücken (Germany), invited by Prof. Frank-Olaf Schreyer.
- Contributed talk: “Surfaces with many real singularities”, at the Workshop “Topology of Real Algebraic Varieties”, Institut Henri Poincare, Paris (France).

**Publications 2005**Accepted for Publication

1. “A Septic with 99 Real Nodes”, in: Rend. Sem. Mat. Univ. Pad.  
 (with Stephan Holzer): “Illustrating the Classification of Real Cubic Surfaces”, in: Proc. of AGGM '04 at Nice (Springer).

Submitted

2. “An Algorithm for Locating Interesting Examples within Families”.

***Dr. Pavel Chalmoviansky***

He is working as a post-doctoral researcher in the SFB project 1315.

**Scientific Achievements 2005****Evolution of Approximate Parameterization of Curves**

The approximation of the intersection curve is formulated as a coupled system of ODE. The first is a tracing of the given implicitly defined curve. The other is the evolution of the approximate parameterization using rational Bezier curve. Using Runge-Kutta methods for approximation of the solution of the ODE, we get the local approximation of order 4 for regular parts of the algebraic curve. The singularities of certain types can be used as starting points of the evolution. The a posteriori error for the approximation was considered. The paper was published as SFB Report and submitted.

**Variational Barycentric Coordinates**

We provide a general construction of barycentric coordinates for arbitrary finite set of points. The points are lifted into a space of higher dimension. Using an auxiliary set of functions, we compute an auxiliary point in the higher dimensional space, which is projected to the variety of feasible solutions. The construction is universal (any set of barycentric coordinates can be constructed in this way), re-

produces affine coordinates and is affinely invariant. Additionally, we provide several constructions of barycentric coordinates for planar polygons. This is an on-going work.

### **Scientific Cooperations**

#### External

Bert Juettler, Institute of Applied Geometry, JKU Linz  
Dalibor Lukas, TU Ostrava, Czech Republic

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

#### Conferences

Spring Conference on Computer Graphics 2005 (also active participation in organization of the review process), May 2005  
SIAM Conference on Computing and Geometric Design, November, 2005

#### Scientific Talks

Invited Talk at TU Ostrava, April 2005

### **Publications 2005**

#### Appeared

1. Bert Juettler, Pavel Chalmoviansky, Mohamed Shalaby, Elmar Wurm. Approximate Algebraic Methods for Curves and Surfaces and their Applications, Proceedings of SCCG2005 (in print also as ACM Siggraph publication).

#### Submitted

2. Pavel Chalmoviansky, Bert Juettler. A Circle-preserving Subdivision Scheme Based on Local Algebraic Fits. (to appear in AiCM)
3. Pavel Chalmoviansky and Bert Juettler. Predictor-Corrector Technique for Approximate Parameterization of intersection Curves (submitted)
4. Dalibor Lukas, Pavel Chalmoviansky. A Sequential Coupling of Optimal Topology and Multilevel Shape Design Applied to 2-Dimensional Nonlinear Magnetostatics (submitted)

### ***Dr. Ibolya Szilagyi***

#### **Introduction**

Ibolya Szilagyi finished her PhD study supervised by J. Schicho in September 2005. The topic of her PhD thesis is symbolic and numerical algorithms for cubic surfaces. She also worked as a researcher in the SFB project 1303. After her PhD was finished, she got a position as a university teacher at Karoly Eszterhazy College in Eger, Hungary.

### **Scientific Achievements 2005**

#### Local parametrization:

Several techniques for parametrizing a rational surface as a whole exist. In many applications, it is sufficient to parametrize only a small portion of the surface. Sz. investigated such local parametrization in the case of nonsingular cubic surfaces. Together with B. Jüttler and J. Schicho, she gave several algorithms for constructing such local parametrizations that cover the surface exhaustively.

### Stability of implicitization

Despite the fact that the implicitization problem for rational curves and surfaces makes sense when the input is only known up to a certain error level, and the fact that there are already several algorithms known for numerically solving this problem, there was previously no investigation of the numerical stability of this problem and these algorithms. Together with Schicho, Sz. introduced a measure, called condition number, for the stability which depends on the numerical input and on some discrete information corresponding to the estimated degree of the unknown implicit equation. The numerical error can be controlled by this condition number.

Together with M. Aigner and B. Jüttler, Sz. also investigated the geometrical consequences of numerical instability in the implicitization process.

### Scientific Cooperations

#### Internal

J. Schicho

#### External

M. Aigner (Linz)

B. Jüttler (Linz)

### Participation at Conferences, Scientific Visits and Talks

#### Conferences

Computational Methods for Algebraic Spline Surfaces (COMPASS; Oslo 2005): “A condition number for the implicitization problem”, contributed talk

#### Scientific Visits and Talks

Workshop on Algebraic Geometry and Singularities: “Numerical stability of implicitization”, talk.

SFB status seminar: “Geometric and algebraic stability of implicitization”, talk.

### Publications 2005

1. Symbolic and numeric techniques for cubic surfaces. PhD thesis, University of Linz.

#### Accepted

2. J. Schicho, I. Szilagyi: A condition number for the implicitization problem. *J. Symb. Comp.* 40/6 (2005), pp 1291-1301.

3. B. Jüttler, J. Schicho, I. Szilagyi: Local parametrization of cubic surfaces. *J. Symb. Comp.*

4. M. Aigner, B. Jüttler, J. Schicho, I. Szilagyi: Implicitization and distance bounds. *Proc. AGGM 2004*, Springer, to appear

### ***Michael Barton***

He is employed for one year of his PhD study as a researcher in the SFB project 1315.

### **Work before joining RICAM (those who joined RICAM 2005)**

Spatial displacement preserving points on given objects (plane, sphere, line) were observed. Dual quaternions and Study's representation of group of congruences were studied. Especially, spatial dis-

placement with three line trajectories were researched. Only one non-trivial motion has been found. This research has been done on two institutes, namely:

Charles University in Prague, Faculty of mathematics and physics  
Czech Technical University in Prague, Faculty of mechanical engineering.

## **Scientific Achievements 2005**

Degree reduction method for solving polynomial equations

An algorithm for solving polynomial equations in one variable is presented. A new method is compared with Bezier clipping. Algorithm: Given polynomial function over given interval is represented by Bezier curve. The best quadratic approximation in L<sub>2</sub> norm is found. The quadratic boundaries are computed. Its roots are found and new interval obtained. The convergence rate is cubical in spite of quadratic clipping's rate. An algorithm is being implemented into C code to compare speed of both algorithms.

## **Scientific Cooperations**

### External

Bert Juettler, Institute of Applied geometry, JKU Linz

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

### Conferences

- The International Conference Presentation of Mathematics '05, Liberec, 20. –23.9. 2005
- 25<sup>th</sup> Conference on geometry and computer graphics, Jizerske Hory, 12. –16.9. 2005
- 14<sup>th</sup> Annual Conference of Doctoral Students - WDS 2005, Prague, 7. –10.6. 2005

## **Publications 2005**

### Appeared

1. *Prostorové problémy související s polybem*, Proceedings of the 25<sup>th</sup> Conference on geometry and computer graphics

### Submitted

2. *Spatial displacement with three line trajectories*, Proceedings of The International Conference Presentation of Mathematics '05

## ***Tobias Beck***

He is working in the SFB project 1303, as a PhD student under the advise of J. Schicho.

## **Scientific Achievements 2005**

The work on the Newton-Puiseux algorithm for multivariate power series roots done in 2004 has been fixed in a RICAM report. One of the results was a representation for algebraic power series. He has explored how to manipulate this representation and use it for effectively executing certain arithmetic operations. This resulted in implementations in two computer algebra systems, Maple and Magma. A paper has been submitted.

He has done work on the efficient parametrization of algebraic curves which are implicitly defined by a sparse polynomial. Therefore he has used methods of toric geometry to construct a particularly nice

birational model of such a curve. Namely the curve is embedded in a toric surface whose construction is guided by the shape of the Newton polygon of the defining equation and thus takes its sparsity into account. He showed how a parametrization algorithm can benefit from this special representation in terms of lower complexity. A paper has been accepted.

The main achievement of 2005 was the development and implementation of an algorithm for computing the adjoint space of an algebraic surface. He used the power series machinery developed earlier to produce an "analytic resolution" of a given surface and finally derived conditions for computing adjoint spaces from this data. Adjoint spaces are the central ingredient of Schicho's Parametrization algorithm for surfaces. He is currently recording the theoretical background.

### **Scientific Cooperations**

#### Internal

Together with Klaus Scheicher he is working on an application of Puiseux expansions to carry over results from geometric number theory to finite fields.

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

#### Conferences

He attended the winter school YMIS'05 ("First meeting for young mathematicians In Sedano") to learn some of the algebraic tools used in geometry.

#### Scientific Talks

- February 22, YMIS'05, Sedano: "Computing Multivariate Power Series Roots" In 2004 he generalized the Newton-Puiseux algorithm for curves, resulting in an easily implementable algorithm for computing the multivariate power series roots of an algebraic equation. At this workshop the algorithm was for the first time presented to an international audience.
- September 21, "Workshop on Resolution of Algebraic Varieties", Kaiserhaus: "An Economic Model for Hypersurfaces" At this periodical workshop he explained a central part of our work on the efficient parametrization of algebraic curves which are implicitly defined by a sparse polynomial. Namely he presented the part that produces a particularly well-fit birational model of the curve. The toric construction was explained in a general setting, applicable to hypersurface of arbitrary dimension.

### **Publications 2005**

#### Accepted

1. Parametrization of Algebraic Curves Defined by Sparse Equations, with Josef Schicho (see also RICAM Report 2005-08), AAECC.

#### Submitted

2. Approximate Roots in Graded Rings, with Josef Schicho (see also RICAM Report 2005-03)

### ***José Manuel García Vallinas***

#### **Introduction**

José Manuel García started to write his PhD thesis under the supervision of J. Schicho, in the frame of the SFB project 1315. The topic of his thesis is root-parametrizations.

## Scientific Achievements 2005

As he just started with working on the thesis, there are no scientific results yet.

### Participation at Conferences, Scientific Visits and Talk

#### Conferences

"Automorphisms of the rational and elliptic curves ", Workshop on Algebraic Geometry and Singularities, September 19-22, Tirol, Austria.

“Marriage Problem”, UWPM 2005, October 8-11, Roznov pod Radhostem, Czech Republic.

## ***Janka Pilnikova***

### Introduction

Janka Pilnikova is a PhD student supervised by Prof. Dr. Josef Schicho. Her research interest is algebraic and arithmetic geometry. She is working on her thesis on parametrizing surfaces over the rational numbers using the Lie algebra of the surface, in the frame of the SFB project 1303.

## Scientific Achievements 2005

Parametrizing varieties using Lie algebras.

Lie algebra of a variety is the Lie algebra of the group of automorphisms of the variety. If the two varieties are isomorphic, also their Lie algebras are isomorphic and using the isomorphism of varieties we can find an isomorphism of their Lie algebras. In many interesting cases also the other implication is valid: Using an isomorphism of the Lie algebras of two varieties one can construct an isomorphism of the varieties and consequently parametrize the given variety. Together with J. Schicho and W.A. de Graaf, Janka Pilnikova worked out this method to parametrize both types Del Pezzo surfaces of degree 8 over the rational numbers. The paper is submitted to LMS, the algorithm is implemented in Magma.

Splitting of central simple algebras.

The problem is for a given central simple (associative) algebra decide whether it is isomorphic to the full matrix algebra, and find an isomorphism in the affirmative case. In some cases it can appear as a substep of the previous algorithm on parametrizing varieties using Lie algebras. Janka Pilnikova solved the problem for the algebras of degree 4 by reducing to the norm equation. The algorithm is implemented in Magma, the paper is in preparation.

### Scientific Cooperations

#### Internal

Josef Schicho

#### External

Willem A. de Graaf, University of Trento, Italy

### Participation at Conferences, Scientific Visits and Talk

#### Conferences

- "Symmetries for Solving Diophantine Equations", SFB-Statusseminar, March 31 – April 2, Strobl, Austria
- "A Lie algebra method for rational parametrization of Severi-Brauer surfaces", MEGA 2005, May 27 - June 1, Alghero, Italy

- "Using Lie algebras to parametrize certain types of algebraic varieties II", Workshop on Lie Algebras, their Classification and Applications, July 24-28, University of Trento, Italy
- "Rational parametrizations via Lie algebras II", Magma Workshop on Group Theory and Algebraic Geometry, August 22-26, University of Warwick, UK
- "Rational parametrization using Lie algebras", Workshop on Algebraic Geometry and Singularities, September 19-22, Tirol, Austria
- "Splitting central simple algebras of degree 4", Darstellungstheorie and Nikolaus Conference, December 8-10, Aachen, Germany

#### Scientific Visits and Talks

- "Racionalna parametrizacia Severi-Brauerovych ploch", seminar talk, April 14, Comenius University, Bratislava, Slovakia
- "Splitting central simple algebras over the rational numbers", seminar talk, November 10, University of Trento, Italy

#### **Publications 2005**

##### Accepted

1. Willem A. de Graaf, Michael Harrison, Jana Pilnikova and Josef Schicho. A Lie algebra method for rational parametrization of Severi-Brauer surfaces. *Journal of Algebra*, to appear.

##### Submitted

2. Willem A. de Graaf, Jana Pilnikova and Josef Schicho. Parametrizing Del Pezzo surfaces of degree 8 using Lie algebras. Submitted to London Mathematical Society.

#### **Scientific plans for 2006**

P. plans to finish and defend her PhD thesis.

Another goal is to design and implement algorithms for splitting algebras using lattice reduction methods, so that the time-expensive solving of norm equations is avoided (central simple algebras of degree 3 and 4)

## **2.4. GROUP “FINANCIAL MATHEMATICS”**

**Group Leaders:**

Univ.-Doz. Dr. Hansjörg Albrecher  
o.Univ.-Prof. Dr. Walter Schachermayer

**Researchers funded via ÖAW/Upper Austrian government funds:**

Dr. Jürgen Hartinger  
Dr. Karel Janeček  
Dr. Gottlieb Pirsic  
Dr. Jörn Saß  
Dr. Klaus Scheicher  
Univ.-Doz. Dr. Arne Winterhof

**Researchers externally funded:**

Mag. Nina Brandstätter  
DI Markus Hahn  
Univ.-Doz. Dr. Wilfried Meidl  
DI Wolfgang Putschögl  
Mag. Christiaan van de Woestijne

***Introduction by Group Leader Prof. Walter Schachermayer***

The Financial Mathematics Group was restructured during 2005, with Dr. Janeček and Doz. Meidl leaving RICAM and Doz. Albrecher (Graz University of Technology/University of Aarhus) starting as new group leader in October. In addition, Dr. Hartinger has been hired, who received his PhD degree in Graz working on the development of efficient simulation techniques for finance and insurance and at RICAM will in particular focus on analytical aspects of risk analysis.

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. In particular, the following research topics are currently covered:

- Portfolio optimization under transaction costs and incomplete information
- Risk measures
- Valuation and semi-static hedging of financial derivatives in general market models
- Dependence and economic environment in risk theory
- Development of efficient rare-event simulation techniques in the presence of heavy tails
- Parameter estimation based on Markov Chain Monte Carlo
- Stochastic Analysis
- Discrepancy and Quasi-Monte Carlo methods
- Coding Theory and Cryptology

There are currently two FWF projects led by group members (Dr. Sass and Doz. Winterhof) and a third one (led by Doz. Albrecher) with two PhD students at RICAM (DI Kortschak and DI Thonhauser) will start in January 2006, so that about half of the group members are then externally funded. 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.

***Univ.-Doz. Dr. Hansjörg Albrecher*****Work before joining RICAM**

H. Albrecher joined RICAM as group leader in October 2005. Since 2001 he holds a faculty position at the Department of Mathematics at Graz University of Technology. From April 2005 to September 2005 he was a Visiting Associate Professor at the Department of Mathematical Sciences, University of Aarhus (Denmark). His main research focus is in the analysis of risk measures in finance and insurance, both from an analytic and a numerical viewpoint. This includes for instance the study of ruin-related quantities in general collective risk models (in particular in the presence of dependence and economic factors such as interest, inflation and dividend payments) as well as the development of efficient hedging strategies for exotic options in general market models.

**Scientific Achievements 2005**

Research (partly before having joined RICAM):

H. Albrecher worked on a general model for the surplus process in collective risk theory that enables the analysis of several measures of risk (such as the probability of ruin and the distribution of the deficit at ruin) from an integrating viewpoint, providing a unified approach to several popular stochastic models. In particular, this approach allows for the first time to retrieve analytic formulae for risk models with causal dependence structure among the risks in the portfolio ([4,14] and, jointly with O. Boxma, [7]). For these results, H. Albrecher received the Gauss-Prize 2005 of the German Association for Insurance and Financial Mathematics.

Together with J. Teugels, a risk model that allows for dependence between interclaim times and claim sizes was investigated in [11]. For light-tailed claim sizes, classical random walk techniques are extended to study the sensitivity of asymptotic expressions for the ruin probability on the degree of dependence. It turns out that the Laplace transform of the increment distribution can be expressed explicitly through the copula structure of the interclaim time and claim size, giving rise to ordering results for the ruin probability with respect to dependence orderings.

In many practical situations in insurance and finance, the coefficient of variation of some underlying random quantity is used to approximatively assess the involved risk. Given a set of data, the sample coefficient of variation is then often used for that purpose. In [8], H. Albrecher and J. Teugels investigate the behaviour of a closely related measure of risk, if the underlying random quantity has infinite fourth moment. Based on Karamata theory of regular variation, they obtain explicit asymptotic expressions for arbitrary moments of this quantity. As a by-product, this leads to a new estimation procedure of the Pareto index from an iid data set in the critical case of infinite second moment of the underlying distribution. Currently, this result is being complemented by weak law results in joint work with S. Ladoucette.

For collective risk models that consider dividend payments according to a linear barrier strategy, analytic expressions for several risk-related quantities could be obtained in joint work with J. Hartinger and R. Tichy [2]. For a horizontal dividend barrier and relaxed assumptions on the claim number process in the portfolio, exact solutions for arbitrary moments of the discounted dividend payments were derived together with M. Claramunt and M. Marmol [5]. Whereas the barrier height is often chosen so as to maximize the expected dividend payments, these results allow to quantitatively underpin the fact that a consideration of higher moments in the choice of the strategy is important.

In several applications, the claim number process is better described by a Cox process with stochastic intensity of shot noise type rather than a homogeneous Poisson process (in particular in insurance lines prone to claims due to natural catastrophes or other external events). In joint work with S. Asmussen [13], H. Albrecher worked out asymptotic results for a corresponding risk portfolio for both light- and heavy-tailed claim sizes. Moreover, an adaptive premium rule based on the past claim experience within the portfolio was implemented.

Another collaboration with S. Asmussen [12,15] deals with the asymptotic behaviour of sums of two dependent heavy-tailed risks, which is highly relevant for risk management techniques in current practice. Within the class of subexponential distributions, the sensitivity of the asymptotic behaviour with respect to varying degree of dependence is investigated in terms of the underlying copula function. For several specific dependence structures, explicit answers are given.

In traditional dynamic hedging of a financial derivative in terms of a position in the underlying and a riskless asset, the hedge portfolio has to be adjusted continuously in time, which is practically not feasible. Moreover, transaction costs and illiquidity of the required products in distressed periods can be problematic issues in practice. In particular for exotic options, static hedging strategies in terms of vanilla options and the underlying may provide efficient alternatives. Here a static hedging portfolio is set up at the beginning of the contract that does not need adjustment during the lifetime of the option, usually at the price of a super-replication. For Asian options, such a static super-hedging strategy was developed jointly with W. Schoutens, J. Dhaene and M. Goovaerts [3,6] using comonotonicity techniques. Moreover, this static super-hedge is optimal in some sense.

In the framework of the above topics, an FWF research project P18392 "Mathematical Models for Insurance Risk" led by H. Albrecher has been granted, and two of his PhD students will join the Financial Mathematics group at RICAM in January 2006, funded by this project.

## **Scientific Cooperations**

### Internal

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

Dr. H. Egger: Inverse problems for local Levy models

Doz. Dr. M. Burger: Hamilton-Jacobi-Bellman equations

### External

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

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

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

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

Dr. Claudio Macci (University Tor Vergata, Rome): Large deviation techniques

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

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

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

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

University Center of Statistics, Katholieke Universiteit Leuven, Belgium,

Invited research visit: November 21-December 2, 2005.

Talk: "Ruin Theory with Dependent Risks"

Mathematisches Kolloquium, Technische Universität Graz:

Invited talk: "Ruintheorie für Versicherungssportfeuilles mit abhängigen Risiken", November 18, 2005.

Workshop on New Mathematical Methods in Risk Theory, Florence:

Talk: "A unified approach to the analysis of some popular collective risk models", October 6-8, 2005.

Workshop 'Portfolio Risk Management', TU Vienna:

Invited talk: "Ruin Estimates for an Insurance Portfolio with Dependent Risks", September 26, 2005.

7th Hellenic European Research Conference on Computer Mathematics and its Applications, Athens:  
Invited talk: "A Unified Approach to the Analysis of Some Popular Models in Collective Risk Theory", September 22-24, 2005.

Workshop of the German Academy of Actuaries, Günzburg:  
Invited talk: "Ruintheorie mit Abhängigkeiten" September 10-11, 2005.

Laboratory of Actuarial Mathematics, University of Copenhagen, Denmark,  
Invited visit: June 6-10, 2005,  
Series of 9 Lectures: "Mathematical Methods in Reinsurance"

Radon Institute for Computational and Applied Mathematics, Linz:  
Talk: "Static Hedging of Asian Options under General Market Models", May 13, 2005.

Conference on "Risk Measures and Risk Management: General Aspects", Eindhoven:  
Invited talk: "Asymptotic Analysis of Measures of Variation", May 9-11, 2005.

Department of University of Karlsruhe:  
Invited research visit: May 2-3, 2005,  
Talk: "Dividend Models in Risk Theory".

Center for Analytical Finance, Aarhus University:  
Invited talk: "Static Hedging of Asian Options under Levy Models", April 12, 2005.

Department of Mathematics, Graz University of Technology:  
Habilitationskolloquium: "Measures of Risk in Insurance: Mathematical Aspects", March 3, 2005.

Department of Mathematics, University of Zagreb:  
Invited research visit: January 25-26, 2005,  
Talk: "On Some Generalizations of Classical Ruin Theory".

## **Publications 2005**

### Appeared

1. H. Albrecher: A note on the asymptotic behaviour of bottleneck problems. *Operations Research Letters* 33 (2005), No. 2, 183-186.
2. H. Albrecher, J. Hartinger, R.F. Tichy: On the distribution of dividend payments and the discounted penalty function in a risk model with linear dividend barrier. *Scandinavian Actuarial Journal* (2005), No.2, 103-126.
3. H. Albrecher, W. Schoutens: Static hedging of Asian options under stochastic volatility models using Fast Fourier transform. In: *Exotic Options and Advanced Levy Models*, A. Kyprianou et al. (eds), pp. 129-148, Wiley, Chichester, 2005.
4. H. Albrecher: Discussion of "The Time Value of Ruin in a Sparre Andersen Model" by H. Gerber and E. Shiu. *North American Actuarial Journal* 9 (2005), No. 2, 71-74.
5. H. Albrecher, M.M. Claramunt, M. Marmol: On the distribution of dividend payments in a Sparre Andersen model with generalized Erlang(n) interclaim times. *Insurance: Mathematics & Economics* 37 (2005), No. 2, 324-334.
6. H. Albrecher, J. Dhaene, M. Goovaerts, W. Schoutens: Static hedging of Asian options under Levy models. *Journal of Derivatives* 12 (2005), No. 3, 63-72.
7. H. Albrecher, O. Boxma: On the discounted penalty function in a Markov-dependent risk model. *Insurance: Mathematics & Economics* 37 (2005), No. 3, 650-672.

Accepted

8. H. Albrecher, J.L. Teugels: Asymptotic Analysis of a Measure of Variation. *Theory of Probability and Mathematical Statistics* (2006), to appear.
9. 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.
10. H. Albrecher: Some Extensions of the Classical Ruin Model in Risk Theory. *Grazer Math. Berichte* (2006), to appear.
11. H. Albrecher, J.L. Teugels: Exponential behavior in the presence of dependence in risk theory. *Journal of Applied Probability* 43 (2006), No. 1, to appear.
12. H. Albrecher, S. Asmussen and L. Rojas-Nandayapa: On the tail behavior of heavy-tailed dependent sums. *Proceedings of the Workshop on New Mathematical Methods in Risk Theory*, Florence 2005, to appear.
13. H. Albrecher, S. Asmussen: Ruin probabilities and aggregate claims distributions for shot noise Cox processes. *Scandinavian Actuarial Journal* (2006), to appear.

Submitted

14. H. Albrecher: A unified approach to the analysis of some popular collective risk models.
15. H. Albrecher, S. Asmussen: Tail asymptotics for the sum of two heavy-tailed dependent risks.

***Prof. Walter Schachermayer*****Publications 2005**Appeared:

1. F. Delbaen, W. Schachermayer: The Mathematics of Arbitrage. Springer Finance, xvi+371 p., ISBN 3-540-21992-7 (2005).
2. M. Drmota, W. Schachermayer, J. Teichmann: A hyper-geometric approach to the BMV-conjecture. *Monatshefte für Mathematik*, Vol. 146 (2005), pp. 179-201.
3. W. Schachermayer: A Note on Arbitrage and Closed Convex Cones. *Mathematical Finance*, Vol. 15 (2005), No. 1, pp. 183-189.
4. J. Hugonnier, D. Kramkov, W. Schachermayer: On Utility Based Pricing of Contingent Claims in Incomplete Markets. *Mathematical Finance*, Vol. 15 (2005), No. 2, pp. 203-212.
5. E. Jouini, C. Napp, W. Schachermayer: Arbitrage and state price deflators in a general intertemporal framework. *Journal of Mathematical Economics*, Vol. 41 (2005), pp. 722-734.

Accepted:

6. D. Rokhlin, W. Schachermayer: A note on lower bounds of martingale measure densities. *Illinois Journal of Mathematics* (2006), to appear.
7. E. Jouini, W. Schachermayer, N. Touzi: Law invariant risk measures have the Fatou property. *Advances in Math. Economics* (2006), to appear.
8. W. Schachermayer, J. Teichmann: How close are the Option Pricing Formulas of Bachelier and Black-Merton-Scholes? *Mathematical Finance* (2006), to appear.
9. W. Schachermayer: The Notion of Arbitrage and Free Lunch in Mathematical Finance. *Publication of the Académie des Sciences Paris* (2006), to appear.

Submitted:

10. W. Schachermayer, J. Teichmann: Solution of a problem in Villani's book.
11. L. Campi, W. Schachermayer: A Super-Replication Theorem in Kabanov's Model of Transaction Costs.

12. E. Jouini, W. Schachermayer, N. Touzi: Optimal risk sharing for law invariant monetary utility functions.

### Research Visits, Conferences and Talks

Mathematics Institute, University of Munich, Germany;

Research Visit: November 17-18, 2005;

Invited talk: "Optimal risk sharing for law invariant monetary utility functions", November 17, 2005.

1. Gemeinsamer Workshop aller Projekte des "Mathematik und..."-Calls, Wiener Wissenschafts-, For-

schungs- und Technologiefonds (WWTF), Vienna, Austria;

Invited presentation: "Optimal risk sharing for law invariant monetary utility functions", November 15, 2005.

math-space, Wien;

Invited talk: "Wie verlässlich ist der Zufall? - Mathematik in Finanzmärkten", November 10, 2005.

Aktionstag "Education meets Science", Wiener Wissenschaftstage, math-space, Vienna, Austria;

Invited talk: "Was macht die Mathematik auf den Finanzmärkten", October 3, 2005.

Annual Meeting of the Österreichische Physikalische Gesellschaft (ÖPG), Symposium "Brownian Mo-

tion, an Interdisciplinary Phenomenon", University of Vienna, Austria;

Invited plenary talk: "Brownian motion and the movements of the stock market", September 29, 2005.

Wiener Vorlesungen: Albert Einsteins Werk, Wiener Rathaus, Wien, Austria

Podiumsdiskutant: "Einsteins Theorie der Brownschen Molekularbewegung und ihre wissenschaftliche Anwendung heute", September 27, 2005.

16th international Congress of the Austrian Mathematical Society (ÖMG), University of Klagenfurt, Austria (September 18-23), 2005;

Research Visit: September 18-21, 2005;

Invited talk: "Die Rolle der Mathematik auf den Finanzmärkten", September 20, 2005.

4th semester of the UNESCO Chair at LAMSIN: "Mathematical Modelling in Finance", Tunis, Tunisia (September 12-17, 2005);

Invited Visit: September 12-16, 2005;

Series of 10 lectures: "Mathematics of Arbitrage", September 12-16, 2005.

PDE and Mathematical Finance, Institut Mittag-Leffler, Stockholm, Sweden (August 15-19, 2005);

Research visit: August 16-19, 2005;

Invited Talk: "Optimal risk sharing for law invariant monetary utility functions", August 17, 2005.

Workshop on "Evolution Equations for Deterministic and Stochastic Systems" (EU RTN HPRN-CT-2002-00281), Centro di Ricerca Matematica Ennio de Giorgi, Scuola Normale Superiore, Pisa, Italy;

Research visit: May 22-27, 2005;

Series of 6 lectures: "Optimal Investment in Incomplete Financial Markets" May 23-25, 2005.

Isaac Newton Institute for Mathematical Sciences, Cambridge, UK;

Research Visit: April 25-29, 2005;

Organizer of the workshop on "Fundamentals of Mathematical Finance" within the Quantitative Finance programme;

Invited opening talk: "Optimal risk sharing for law invariant monetary utility function", April 25, 2005.

Research seminar on "Stochastische Analysis und Stochastik der Finanzmärkte", University of Technology/ Humboldt University, Berlin, Germany

Talk: "Optimal risk sharing with law invariant monetary utility functions", April 14, 2005.

Schmetterer Gedenkkolloquium, April 4-5, 2005, Austrian Academy of Sciences, Vienna, Austria;  
Invited Talk: "Anwendungen der Wahrscheinlichkeitstheorie auf die Finanzmathematik", April 5, 2005.

FAM-Seminar, Vienna University of Technology, Austria;

Talk: "Optimal Design of Risk Exchange for Cash-Invariant Risk Measures", February 15, 2005.

Journée de Présentation des Mathématiques, Académie des Sciences, Paris, France;

Invited Talk: "Introduction aux notions d'arbitrage: Qu'est-ce qu'un Free Lunch?", February 1, 2005.

### ***Dr. Jürgen Hartinger***

#### **Work before joining RICAM**

Dr. Hartinger joined the institute in October 2005. Before, his scientific focus were stochastic and quasi-stochastic simulation methods in financial engineering. During and after his PhD project "Quasi-Monte Carlo techniques in financial and actuarial mathematics" he was employed in the FSP "Number-theoretic algorithms and their applications" in Graz and Linz. From October 2004, he held a temporary position as research and teaching assistant at the Graz University of Technology.

#### **Scientific Achievements 2005**

In 2005, Dr. Hartinger was interested in new aspects of Quasi-Monte Carlo (QMC) methods inspired by financial applications. In [2] and [4] so-called corner avoidance properties, one of the backbones of QMC error estimates for unbounded integrands, of various low discrepancy sequences are studied. Methods for the generation of low-discrepancy sequences with respect to non-uniform distributions with appropriate corner avoidance properties are discussed in [3]. Risks induced from low frequency-high impact events, called rare events, require properly designed simulation algorithms. QMC methods for the estimation of rare events are studied in [5].

After joining RICAM, a close cooperation between Dr. Hartinger and Univ.-Doz. Albrecher on various aspects of ruin theory (e.g. [1]) was relaunched. Actually, the main focus is laid on the analysis of the discounted penalty function and the moment-generating function of discounted dividends in several generalizations of the classical Cramer-Lundberg model under various dividend strategies. First results in this direction were recently obtained and are expected to be submitted very soon.

#### **Scientific Cooperations**

##### Internal

Hansjörg Albrecher (Financial Mathematics): ruin theory, discounted penalty and dividend strategies.

##### External

Reinhold Kainhofer (Vienna): QMC – corner avoidance properties, financial applications

Dominik Kortschak (Graz): QMC – rare event sampling

Giray Ökten (Tallahassee): QMC – actuarial applications

Robert F. Tichy (Graz): various aspects of QMC theory and ruin theory  
 Stefan Thonhauser (Graz): ruin theory, discounted penalty and dividend strategies  
 Art Owen (Stanford): QMC – corner avoidance properties  
 Volker Ziegler (Vienna/Graz): QMC – corner avoidance properties

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

#### Conferences

Workshop: Interface between Quantitative Finance and Insurance, Edinburgh (Great Britain).  
 Fifth IMACS Seminar on Monte Carlo Methods (MCM 2005), Tallahassee (USA), invited talk in the special session “Monte Carlo and Quasi-Monte Carlo methods in finance”: QMC methods and rare event sampling  
 Summer School: Modelling mortality dynamics for pensions and annuity business, Trieste (Italy).

#### Scientific Talks

TU Vienna (Institute of Financial and Actuarial Mathematics): QMC methods and rare event sampling.

#### Lectures

Winter term 04/05 (Graz University of Technology): Analysis I (exercise course), Mathematics I (exercise course, civil engineer)  
 Summer term 2005 (Graz University of Technology): Financial and Actuarial Mathematics I, Analysis II (exercise course), Mathematics I/II /(exercise course, civil engineer)

### **Publications 2005**

#### Appeared

1. H. Albrecher, J. Hartinger, and R. F. Tichy: On the distribution of dividend payments and the discounted penalty function in a risk model with linear dividend barrier, Scandinavian Actuarial Journal 2005 (2), 103--126.
2. J. Hartinger, R.F. Kainhofer and V. Ziegler: On the corner avoidance properties of various low-discrepancy sequences, Electronic Journal of Combinatorial Number Theory 5(3), 2005, A 10.

#### Accepted

3. J. Hartinger and R. Kainhofer: Non-uniform low-discrepancy sequence generation and integration of singular integrands, 2005, H. Niederreiter & D. Talay, eds, Proceedings of MCQMC 2004, Juan-Les-Pins France, June 2004, Springer Verlag, Berlin.

#### Submitted

4. J. Hartinger and V. Ziegler V.: A note on corner avoidance of random start-Halton sequences.
5. J. Hartinger and D. Kortschak: Quasi-Monte Carlo techniques and rare event sampling, RICAM report 26-05.

### ***Dr. Karel Janeček***

#### **Introduction**

(Half-time employment at RICAM since March 2005, active at RICAM until June 2005)  
 The main topic of research has been optimal control under transaction costs. This is an on-going research from Dr. Janeček's Ph.D. studies at Carnegie Mellon University, Pittsburgh. Another line of research is the duality approach to optimal control.

## Scientific Achievements 2005

A new working paper “Optimal investment with proportional profit-share fee” is close to completion. The paper analyses the optimal trading strategy under the so-called High-Water Mark fee policy that is of a standard use in the industry.

Paper modeling futures contracts under transaction costs has been finalized. Prof. Shreve is in the process of preparing the final draft for submission. The new approach includes modeling of futures contracts trading rather than stock trading, which appears to be an original concept.

A paper “Optimal investment strategy with liquidity constraints” is in working process.

By cooperation with Prof. Schachermayer, analysis of a duality approach to the problem of transaction costs analysis has been performed.

## Scientific Cooperation

### Internal Cooperation with

Karl Kunisch (RICAM), Jörn Saß (RICAM):

Numerical analysis of optimal control under transaction costs.

Walter Schachermayer

Topics concerning the duality approach to the transaction costs analysis.

### External Cooperation with

Steven E. Shreve, Carnegie Mellon University:

The asymptotic analysis of optimal control under transaction costs, futures trading

## Participation at conferences

- IMA Workshop, May 3 – May 7, 2004, University of Minnesota, MN 55455
- Bachelier Finance Society, Third World Congress, July 21-24, 2004, Intercontinental Hotel, Chicago, IL
- Stochastic Analysis and its Applications, January 6-7, 2005, Prague.
- Talk: Futures trading model with transaction costs
- CARISMA workshop “New Directions in Risk Modeling”, May 18-9, 2005, London.

## Publications

### Appeared

“Asymptotic analysis for optimal investment and consumption with transaction costs”, Janeček, K., Shreve, S., Finance and Stochastics 8, 181-206 (2004)

### Submitted

“What is a realistic aversion to risk for real-world individual investors?”, working paper.

“The low risk free rate is not too low”, working paper.

***Dr. Gottlieb Pirsic*****Introduction**

In addition to his ongoing work in the area of quasi-Monte Carlo methods (see the Introduction paragraphs of previous annual reports), due to the organizational restructuring of the group, Dr. Pirsic also spent some time acquiring more knowledge in the fields of Stochastics, Stochastic Analysis and Mathematical Finance.

**Scientific Activities 2005**

Somewhat following the spirit of the work on cyclic digital nets [2],[3], some new point set constructions were investigated. This was partly (points 1., 2. below) collaboration with Fritz Pillichshammer (Linz) and Josef Dick (Sydney). The considered constructions were

1. hybrids of (t,m,s)-nets and lattice rules
2. Kronecker sequences in the q-adic field  $Q_p$ , with special regard to analysis by characters on the q-adic integers
3. the application to (t,m,s)-nets of methods (due to Mullen) for the construction of infinite mutually orthogonal latin squares by infinite field extensions of finite fields

Another point was the research of cohomological methods in coding theory, in particular of evaluation codes on complete intersection varieties, in view of a possible translation to net theory.

A common construction of the Wiener process (or Brownian motion) is by use of the Faber-Schauder basis. As the functions of this basis are nothing but anti-derivatives of Haar functions, which themselves are closely related to Walsh functions, the anti-derivatives of Walsh functions (Walk functions) were considered.

As Walk functions (just like the Schauder functions) form a non-orthogonal basis with respect to the  $L_2$  scalar product, several orthogonalizations were derived. The reason for considering such orthogonalizations is that one of the objectives is to relate Korobov function classes with respect to the Walk basis to the Walsh-Korobov function classes, with a view to possibly obtain numerical integration bounds. This relation (Walk functions themselves lie in this class with parameter 1) turned out not to be practically advantageous in its current form and further investigation is needed.

Finally, the construction of the Brownian motion by Walk functions was obtained, and the convergence speed was shown to exactly equal that of the construction by Schauder functions (whereas initially a mildly better rate was to be expected due to the “random walk” nature of the Walk functions inspiring their name). This result will be submitted soon.

In a similar vein, also a Walsh expansion of the exponentiated Brownian motion (with applications in the modelling of stock price behavior) was derived, but the coefficients turned out to be too involved for practical implementation.

Malliavin Calculus is an important tool in Stochastic Finance, usually applied in the continuous time setting. In the discrete time setting, several existing approaches were examined; in particular the finite time-horizon approach as introduced in a paper of Leitz-Martini and the infinite time-horizon approach of Privault and Schoutens. For the former, the Itô formula in space and time could be derived.

**Scientific Cooperations**External:

F. Pillichshammer (Univ. Linz), J. Dick (Univ. New South Wales): Low-discrepancy sequences

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

- 16 May – 20 May, Developments in Quantitative Finance: Monte Carlo Methods, Isaac Newton Institute for Mathematical Sciences, Cambridge
- 10 Oct – 14 Oct, International Workshop on Sequence Design and its Applications in Communications, Shimonoseki (Yamaguchi, Japan)

Scientific Talks

- 26 Jan, RICAM GROUP SEMINAR - Financial Mathematics: Digital Nets in Analytical, Algebraical and Combinatorial Context - From Numerical Integration via Infinite Finite Field Extensions to Infinite Latin Squares
- 7 Jul, University Salzburg, Workshop on digital nets: A small taxonomy of digital nets
- 8 Jul, RICAM GROUP SEMINAR - Financial Mathematics: A Brownian path construction by Walsh functions
- 24 Oct, RICAM GROUP SEMINAR – Financial Mathematics: QMC: high dimensional point sets, well distributed, widely related
- 5 Dec, RICAM GROUP SEMINAR - Financial Mathematics: A Malliavin calculus for the discrete time setting

**Publications 2005**Appeared

1. H. Maharaj, G.L. Matthews, G. Pirsic, Riemann-Roch spaces of the Hermitian function field with applications to algebraic geometry codes and low-discrepancy sequences. *J. Pure Appl. Algebra* 195 (2005), no. 3, 261—280

Accepted

2. J. Dick, G. Pirsic, F. Pillichshammer, Cyclic digital nets, hyperplane nets and multivariate integration in weighted Sobolev spaces, *SIAM Journal on Numerical Analysis*, to appear.

Submitted

3. G. Pirsic, A small taxonomy of integration node sets

***Dr. Jörn Sass*****Scientific Achievements 2005**

In 2005 the work of Dr Sass was focused on portfolio optimization under transaction costs, under partial information, and on parameter estimation in Markov switching models.

Usually transaction costs are defined in three different ways: proportionally to the volume of trade (proportional cost), proportionally to the portfolio value (fixed cost) or consisting of a constant component (constant cost) and proportional cost. In [1] the utility maximization of the terminal wealth in the discrete time CRR model is treated for very general utility functions and fees which cover combinations of all these cost structures. In a cooperation with Prof Schäl it is shown in a general discrete-time model with proportional transaction costs that a numeraire portfolio exists (in preparation). In continuous time [2] considers a combination of fixed and proportional costs. For a suitable class of stationary trading strategies the asymptotic growth rate is maximized using renewal theoretic arguments. The surprising result that an optimal solution exists under very weak conditions is shown in [5].

Further progress has been made in a joint work with Prof Kunisch on the computation of the boundaries of the trading regions for proportional transaction costs and finite time horizon. The procedure for the 1-dimensional case is implemented and now the multi-dimensional case is looked at.

Portfolio optimization under partial information deals with the case that the possibly stochastic appreciation rates of the stocks (drift of the stock returns) cannot be observed, the stock prices are the only information an investor has available. For the drift as a continuous time Markov chain, in [3] the utility maximization problem is solved for a shortfall constraint on the expected loss in utility. And in [4], convex constraints are imposed on the strategies which yield more robust strategies. In fact the computation of optimal portfolio policies is the aim of the FWF project P17947 which started in February and which is lead by Dr. Sass. In this project, current work with DI Puschögl deals with non-constant volatility models under partial information.

Another part of the project includes parameter estimation in these hidden Markov models which can be generalized to Markov switching models. In [6] a method of moments combined with a linear regression is used to estimate parameters, in [7] MCMC methods can improve the widely used EM algorithm. This work motivates to improve the results using methods from inverse problems: A related method to estimate parameters in a simple Lévy process is considered with Dr Egger, improvements of the EM algorithm are discussed with Dr Resmerita.

## **Scientific Cooperations**

### Internal (name, topic, publication(s))

- H. Egger, parameter estimation for a simple Lévy process, in progress.
- M. Hahn, parameter estimation in Markov switching models, [7], continued.
- K. Kunisch, numerical solution of free boundary problems arising in finance, in progress.
- W. Puschögl, portfolio optimization for stochastic volatility models under partial information, advanced.
- E. Resmerita, EM algorithm for infinite dimensional filters, discussed

### External (name, affiliation, topic, publication(s))

- R.J. Elliott, University of Calgary, method of moments for Markov switching models, [6].
- S. Frühwirth-Schnatter, JKU Linz, MCMC methods for Markov switching models, [7], continued.
- Gabih, Universität Leipzig, utility maximization under risk constraints, [3], in progress.
- U.G. Haussmann, UBC Vancouver, portfolio optimization under partial information, Lévy processes, advanced.
- Irle, Universität Kiel, portfolio optimization under transaction costs, [2,5], continued.
- V. Krishnamurthy, UBC Vancouver, method of moments for Markov switching models, [6].
- M. Schäl, Universität Bonn, Numeraire portfolio under transaction costs, advanced.
- R. Wunderlich, FH Zwickau, Utility maximization under risk constraints, [3], in progress.

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

### Conferences

- GAMM-Workshop "Stochastische Modelle und Steuerung", Moritzburg, Germany, March 15-18.Talk: Portfolio Optimization under Partial Information: An HMM for Stock Returns with Jumps.
- Stochastic Calculus and its Applications to Quantitative Finance and Electrical Engineering, Calgary, Canada, July 24-27.Talk: Portfolio Optimization under Partial Information: An HMM for Stock Returns with Jumps.
- Second Brazilian Conference on Statistical Modelling in Insurance and Finance, Maresias, Brazil, August 28-September 3.Talk: Utility maximization with bounded shortfall risk in an HMM for the stock returns.

- Operations Research 2005, Bremen, Germany, September 7-9. Talk: Portfolio optimization under partial information and convex constraints in a hidden Markov model.
- Mathematik 2005 Klagenfurt, Austria, September 18-23. Talk: Improved portfolio policies under partial information.
- PRisMa 2005: One-Day Workshop on Portfolio Risk Management, TU Vienna, Austria, September 26. Invited talk: Reducing the risk of optimal portfolio policies.

**Scientific Visits**

- Mathematisches Seminar, Universität Kiel, Germany, June 21.
- Institut für angewandte Mathematik, Universität Bonn, Germany, June 22-24.
- Department of Mathematics, UBC, Vancouver, Canada, July 28-August 4.
- Institute of Financial and Actuarial Mathematics, TU Wien, Austria, December 13.
- Department of Mathematics, Fraunhofer IWTM, Kaiserslautern, Germany, November 2-4.

**Scientific Talks**

Talks at conference and workshops are listed under 'Conferences' above.

- Optimality of good portfolio policies under fixed and proportional transaction costs. Invited talk at Department of Mathematics, Fraunhofer IWTM, Kaiserslautern, Germany, November 3.

**Lectures**

Personenversicherung (life insurance mathematics), winter 2005/6, JKU Linz

**Publications 2005****Appeared**

1. J. Sass (2005): Portfolio optimization under transaction costs in the CRR model. Mathematical Methods of Operations Research 61, 239-259.
2. A. Irle, J. Sass (2005): Good portfolio strategies under transaction costs: A renewal theoretic approach. In: M. Do Rosário Grossinho, A.N. Shiryaev, M.L. Esquivel, P.E. Oliveira (eds.): Stochastic Finance, Springer, New York, 321-341.
3. A. Gabih, J. Sass, R. Wunderlich (2005): Utility maximization with bounded shortfall risk in an HMM for the stock returns. In: N. Kolev, P. Morettin (eds.): Proceedings of the Second Brazilian Conference on Statistical Modelling in Insurance and Finance, Maresias, August 28 -- September 3, 2005, Institute of Mathematics and Statistics, University of São Paulo, 116-121.

**Accepted**

4. J. Sass: Portfolio optimization under partial information and convex constraints in a hidden Markov model, to appear in Operations Research 2005 Proceedings.

**Submitted**

5. A. Irle., J. Sass: Optimal portfolio policies under fixed and proportional transaction costs.
6. R. J. Elliott, V. Krishnamurthy, J. Sass: Moment based regression algorithm for drift and volatility estimation in continuous time Markov switching models.
7. M. Hahn, S. Frühwirth-Schnatter, J. Sass: Markov chain Monte Carlo methods for parameter estimation in multidimensional continuous time Markov switching models.

***Dr. Klaus Scheicher*****Introduction**

Dr. Scheicher's research field are quasi Quasi Monte Carlo (QMC) Algorithms and their applications to Mathematical Finance. This research area gives a link between number theory and applied mathematics. QMC algorithms may be used for problems in numerical integration and optimization. Asymptotically, QMC algorithms provide better rates of convergence than Monte Carlo methods; however, there are several restrictions to be considered. One actual research topic is the application of these concepts to the simulation of stochastic processes.

**Scientific Achievements 2005**

Discretization methods to simulate stochastic differential equations belong to the main tools in mathematical finance. For Ito processes, there exist several Euler- or Runge-Kutta-type methods which are analogues of well known approximation schemes in the non-stochastic case. However, in the multidimensional case, there appear several difficulties, caused by the mixed second order derivatives. These mixed terms (or more precisely their differences) correspond to special random variables called Levy area terms. Generating samples from their distribution is a challenging simulation problem. In [6], a method to approximate such random variables is proposed. This new concept seems to be a promising approach for the application of QMC methods as well as variance reduction techniques.

The papers [1,2] are dealing with generalizations of the b-ary expansion of real numbers, i.e. canonical number systems (CNS) and beta-expansions. Recently, a unified notation for both of these concepts, so called Shift Radix Systems (SRS) was introduced. In [2], geometric properties of the tilings giving the Markoff partitions of the dynamical systems associated to these number systems were studied. In [4], a symmetric version of SRS was studied. In [3], the theory of beta-expansions was transferred to algebraic function fields. Some results have been proved that correspond to open problems in the real case. Analogous results for CNS will be proved in [5].

**Scientific Visits**

|               |                    |                                      |
|---------------|--------------------|--------------------------------------|
| 5. April      | Montanuniv. Leoben |                                      |
| 15.-21. May   | Cambridge          | Developments in Quantitative Finance |
| 19.-23. Sept. | Klagenfurt         | ÖMG Tagung                           |

**Scientific Talks**

|           |            |   |
|-----------|------------|---|
| 5. April  | Leoben     | Number systems with positive characteristic |
| 13. April | RICAM      | From number systems to shift radix systems  |
| 22. Sept. | Klagenfurt | Number systems with positive characteristic |
| 21. Oct.  | RICAM      | Number systems and fractal tilings          |

Lecture

Monte Carlo Simulation in der Finanzmathematik (JKU Linz, WS 05/06)

**Scientific Cooperations**Internal Cooperations

T. Beck (Symbolic Computation Group): Algebra

External Cooperations

H.Brunotte (Düsseldorf):Algebra  
 S. Akiyama (Univ. Niigata, Japan): Algebra  
 J. Thuswaldner (Montanuniv. Leoben): Algebra

**Publications**Accepted

1. S. Akiyama, K. Scheicher, From number systems to shift radix systems, to appear in Nihonkai Math. J.
2. S. Akiyama, K. Scheicher, Intersecting two dimensional fractals with lines, to appear in Acta Sci. Math. (Szeged).
3. K. Scheicher, Beta-expansions in algebraic function fields over finite fields, to appear in Finite Fields Appl.

Submitted

4. S. Akiyama, K. Scheicher, Symmetric shift radix systems and finite expansions, submitted to Theoret. Comput. Sci.

Work in progress

5. T. Beck, H. Brunotte, K. Scheicher, J. Thuswaldner, Number theoretical tilings in function field spaces.
6. K. Scheicher, Efficient simulation of Levy areas.
7. K. Scheicher, Metric properties of Ostrogradskii's second algorithm for Laurent series.

***Univ.-Doz. Dr. Arne Winterhof*****Scientific Achievements 2005**

Dr. Winterhof led the FWF project S8313 (Number theoretic methods in cryptography and pseudorandom number generation, employees: Univ.-Doz. Dr. W. Meidl, Mag. N. Brandstätter and Mag. C. van de Woestijne).

In 2005 Dr. Winterhof's research focused on pseudorandom number generation (in view of quasi-Monte Carlo applications to financial mathematics), cryptography and exponential sum applications to quantum computation.

Nonlinear pseudorandom number generation

Nonlinear methods are attractive alternatives to linear methods for the generation of pseudorandom numbers. In [14,15] Mag. El Mahassni, Prof. Shparlinski (both Macquarie University Sydney) and Dr. Winterhof extended results on the distribution of pseudorandom numbers obtained from nonlinear congruential generators modulo a prime to composite modulus. In particular, they proved a stronger discrepancy bound 'on average' over all initial values which was even new in the case of prime modulus. The proofs are based on new bounds on exponential sums. In the case of inversive congruential generators with power of 2 modulus Prof. Niederreiter (NU Singapore) and Dr. Winterhof proved a much better discrepancy bound in [8]. These authors analysed the distribution of some new explicit nonlinear generators in [7,26], as well.

The linear complexity is a quality measure for the intrinsic structure of pseudorandom numbers. As discrepancy bounds, lower bounds on the linear complexity of an arbitrary nonlinear congruential generator are rather weak. Essential improvements for some special nonlinear generators with Dickson polynomials and Redei functions are given by Prof. Aly (Cairo University), Dr. Meidl (since September Sabanci University Istanbul) and Dr. Winterhof in [12,18]. The article [9] of Prof. Niederreiter and

Dr. Winterhof deals with the existence problem of some special permutations called R-orthomorphisms which are suitable to construct nonlinear pseudorandom numbers with small discrepancy.

Nonlinear generators of higher order provide longer periods. Prof. Topuzoglu (Sabanci University Istanbul) and Dr. Winterhof proved lower bounds on the linear complexity of these generators in [11]. Dr. Meidl and Dr. Winterhof studied multisequences of explicit inversive generators in [6]. Their results imply that these generators are highly suitable for parallelization.

A survey article on recent developments on pseudorandom sequences for quasi-Monte Carlo methods and cryptography was written by Prof. Topuzoglu and Dr. Winterhof [25].

### Cryptographic functions and sequences

The successful research on theoretical results that support the assumption that certain cryptosystems are secure has been continued. In the series of papers [2,17,27] Mag. Brandstätter (RICAM, Financial Mathematics), Dr. Kiltz (University of California, San Diego), Prof. Lange (University of Copenhagen) and Dr. Winterhof proved several lower bounds on functions related to cryptosystems based on the discrete logarithm problem. Dr. Adelmann (TU Braunschweig) and Dr. Winterhof analyzed also functions related to the integer factoring problem in [1]. Prof. Aly and Dr. Winterhof deduced an explicit formula for the interpolation polynomial of the Lucas logarithm. In the series of papers [4,16,19] Mag. Brandstätter, Prof. Garaev, Prof. Luca (both Universidad Morelia, Mexico) and Dr. Winterhof analyzed cryptographic sequences constructed with the Legendre symbol.

In [23,24] Prof. Shparlinski and Dr. Winterhof modified polynomial time algorithms for recovering a 'hidden' element of a finite field if only some partial information is given. These results can be applied to the bit security of cryptosystems based on the discrete logarithm.

Each Boolean function can be naturally regarded as a binary sequence. The nonlinearity is a quality measure for Boolean functions. In [3,22,28] Mag. Brandstätter, Prof. Shparlinski and Dr. Winterhof proved lower bounds on the nonlinearity of Boolean functions corresponding to linear recurrence sequences and sequences with small autocorrelation, respectively.

### Exponential sums and their application to quantum computing

By Kerckhoff's principle, the security of a cryptosystem shall not be based on keeping the algorithm secret but solely on keeping the key secret. The security of many cryptographic sequences is only based on a secret period. In [20] Dr. Piroi (RICAM, Symbolic Computation) and Dr. Winterhof proved the existence of a polynomial time quantum algorithm for the period finding problem for all binary sequences with moderate autocorrelation. In [10] Prof. Shparlinski and Dr. Winterhof investigated the same problem for nonbinary sequences and showed that even only a few bits of the sequence elements are enough to determine the period of a sequence of moderate autocorrelation using a quantum algorithm of Hales and Hallgren.

In [5] Prof. Klappenecker (Texas University), Prof. Rötteler (NEC, Princeton), Prof. Shparlinski and Dr. Winterhof constructed complex n-dimensional vector systems which are almost orthogonal and might turn out to be useful for quantum computing. These constructions are based on results of analytic number theory, in particular, on exponential sum bounds. In [21] some of these constructions were improved using exponential sums over elliptic curves.

## Scientific Cooperations

### Internal

N. Brandstätter, W. Meidl (Financial Mathematics): Cryptography and pseudorandom numbers  
 F. Piroi (Symbolic Computation): Quantum period reconstruction  
 C. van de Woestijne (Financial Mathematics): Polynomial equations over finite fields

### External

H. Aly (Cairo): Cryptographic functions and sequences  
 C. Adelmann (Braunschweig): Cryptographic functions  
 A. Klappenecker (Texas): Quantum computing

- 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  
 H. Niederreiter (Singapore): Orthomorphisms, pseudorandom numbers  
 M. Rötteler (Princeton): Quantum computing  
 I. Shparlinski (Sydney): Cryptography, pseudorandom numbers, quantum algorithms  
 A. Topuzoglu (Istanbul): Pseudorandom numbers

**Lectures, Conferences, Scientific Visits and Talks**Lectures

- Winter term 04/05: Pseudorandom number generation (JKU Linz)  
 Summer term 05: Coding theory (JKU Linz)  
 Winter term 05/06: Cryptography (JKU Linz)

Conferences

- OeMG/DMV conference, Klagenfurt, invited talk in special session on cryptography: Linear complexity and related quality measures for cryptographic sequences  
 Workshop on Coding and Crpytography, Bergen (Norway), talk: Interpolation of functions related to RSA and factoring

Scientific Visits

- Sabanci University Istanbul: two weeks

Invited Scientific Talks

- TU Munich: Linear complexity and related complexity measures for sequences  
 Uni Düsseldorf: Number theoretic methods for geneation and analysis of pseudorandom numbers  
 TU Vienna: New results on the linear complexity of nonlinear pseudorandom number generators

**Publications 2005**Appeared

1. C. Adelmann and A. Winterhof, Interpolation of functions related to the integer factoring problem (Extended abstract), Workshop on Coding and Cryptography (WCC) 2005, 62--70.
2. N. Brandstätter, T. Lange and A. Winterhof, Interpolation of the discrete logarithm in finite fields of characteristic two by Boolean functions (Extended abstract), Workshop on Coding and Cryptography (WCC) 2005, 47--54.
3. N. Brandstätter and A. Winterhof, Nonlinearity of binary sequences with small autocorrelation, Proceedings of the Second International Workshop on Sequence Design and its Applications in Communications (IWSDA'05), 44--47.
4. N. Brandstätter and A. Winterhof, Some notes on the two-prime generator, IEEE Transactions on Information Theory 51 (2005), 3645—3657.
5. A. Klappenecker, M. Rötteler, I. Shparlinski and A. Winterhof, On approximately symmetric informationally complete positive operator-valued measures and related systems of quantum states, Journal of Mathematical Physics 46 (2005), no.8, 082104, 17pp.
6. W. Meidl and A. Winterhof, On the joint linear complexity profile of explicit inversive multisequences, Journal of Complexity 21 (2005), 324—336.
7. H. Niederreiter and A. Winterhof, On the distribution of some new explicit nonlinear congruential pseudorandom numbers, in T. Helleseth et al. eds.: Sequences and Their Applications-SETA 2004, Lecture Notes in Computer Sciences 3486 (2005), 266--274.

8. H. Niederreiter and A. Winterhof, Exponential sums and the distribution of inversive congruential pseudorandom numbers with power of two modulus, *International Journal of Number Theory* 1 (2005), 431–438.
9. H. Niederreiter and A. Winterhof, Cyclotomic R-orthomorphism of finite fields, *Discrete Mathematics* 295 (2005), 161–171.
10. I. Shparlinski and A. Winterhof, Quantum period reconstruction of noisy sequences, (extended abstract), *EQIS'05*, 7–8.
11. A. Topuzoglu and A. Winterhof, On the linear complexity profile of nonlinear congruential pseudorandom number generators of higher orders, *Applicable Algebra in Engineering, Communication and Computing* 16 (2005), 219–228.

Accepted

12. H. Aly and A. Winterhof, On the linear complexity profile of nonlinear congruential pseudorandom number generators with Dickson polynomials, *Designs, Codes and Cryptography*.
13. H. Aly and A. Winterhof, Polynomial representations of the Lucas logarithm, *Finite Fields and Their Applications*.
14. E.D. El-Mahassni, I. Shparlinski and A. Winterhof, Distribution of nonlinear congruential pseudorandom numbers for almost squarefree integers, *Monatshefte für Mathematik*.
15. E. D. El-Mahassni and A. Winterhof, On the distribution of nonlinear congruential pseudorandom numbers in residue rings, *International Journal of Number Theory*.
16. 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*.
17. E. Kiltz and A. Winterhof, Polynomial interpolation of cryptographic functions related to Diffie-Hellman and discrete logarithm problem, *Discrete Applied Mathematics*.
18. W. Meidl and A. Winterhof, On the linear complexity profile of nonlinear congruential pseudorandom number generators with Redei functions, *Finite Fields and Their Applications*.
19. W. Meidl and A. Winterhof, Some notes on the linear complexity of Sidelnikov-Lempel-Cohn-Eastman sequences, *Designs, Codes and Cryptography*.
20. F. Piroi and A. Winterhof, Quantum period reconstruction of binary sequences, *Proceedings AAECC 16*, to appear.
21. I. Shparlinski and A. Winterhof, Constructions of approximately mutually unbiased bases, *Proc. LATIN'06*, to appear.
22. I. Shparlinski and A. Winterhof, On the nonlinearity of linear recurrence sequences, *Applied Mathematics Letters*.
23. I. Shparlinski and A. Winterhof, On the linear complexity of bounded integer sequences over different moduli, *Information Processing Letters*.
24. I. Shparlinski and A. Winterhof, Noisy interpolation of sparse polynomials in finite fields, *Applicable Algebra in Engineering, Communication and Computing*.
25. A. Topuzoglu and A. Winterhof, Pseudorandom sequences, in *Topics in Geometry, Cryptography and Coding Theory*, Springer, Berlin, to appear.
26. A. Winterhof, On the distribution of some new explicit inversive pseudorandom numbers and vectors, *Proceedings MC2QMC 2004*.

Submitted

27. N. Brandstätter and A. Winterhof, Approximation of the discrete logarithm in finite fields of even characteristic by real polynomials.
28. N. Brandstätter and A. Winterhof, Linear complexity profile of binary sequences with small correlation measure.

**Nina Brandstätter**

Mag. Brandstätter has been employed as a PhD student in the FWF project S83 (Numbertheoretic algorithms and applications) since April 2004.

**Scientific Achievements 2005**

In 2005 Mag. Brandstätter's research focused on cryptographic functions and sequences.

In [1] Mag. Brandstätter, Prof. Lange (University of Copenhagen) and Dr. Winterhof proved a lower bound on the nonlinearity of Boolean functions describing 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 [2,5] Mag. Brandstätter and Dr. Winterhof proved lower bounds on the nonlinearity of Boolean functions in terms of the autocorrelation of the corresponding sequence.

In [3] Mag. Brandstätter and Dr. Winterhof analyzed the autocorrelation of a particular interesting cryptographic sequence, the two prime generator.

In [4] Mag. Brandstätter and Dr. Winterhof proved complexity lower bounds on real polynomials representing the discrete logarithm in a finite field of characteristic two.

**Scientific Cooperations**Internal

Dr. Winterhof (Financial Mathematics): Cryptographic functions and sequences

External

T. Lange (Kopenhagen): Boolean functions

I. Shparlinski (Sydney): Cryptography

A. Topuzoglu (Istanbul): Pseudorandom numbers

**Conferences, Scientific Visits and Talks**Conferences

Workshop on Coding and Crpytography, Bergen (Norway), Talk: Interpolation of the discrete logarithm in a finite field of characteristic two

International Workshop on Sequence Design and Applications, Yamaguchi (Japan), Talk: Nonlinearity of binary sequences with small autocorrelation

Scientific Visits

Sabanci University Istanbul: one week

**Publications 2005**Appeared

1. N. Brandstätter, T. Lange and A. Winterhof, Interpolation of the discrete logarithm in finite fields of characteristic two by Boolean functions (Extended abstract), Workshop on Coding and Cryptography (WCC) 2005, 47--54.
2. N. Brandstätter and A. Winterhof, Nonlinearity of binary sequences with small autocorrelation, Proceedings of the Second International Workshop on Sequence Design and its Applications in Communications (IWSDA'05), 44--47.
3. N. Brandstätter and A. Winterhof, Some notes on the two-prime generator, IEEE Transactions on Information Theory 51 (2005), 3645—3657.

**Submitted**

4. N. Brandstätter and A. Winterhof, Approximation of the discrete logarithm in finite fields of even characteristic by real polynomials.
5. N. Brandstätter and A. Winterhof, Linear complexity profile of binary sequences with small correlation measure.

***Markus Hahn*****Work before joining RICAM**

After graduating at the University Linz in October 2003 with his diploma thesis on option pricing under transaction costs which was supervised by Prof Larcher and for which he received the Ludwig-Scharinger-Award 2004, DI Hahn was employed at the Institute for Financial Mathematics at University Linz from November 2003 until January 2005, financed by the FWF project S 8305. Working on his Ph.D., he has been concerned with portfolio optimisation under partial information, with a special interest on related parameter estimation problems. Since February 2005 he is working in the Financial Mathematics Group (in the FWF project P17947, Dr Sass).

**Scientific Achievements 2005**

In 2005, DI Hahn was mainly concerned with parameter estimation in Markov switching models using Markov chain Monte Carlo (MCMC) methods. In this problem, the widely used expectation maximization algorithm turns out not to be successful when dealing with parameters as encountered in financial time series. In cooperation with Prof Frühwirth-Schnatter and Dr Sass, DI Hahn developed a continuous time algorithm as well as an approximating discrete time method providing stable results for historical financial data.

**Scientific Cooperations****Internal**

Cooperation with DI Putschögl and Dr Sass within the FWF project.

**External**

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

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

- Tutorial on Bayesian Statistics and Marketing, Institute for Applied Statistics, Johannes Kepler University Linz, Austria, September 19--20.
- Mathematik 2005, Annual Meeting of the Austrian Mathematical Society, Klagenfurt, Austrian Mathematical Society, September 18--23. Talk: MCMC Methods for Parameter Estimation in an HMM-Model for Stock Returns.
- Workshop on Model Choice and Validation, Sonderforschungsbereich 386 "Statistical Analysis of Discrete Structures", Munich, Germany, October 6--8. Poster presentation: MCMC Methods for Parameter Estimation in continuous time Markov switching stock models.
- Fraunhofer-HVB-Finance-Tagung für den wissenschaftlichen Nachwuchs, Fraunhofer ITWM and Hypo Vereinsbank, Kaiserslautern, Germany, October 13--14. Invited talk: MCMC Methods for Parameter Estimation in an HMM-Model for Stock Returns.

**Lectures**

Financial Mathematics project at "Applied mathematics week" for intellectually gifted high school pupils organised by "Stiftung Talente", February 2005.

**Publications 2005****Submitted**

1. M. Hahn, S. Frühwirth-Schnatter, J. Sass: Markov chain Monte Carlo methods for parameter estimation in multidimensional continuous time Markov switching models.

***Univ.-Doz. Dr. Wilfried Meidl*****Scientific Achievements 2005**

Dr. Meidl was part of the group until August 2005 (employed in the FWF project S8313 "Number theoretic methods in cryptography and pseudorandom number generation", leader Dr. Winterhof). He then accepted a position as a lecturer at Sabanci University of Istanbul.

His research in 2005 focused on cryptographic functions. For the papers [2,6,7] see Dr. Winterhof.

In [1] an exact formula for the expected 1-error linear complexity of a  $2^n$  periodic binary sequence was given.

In [3] the linear complexity of a multisequence and the linear complexity of a corresponding single sequence over an extension field are compared.

The paper [4] presents enumeration results on the linear complexity profile and the related lattice profile, a complexity measure based on Marsaglia's lattice test, of sequences over finite fields. In particular the number of sequences with prescribed profiles is calculated. In [5] a survey of several features of the linear complexity profile and the lattice profile is given. Moreover, a relationship is utilized to completely describe the lattice profile of sequences over a finite field in terms of the continued fraction expansion of its generating function.

**Scientific Cooperations**

N. Brandstätter, A. Winterhof (Financial Mathematics): Cryptography and pseudorandom numbers

**Talks****Invited Scientific Talks**

University Klagenfurt: Linear complexity, a measure for the quality of sequences for stream ciphers  
 TU Vienna: New results on the linear complexity of nonlinear pseudorandom number generators

**Publications 2005****Appeared**

1. W. Meidl, On the stability of  $2^n$  periodic binary sequences, IEEE Trans. Inform. Theory 51 (2005), 1151—1155.
2. W. Meidl and A. Winterhof, On the joint linear complexity profile of explicit inversive multisequences, Journal of Complexity 21 (2005), 324—336.
3. W. Meidl, Discrete Fourier transform, joint linear complexity and generalized linear complexity of multisequences, Proceedings of SETA'04, Lecture Notes in Computer Science 3486 (T. Helleseth et al., eds), Springer-Verlag, Berlin Heidelberg, 2005, 101—112.

Accepted

4. W. Meidl, Enumeration results on linear complexity profiles and lattice profiles, JoC, to appear.
5. W. Meidl, Continued fraction for formal Laurent series and the lattice structure of sequences, AAECC, to appear.
6. W. Meidl and A. Winterhof, On the linear complexity profile of nonlinear congruential pseudorandom number generators with Redei functions, Finite Fields and Their Applications.
7. W. Meidl and A. Winterhof, Some notes on the linear complexity of Sidelnikov-Lempel-Cohn-Eastman sequences, Designs, Codes and Cryptography.

***Wolfgang Putschögl*****Work before joining RICAM**

Wolfgang Putschögl completed his Diploma in 'Technische Mathematik' in January 2005 at the Johannes Kepler University Linz. His diploma thesis on 'optimal investment and consumption with transaction costs' was supervised by Prof Larcher. Since March 2005 he is a Ph.D student in the Group Financial Mathematics at the RICAM supported by the FWF project P 17947-N12, 'Computing Optimal Portfolio Policies under Partial Information', project leader is Dr Sass.

**Scientific Achievements 2005**

In 2005 the work of DI Putschögl was focused on the computation of optimal trading strategies in the context of utility maximization under partial information for different non-constant volatility models, e.g. the CEV model and the Hobson-Rogers model. These explicitly derived strategies were applied to simulated and market data. DI Putschögl gave several talks on his results and received the 'best conference talk award' at the Fraunhofer-HVB-Finance Workshop for young scientists.

**Scientific Cooperations**Internal

Cooperation with DI Hahn and Dr Sass within the FWF project.

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

- Tutorial on Bayesian Statistics and Marketing, Institut für angewandte Statistik (IFAS), Linz, Austria, September 19-21.
- Mathematik 2005 Klagenfurt, Austria, September 18-23. Talk: Portfolio optimisation under partial information.
- PRisMa 2005 Workshop on Portfolio Risk Management, Institute for Financial and Actuarial Mathematics (FAM), Vienna, Austria, September 26.
- Fraunhofer-HVB-Finance Workshop für den wissenschaftlichen Nachwuchs, Kaiserslautern, Germany, October 12-13. Invited talk: Optimal portfolio policies under partial information using stochastic volatility models.

Lectures

Finanzmathematik 1 (Financial mathematics I), winter 2005/6, FH-Linz

## Publications 2005

### Submitted

A joint paper with DI Hahn and Dr Sass on utility maximization with non-constant volatility models and partial information will be submitted shortly.

## *Christiaan van de Woestijne*

### Work before joining RICAM

Mag. van de Woestijne has been working in a Ph.D. project at University of Leiden, under supervision of Prof. H.W. Lenstra, Jr.. He has been employed in the FWF project S8313 (Number theoretic methods in cryptography and pseudorandom number generation, leader Dr. Winterhof) since October 2005. His main research interests are number theory, finite fields, symbolic computation, complexity of algorithms and combinatorics.

## Scientific Achievements 2005

Mag. van de Woestijne obtained one of two Distinguished Student Author Awards, awarded by the ACM Special Interest Group on Symbolic and Algebraic Manipulation.

In 2005 Mag. van de Woestijne finished redaction of his Ph.D. thesis on deterministic algorithms for solving equations over finite fields. He applied results of his thesis to construct an efficient deterministic algorithm for finding rational points on elliptic curves over finite fields, a problem that has been open for at least 20 years. Moreover, he started joint work with Dr. Winterhof on Waring's problem in finite fields, diagonal equations over finite fields and applications to coding theory. Moreover, he started intensive discussions with Prof. Schicho (symbolic computation) on rational parametrisations of algebraic surfaces with a rational pencil.

## Scientific Cooperations

### Internal

Dr. Winterhof (Financial Mathematics): finite fields and coding theory

Prof. Schicho (Symbolic Computation): rational parametrisation of algebraic surfaces

### External

Prof. Lenstra (University of Leiden): deterministic algorithms in algebra and algebraic geometry

## Participation at Conferences, Scientific Visits and Talk

### Conferences

ISSAC 2005, Beijing (China): obtained one of two Distinguished Student Author Awards, awarded by the ACM Special Interest Group on Symbolic and Algebraic Manipulation

### Scientific Talks

Algebraic Geometry Seminar of the Symbolic Computation group at RICAM: Deterministic equation solving over finite fields

Zahlentheoretisches Kolloquium at TU Graz (invited talk): Deterministic equation solving over finite fields

**Publications 2005**Appeared

1. Christiaan van de Woestijne, Deterministic equation solving over finite fields. Proc. ISSAC 05, Beijing, China, ACM press (2005), 348--353.

Submitted

2. Ph.D. thesis “Deterministic equation solving over finite fields”, submitted for defence in 2006.

## 2.5. GROUP “ANALYSIS OF PARTIAL DIFFERENTIAL EQUATIONS”

### **Group Leaders:**

o.Univ.-Prof. Dr. Peter Markowich  
Univ.-Prof. Dr. Christian Schmeiser

### **Researchers funded via ÖAW/Upper Austrian government funds:**

Dr. Shun-Yin Henry Chu  
Dr. Marco Di Francesco  
Dr. Yasmin Dolak-Struß  
Dr. Arjan Kuijper (half-time employed at RICAM)  
Dr. Lukas Neumann

### ***Introduction by Group Leader Prof. Peter Markowich***

In 2005, the composition of the group and the scientific orientation changed partially. N. Matevosyan left RICAM, and two new PostDocs, A. Kuijper and L. Neumann, have been employed. Using the expertise of A. Kuijper, a new research subject is the analysis of partial differential equations occurring in computer vision. This will create new cooperations within RICAM and with a new activity of P. Markowich in Vienna. The other new PostDoc, L. Neumann, recently obtained his PhD in Vienna and works in one of the central research areas of the group leaders, the asymptotic analysis of kinetic transport equations. Both new PostDocs are already involved in international cooperations which will be continued.

The work of Y. Dolak-Struss is in the field of Mathematical Biology. Particularly noteworthy is a new RICAM internal cooperation activity with the group 'Inverse Problems' concerning parameter estimation in chemotaxis models. The work of S.Y. Chu on asymptotic behaviour of the Cahn-Hilliard equation is also pursued within an internal cooperation. Mathematically, it is connected to some of the work of Y. Dolak-Struss on singular limits for convection dominated chemotaxis models.

The group leaders have, besides their research work, been involved in the early stages of planning a special semester on 'Mathematics in the Life Sciences' at RICAM.

The research work of the PostDocs is detailed in the following sections.

### ***Dr. Shun-Yin Chu***

#### **Scientific Achievements 2005**

S.Y. Chu worked on developing several interesting problems of anisotropic flows, such as evolution of phase transitions, dynamical movements of bubbles, asymptotic behaviour of the solutions, and vanishing viscosity problems of the the Cahn-Hilliard equation.

For asymptotics in time of the Cahn-Hilliard equation, he derived different kinds of formal approximations by matching asymptotic methods, such as in several dimensional domains. Also he considered various perturbations of stationary solutions in the one-dimensional case and explored the stability of the solution and evolution patterns of parts of high frequency oscillations. He found that the asymptotic structure of the one-dimensional Cahn-Hilliard equation is somehow similar to the solution of the 4-Laplacian diffusion equation. A cooperation related to this problem with Martin Burger, Peter Markowich and Carola Schoenlieb started.

For matching problems by phase transition of one-dimensional solutions of the Cahn-Hilliard equation, compared with work by Carlen, Carvalho, Orlandi, he analyzed solutions with special behaviour at critical second order viscous growth time, where small amplitude oscillations and blowup on an anisotropic curve may appear in this time scale region. A series of estimates of fourth order linearized elliptic operators was investigated.

### **Scientific Cooperations**

#### Internal

Dr. Martin Burger  
Prof. Dr. Peter Markowich  
Prof. Dr. Christian Schmeiser

#### External

Carola Schoenlieb, Technische Universität Wien

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

#### Conferences

Conference on nonlinear PDEs in honor of Luis Caffarelli, Vienna, 24-25 October 2005

### **Publications 2005**

#### Submitted

1. Chu, Shun-Yin: Global Existence of Weak Solutions to 3-D Axisymmetric Prandtl's System with Positive Swirls

### ***Dr. Marco Di Francesco***

#### **Introduction**

Marco Di Francesco's research area concerns linear and nonlinear diffusion equations of various types, with special interest for those arising from nonlinear friction phenomena and from population dynamics. He is also interested in nonlinear conservation laws and other problems arising from gas dynamics and semiconductor devices.

Dr. Marco Di Francesco left RICAM in August 2005. He is now research associate at the University of L'Aquila (Italy).

### **Scientific Achievements 2005**

#### 1. Nonlinear diffusion and optimal transportation.

A classical problem in nonlinear diffusion is detecting typical asymptotic states for large times. In the case of the classical porous medium equation, this problem goes back to the 50' since the work of Barenblatt and Zel'dovich. The problem of improving the rate of convergence towards self-similarity has been of great interest in the recent years, thanks to the emergence in this field of the use of optimal transportation tools and of Wasserstein distances. In collaboration with José Carrillo (University of Barcelona) and Giuseppe Toscani (University of Pavia), an improved rate by mass-centering towards Barenblatt profiles has been obtained by means of new ideas concerning the quadratic Wasserstein distance.

When the nonlinearity function in the diffusion equation is not a power (and it hasn't a power-like behaviour near vacuum), the use of the Wasserstein distance has lead to characterize new asymptotic

states as fixed points of certain renormalization maps. Improvements in this direction have been carried out in collaboration with José Carrillo and Maria Gualdani.

## 2. The Keller-Segel model of chemotaxis with prevention of overcrowding: linear vs nonlinear diffusion.

In collaboration with Yasmin Dolak Struss and Martin Burger, we have performed a detailed studied of a Keller-Segel model with volume filling effect on the whole space. Existence results have been supplemented with a qualitative study of the solutions and with a parallel analysis of the asymptotic behaviour in case of linear and nonlinear diffusion. The introducement of nonlinear diffusion in this subject is quite new in the literature, and it has been recently physically justified. The existence of stationary solutions in a small diffusive regime and the decay of solutions for large diffusions have been proven, whereas the non-existence of stationary solutions occurs in the linear case. In the latter case, we prove intermediate decay to heat-gaussian states. The main technique used relies on several entropy functionals.

## 3. Nonlinear scalar conservation laws.

In collaboration with Corrado Lattanzio (University of L'Aquila) and José Carrillo, a stability result for scalar conservation law with respect to a certain Wasserstein distance has been obtained. It is the first time that optimal transportation tools are used in this context. This result implies also a characterization of the asymptotic states in the spirit of the work performed before for nonlinear diffusions.

## 4. Drift-diffusion-Poisson models \*

In collaboration with Marcus Wunch (University of Vienna), a stability result for the bipolar drift diffusion Poisson model for semiconductor devices has been achieved by use of the Wasserstein distance.

## 5. Population “swarming models” \*

In collaboration with Martin Burger, a systematic study of several models arising in the context of population dynamics with nonlinear diffusion and nonlocal interaction has been performed.

The headings \* concern works under preparation.

## **Scientific Cooperations**

### Internal

Yasmin Dolak Struss, RICAM

### External

Martin Burger, Johannes Kepler University, Linz

José A. Carrillo, University of Barcelona

Maria Pia Gualdani, University of Mainz

Giuseppe Toscani, University of Pavia

Corrado Lattanzio, University of L'Aquila

## **Publications**

### Preprints:

1. J. A. Carrillo, M. Di Francesco and C. Lattanzio, Contractivity of Wasserstein metrics and asymptotic profiles for scalar conservation laws. - Submitted preprint .
2. M. Burger, M. Di Francesco and Y. Dolak, The Keller-Segel model for chemotaxis with prevention of overcrowding: linear vs. nonlinear diffusion. - Submitted preprint .
3. J. A. Carrillo, M. Di Francesco and M. P. Gualdani, Semidiscretization and long-time asymptotics of nonlinear diffusion equations. - Submitted preprint .

**Accepted papers:**

4. J. A. Carrillo, M. Di Francesco and G. Toscani, Strict contractivity of the 2-Wasserstein distance for the porous medium equation by mass-centering. - To appear on Proceedings of the American Mathematical Society.
5. J. A. Carrillo, M. Di Francesco and G. Toscani, Intermediate asymptotics beyond homogeneity and self-similarity: long time behavior for  $ut = \Delta\phi(u)$ . - To appear on Archive for Rational Mechanics and Analysis, Springer.
6. M. Di Francesco, Initial value problem and relaxation limits of the Hamer model for radiating gases in several space variables. - To appear on Nonlinear Differential Equations and Applications (NoDEA).
6. M. Di Francesco and C. Lattanzio, Optimal L1 decay rates to diffusion waves for the Hames model of radiating gases. - To appear on Appl. Math. Letters, Elsevier.

**Attended conferences and schools:**

Summer CIME Course “Calculus of variations and nonlinear differential equations”, Cetraro (Italy), July 2005.

HYKE (EU project) conference in Roma, May 2005.

***Dr. Yasmin Dolak-Struß*****Introduction**

Yasmin Dolak-Struß' research area is the mathematical modeling of cell movement and chemotaxis. A main part of her work in 2005 was dedicated to the analysis and numerical solution of the Keller-Segel model for chemotaxis, which is a drift-diffusion equation for the cell density coupled with an elliptic equation describing the evolution of the chemoattractant. In particular, she was interested in the asymptotic behavior of a special case of this model, accounting for the finite volume of cells and the fact that random movement of cells is often suppressed when a chemical gradient is encountered. Mathematically, this leads to a nonlinear term in the cell flux and a diffusion constant that is small compared to the relevant time and space scales in the problem. Other areas of interest were the identification of chemotaxis parameters from experimental data and the mathematical description of cell movement on the level of individual cells.

**Scientific Achievements 2005****1. The Keller-Segel Model with Volume Filling**

A main topic of research was the analysis of the Keller-Segel model for chemotaxis with volume filling and small diffusion.

In a joint work with M. Burger and M. Di Francesco, the asymptotic behavior of the model for both linear and nonlinear diffusion (with a special choice of the nonlinearity) on unbounded domains was investigated. As it turns out, the long-time behavior of the system depends crucially on the diffusion term. In the linear case, there exist no stationary solutions on unbounded domains, irrespective of the value of the diffusivity. In contrast to this, the asymptotic behavior in the nonlinear case is fully determined by the value of the diffusion constant in the model. Whereas above a threshold value of the diffusivity, all compactly supported solutions are proven to decay asymptotically to zero, below this threshold value, non-decaying solutions do exist and are shown to converge to stationary solutions.

The focus of a joint work with M. Burger and C. Schmeiser was the asymptotic behavior of the model with a linear diffusion term on bounded domains. Of particular interest was the behavior of a certain class of plateau-shaped solutions in multiple space dimensions. For one space dimension, it was shown in a joint work with C. Schmeiser in 2004 that solutions stay exponentially long close to a stationary state, a behavior that is reminiscent of the behavior of phase-separation models like the Cahn-Hilliard

or Allen-Cahn equation. In contrast to this, the behavior in multiple space dimensions occurs on a faster time scale, and can be purely described as the movement of the interface between regions of high and low cell density.

Finally, in a co-operation with V. Calvez, numerical studies of asymptotic behavior of the Keller-Segel model with volume filling term were performed, and results were compared with simulations for the classical Keller-Segel model. As it turns out, the behavior of these two types of chemotaxis models is indeed qualitatively the same.

## 2. Estimation of Chemotactic Parameters using Inverse Methods

The quantification of cell migration parameters has become an important issue for clinicians, especially in the context of leukocyte migration. Clinical investigations of leukocyte chemotaxis are often based on measuring the dependence of different parameters, which are based either on the behavior of individual cells or of the whole cell population. In the latter case, especially the random motility and the sensitivity of cells for the chemical stimulus are important quantities, and various methods to determine these quantities from measurements have been proposed. However, to estimate these parameter values from the data (which is only done by visual comparison of the curves), either some kind of a priori information about the dependence is needed, or the parameters can only be estimated at average values of the signal concentration.

In a joint work with Philipp Kügler, a different approach to this problem is used: using inverse methods, the functional dependence of these quantities on the chemical can be determined systematically. This approach was already tested on self-produced data (in order to compare the obtained results to the true solution, which is known in this case) and to available data from chemotaxis experiments, showing good results. In a next step, the method will also be applied to more complicated experimental setups.

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

- March/Mai 2005: Stay at the Université Paul Sabatier, Toulouse, France
- July 2005: Talk at the European Conference on Mathematical and Theoretical Biology in Dresden, Germany
- September 2005: Talk at the meeting of the Austrian Mathematical Society in Klagenfurt, Austria
- November 2005: Talk at the Workshop on Cell Motility and Cytoskeletal Dynamics at the Wolfgang Pauli Institute, Vienna
- November 2005: Talk at the Bilateral Biomathematics Meeting at the Politecnico di Torino, Italy

## **Scientific Cooperations**

### Internal

Prof. Christian Schmeiser

Prof. Peter Markowich

Marco Di Francesco (Analysis of PDEs)

### External

Martin Burger, Johannes Kepler University, Linz

Vincent Calvez, ENS Paris

Fabio Chalub, Universidade de Lisboa

Philipp Kügler, Johannes Kepler University, Linz

Dietmar Ölz, University of Vienna

Alexander Soreff, TU Vienna

## Publications

### Appeared

1. Y. Dolak, C. Schmeiser: Kinetic models for chemotaxis: Hydrodynamic limits and the back-of-the-wave problem. *J. Math. Biol.* 51(6), pp. 595-615, 2005.
2. Y. Dolak, C. Schmeiser: The Keller-Segel model with logistic sensitivity function and small diffusivity. *SIAM J. Appl. Math.* 66(1), pp. 286-308, 2005.

### Submitted:

3. F. Chalub, Y. Dolak-Struß, P. Markowich, D. Ölz, C. Schmeiser and A. Soreff: Model hierarchies for cell aggregation by chemotaxis (Review article). To appear in M3AS.
4. M. Burger, M. Di Francesco, Y. Dolak-Struß: The Keller-Segel model for chemotaxis with prevention of overcrowding: Linear vs. nonlinear diffusion. RICAM Report 14/2005
5. V. Calvez, Y. Dolak-Struß: The Keller-Segel model with and without density control. Submitted.

## ***Dr. Arjan Kuijper***

### **Work before joining RICAM**

Before joining RICAM, Arjan Kuijper was employed at the IT University of Copenhagen on the European Union sponsored project Deep Structure, Singularities, and Computer Vision (IST-2001-35443).

His work focussed on the development of sophisticated representations of images and shapes by syncretizing principles and methods from scale space theory, singularity theory and algorithmics and to creating efficacious algorithms for solving computer vision tasks on the basis of these.

Most emphasis has been on the application of so-called Symmetry Sets and its relatives in shape description, analysis, and comparison. Besides this, research related to image analysis based on scale space and catastrophe theory was carried out.

### **Scientific Achievements 2005**

The work on Symmetry Sets resulted in a shape descriptor that can be used for indexing, classifying, and comparing shapes [1, 9, 11, 12, 13, 14, 16, 17, and 18]. A related structure, the pre-Symmetry Set [9, 13], has the advantage of a symmetric matrix representation. Several mathematical aspects of this matrix were presented [2], as well as its relationship to the – in shape analysis – well-known skeleton [3].

A case study with respect to extension of the theory to shapes in 3D was presented [4].

As the work on the Symmetry Set is only concerned with the shape at a given resolution (i.e. scale), also the possibility of embedding the shape descriptor in a multi-scale context based on curvature motion was investigated. Results with respect to the changes under the influence of scale, the singularities, and the induced hierarchical structure were presented [5].

The work on Gaussian scale space-based image analysis resulted in a method to derive the scale space hierarchy fast [6, 10]. An investigation of the multi-scale structure of images at critical points in scale space – the scale space saddles – was presented [7].

Current work at RICAM besides abovementioned research includes the analysis other PDE-based image processing methods [15].

### **Scientific Cooperations**

#### Internal

Prof. Dr. Peter Markowich, RICAM/Wolfgang Pauli Institute Vienna, Austria: p-Laplacians [15].

External

Dr. Ole Fogh Olsen, Image group, IT University of Copenhagen, Denmark: Symmetry Sets, singularities, algorithms [1,2,3,4,5,8,9,11,12,13,14]

Prof. Dr. Mads Nielsen, Image group, IT University of Copenhagen, Denmark: Computer Vision, algorithms [9, 12]

Dr. Philip Bille, Theory group, IT University of Copenhagen, Denmark: algorithms [9, 12]

Prof. Dr. Peter Giblin, Dept. of Mathematics, University of Liverpool, United Kingdom: Symmetry Sets and singularities [5, 9, 12].

Dr. Luc Florack, Biomedical Image Analysis, Technical University of Eindhoven, the Netherlands: Scale space [6, 7, 8, and 10].

Prof. Dr. Bart Ter Haar Romeny, Biomedical Image Analysis, Technical University of Eindhoven, the Netherlands: Mathematica programming for scale space implementations [6, 10].

Prof. Dr. Dirk Siersma, Dept. Of Mathematics, Utrecht University, the Netherlands: Symmetry Sets and singularities [5].

L. Muresan, Fuzzy Lab, Hagenberg, Austria: biomedical image analysis.

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

Arjan Kuijper was co-organiser of the First International workshop on Deep Structure, Singularities, and Computer Vision and co-editor of the proceedings [8].

He was member of the program committee of the 5th International Conference on Scale-Space and PDE Methods in Computer Vision, and the First International workshop on Deep Structure, Singularities, and Computer Vision.

In 2005 he was reviewer for the International Conference on Computer Vision (ICCV05) and the European Conference on Computer Vision (ECCV06), the above mentioned conferences, and the journal IEEE Transactions on Image Processing.

Conferences

- First International workshop on Deep Structure, Singularities, and Computer Vision - DSSCV05. Maastricht, the Netherlands, 9-10 June, 2005
- 12th Danish conference on pattern recognition and image analysis -DSAGM05, Copenhagen, August 18-19, 2005.
- 12th IEEE International Conference on Image Processing - ICIP 2005, Genova, Italy, 11-14 September, 2005.
- 5th International Conference on Scale-Space and PDE Methods in Computer Vision (Scale Space 2005), Hofgeismar, Germany, April 7-9, 2005

Scientific Visits

- DSSCV Meeting (Prof. Giblin, Dr. Florack, Prof. Ter Haar Romeny, et al.) Maastricht, the Netherlands, June 8, 2005
- Fuzzy lab (L. Muresan, B. Heise), Hagenberg. December 12, 2005.

Scientific Talks

- Mathematics, Images, and Shapes. Dept. of Mathematics, University of Warwick, United Kingdom. August 2005.
- Images, Shapes, and Mathematics. Wolfgang Pauli Institute, University of Vienna, Austria, September 2005.
- Image analysis considered from a biological and mathematical point of view. Fuzzy lab, Hagenberg, December 2005.

**Publications 2005**Appeared

1. A Symmetry Set Based 2D Shape Descriptor, A.Kuijper, O. F.Olsen.  
12th Danish conference on pattern recognition and image analysis (S.I. Olsen (Ed.), DSAGM05, Copenhagen, August 18-19, 2005), pages 118--125, 2005.
2. Essential Loops and their Relevance for Skeletons and Symmetry Sets, A. Kuijper, O. F. Olsen  
1st International Workshop on Deep Structure, Singularities and Computer Vision - DSSCV05 (Maastricht, the Netherlands, 9-10 June, 2005), LNCS 3753, 24--35, 2005.
3. Geometric Skeletonization using the Symmetry Set, A. Kuijper, O. F. Olsen  
12th IEEE International Conference on Image Processing - ICIP 2005 (Genova, Italy, 11-14 September, 2005), Vol I, 497--500, 2005.
4. Computing 3D Symmetry Sets; A Case Study, A. Kuijper, O. F. Olsen  
1st International Workshop on Deep Structure, Singularities and Computer Vision - DSSCV05 (Maastricht, the Netherlands, 9-10 June, 2005), LNCS 3753, 193--204, 2005.
5. The Structure of Shapes: Scale Space aspects of the (pre-) Symmetry Set, A. Kuijper, O. F. Olsen  
In LNCS 3459 (Proceedings of the 5th International Conference on Scale-Space and PDE Methods in Computer Vision (Scale Space 2005), Hofgeismar, Germany, April 7-9, 2005), pages 291--302, 2005.
6. Exploiting Deep Structure, A. Kuijper  
1st International Workshop on Deep Structure, Singularities and Computer Vision - DSSCV05 (Maastricht, the Netherlands, 9-10 June, 2005), LNCS 3753, 169--180, 2005.
7. Using Catastrophe Theory to Derive Trees from Images, A. Kuijper, L.M.J. Florack  
Journal of Mathematical Imaging and Vision, 23 (3): 219-238, 2005.
8. Deep structure, Singularities, and Computer Vision. Proceedings of the First International Workshop. O.F. Olsen, L.M.J. Florack, and A. Kuijper (Eds.)  
Lecture Notes in Computer Science 3753.

Submitted

9. Alternative 2D Shape Representations using the Symmetry Set, A. Kuijper, O. F. Olsen, P. J. Giblin, and M. Nielsen. Journal paper, submitted 2005.
10. Scale Space Saddles: From Theory to Practice, A. Kuijper  
Journal paper, submitted 2005
11. Shapes, Symmetry Sets, and Matching, A. Kuijper, O.F. Olsen,  
Conference paper, submitted 2005
12. Matching 2D Shapes using their Symmetry Sets, A. Kuijper, O.F. Olsen, P. J. Giblin, and M. Nielsen.  
Conference paper, submitted 2005
13. Describing and Matching 2D Shapes by Their Points of Mutual Symmetry, A. Kuijper, O.F. Olsen,  
Conference paper, submitted 2005
14. Multi-Scale Shape Analysis Using Symmetry Sets, A. Kuijper, O.F. Olsen  
Conference paper, accepted SIAM Conference on Imaging Science, Minneapolis, USA, May 15-17, 2006
15. p-norm PDE's, A. Kuijper, P. Markowich  
Conference paper, accepted SIAM Conference on Imaging Science, Minneapolis, USA, May 15-17, 2006
16. Shapes, Symmetry Sets, and Matching, A. Kuijper, O.F. Olsen.  
Conference paper, submitted 2005.

Technical reports

17. ITU-TR-2005-72 Pre-Symmetry Set Based Shape Matching, A. Kuijper, ISBN 87-7949-106-5
18. ITU-TR-2005-65 Matching 2D Shapes Using Their Symmetry Sets, A. Kuijper, ISBN 87-7949-095-6

***Dr. Norayr Matevosyan*****Scientific Achievements 2005**

In January- February 2005 Dr. Matevosyan focused on the folowing problems:  
Regularity of the free boundary in obstacle like problems. Also work has been done on the topic of level sets methods for obstacle problems.

**Scientific Cooperations**Internal

Cooperation with M. Burger (University of Linz, INDMATH).

External

Colaboration with A. Hakobyan (Yerevan State University).

***Dr. Lukas Neumann*****Work before joining RICAM**

Before joining RICAM, Lukas Neumann was finishing his PhD in the Wissenschaftskolleg “Differential Equations” at the University of Vienna (Faculty of Mathematics) by end of August. His thesis was titled “Long time properties of solutions to collisional kinetic equations”.

He was visiting the Universidad del País Vasco in Bilbao from April to July 2005 funded by the HYKE-Research training Network (HPRN-CT-2002-00282)

**Scientific Achievements 2005**

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. Mouhot) developed a method to study the long time properties of solutions to collisional kinetic equations. This method applies to a large class of collision operators and can give precise rates of convergence to the equilibrium distribution.

**Scientific Cooperations**Internal

o.Univ.-Prof. Dr. Peter Markowich  
ao.Univ.-Prof. Dr. Christian Schmeiser

External

Miguel Escobedo, Universidad del País Vasco  
Michael Lohwasser, Universität Wien  
Clément Mouhot, Université Paris Dauphine  
Christof Sparber, Universität Wien

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

Conference on nonlinear PDEs in honor of Luis Caffarelli, Vienna, 24-25 October 2005

Workshop “Entropy Methods in PDE Theory and in Stochastics”, Mainz, 23-25 November 2005

**Scientific Visits**

April-July 2005: UPV, Bilbao

**Scientific Talks**

June 2005 Talk in the Seminar of the Institute for Mathematics of the UPV

June 2005 Talk in the Group Seminar at RICAM

July 2005 PhD Defense at the University of Vienna

**Publications 2005****Appeared**

1. LN, C. Schmeiser “Convergence to global equilibrium for a kinetic model for fermions”, SIAM J. Math. Anal. 36, pp 1652-1663

**Submitted**

2. C. Mouhot, LN “Quantitative perturbative study of convergence to equilibrium for collisional kinetic models in the torus”, submitted to Nonlinearity

## 2.6. GROUP “OPTIMIZATION AND OPTIMAL CONTROL”

**Group Leaders:**

o.Univ.-Prof. DI. Dr. Karl Kunisch

**Researchers funded via ÖAW/Upper Austrian government funds:**

Dr. Samuel Amstutz

Dr. Roland Griesse

Dr. Boris Vexler

**Researchers externally funded:**

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, specifically 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 are of special importance to our work, especially in the context of the equations of fluid mechanics. Significant progress was made in the area of vortex reduction by the development of new cost functionals. It should be extended from two to three dimensional problems and in the long run pave the way to optimal control of mixing phenomena. Due to the start of Dr. Amstutz in mid-August, topology optimization and associated numerical methods are in the process of becoming another focus area in the group’s research activities.

During the second half of the year 2005 the group was significantly involved in contributing to the organization of the special semester, for example, by organizing two “focus weeks”. Several joint projects with members of the Radon Institute and with outside scientists were started during this semester.

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.”

With respect to the latter further progress has been made jointly with Dr. J. Sass on the computation of the boundaries of the trading regions for proportional transaction costs and finite time horizon. The procedure which was successful for the 1-dimensional case is now being analysed with respect to extendibility to the multi-dimensional case.

As announced in the previous report efforts were also made to make advances on the control of the quantum mechanical systems modelled by the Schrödinger equation. These led to the joint work “K. Ito and K. Kunisch: Optimal Bilinear Control of an Abstract Schrödinger Equation” which is currently under review.

***Dr. Samuel Amstutz*****Work before joining RICAM**

The research of Dr. Amstutz is focused on topological sensitivity analysis and its applications in topology optimization. In short, the topological sensitivity analysis provides information on the behavior of a shape functional when creating a small hole inside the domain. This information is characterized by the so-called topological gradient and can be used as a descent direction for removing matter in topology optimization algorithms. While the first mathematical paper in this area dates back to 1999, determining the expression of the topological gradient is still a challenging issue for many problems. Also, the concern for developing efficient associated algorithms is very recent.

Before joining RICAM, Dr. Amstutz held a postdoctoral position at the Fraunhofer Institute für Techno- und Wirtschaftsmathematik (ITWM, Kaiserslautern, Germany) funded by the European network HYKE. Besides pursuing previously started theoretical studies [1,3,5,6], Dr. Amstutz worked on the construction of a topological shape optimization algorithm coupling the topological sensitivity information and a level-set-based domain representation. This algorithm was validated on classical problems in structural optimization, after which, in cooperation with PD Dr. H. Andrä and PD Dr. O. Iliev, it was applied to the optimal design of a certain class of waste water ceramic filters. A paper reporting this work was accepted [4].

**Scientific Achievements 2005**

Dr. Amstutz was appointed at RICAM on August 16, 2005. The first part of his stay was devoted to completing two papers started earlier, namely the paper [6] dealing with sensitivity analysis with respect to the insertion of an inclusion possibly different from void, and [4] which was under revision at that time. Subsequently a collaboration with Dr. T. Takahashi (in visit in RICAM for the special Radon semester) and Dr. B. Vexler was started on the derivation of topological asymptotic formulas for time-dependent problems. Finally, bibliographic studies were carried out about two issues which should be subject to future research: the treatment of a (local) stress criterion / constraint instead of the classical compliance in structural optimization and the elaboration of filtering / regularization techniques in order to cope with the ill-posedness of topology optimization problems.

**Scientific Cooperations**Internal

Dr. Boris Vexler, group “Optimization and Optimal Control”

External

Nicolas Dominguez, Airbus Toulouse (France)

PD Dr. Heiko Andrä, Fraunhofer ITWM, Kaiserslautern (Germany)

PD Dr. Oleg Iliev, Fraunhofer ITWM, Kaiserslautern (Germany)

Dr. Takéo Takahashi, INRIA & Institut Elie Cartan de Nancy (France)

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

April 13-15, 2005. Third annual meeting of the HYKE network, Rome (Italy)

June 4-9, 2005. “Shape and topological sensitivity seminar”, Rio de Janeiro (Brazil)

October 20-22, 2005. International meeting “Shape optimization and its applications”, Nancy (France)

Scientific Talks

- Topological shape optimization using a level-set method (third annual meeting of the HYKE network, Rome)

- On the topological sensitivity: some theoretical and numerical aspects (series of lectures, Shape and topological sensitivity seminar, Rio de Janeiro)
- On the topological sensitivity: some theoretical and numerical aspects (RICAM group seminar, invited by Prof. Dr. K. Kunisch)
- Introduction to the topological derivative (RICAM group seminar)
- On the use of the topological gradient in shape optimization (invited talk, international meeting “Shape optimization and its applications”, Nancy)

**Publications 2005**Appeared

1. S. Amstutz, I. Horchani, M. Masmoudi. Crack detection by the topological gradient method, *Control and Cybernetics* 34(1), pp. 81-101, 2005.
2. S. Amstutz. The topological asymptotic for the Navier-Stokes equations, *ESAIM:COCV* 11(3), pp. 401-425, 2005.

Accepted

3. S. Amstutz. Topological sensitivity analysis for some nonlinear PDE systems, to appear in *J. Math. Pures Appl.*
4. S. Amstutz, H. Andrä. A new algorithm for topology optimization using a level-set method, accepted in *J. Comput. Phys.*

Submitted

5. S. Amstutz, N. Dominguez. Topological sensitivity analysis in the context of ultrasonic non-destructive testing.
6. S. Amstutz. Sensitivity analysis with respect to a local perturbation of the material property.

***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. Application areas cover in particular reaction-diffusion systems with or without chaotic behaviour, crystal growth problems, as well as magnetohydrodynamic (MHD) systems. Parametric sensitivity analysis of optimal solutions under parameter perturbations continues to be another of his areas of expertise.

**Scientific Achievements 2005**

In 2005, Dr. Griesse has worked on the following topics:

Sufficient Second-Order Optimality Conditions and Convergence Analysis for SQP Methods for Mixed Constrained Optimal Control Problems

Cooperation with Dr. Arnd Rösch and Dipl.-Math. Nataliya Metla

In 2005, the Austrian Science FWF granted support for the FWF-project P18056, applied for jointly by Dr. Roland Griesse and PD Dr. Arnd Rösch (Inverse Problems group). After an international selection process, Dipl.-Math. Nataliya Metla began to work on the project in October 2005.

Simulation and Optimal Control in Magnetohydrodynamics

Magnetohydrodynamics, or MHD, concerns the mutual interaction of electrically conducting fluids and magnetic fields, which has very attractive applications in metallurgy and crystal growth. Dr.

Griesse has worked jointly with Karl Kunisch on the analysis of MHD optimal control problems. He has started a cooperation with Dr. Marco Discacciati, Dr. Joachim Schöberl and Prof. Ulrich Langer (Direct Field Problems group) concerning the implementation of numerical algorithms for MHD simulation and control, using the software *NGSolve* by J. Schöberl. This software supports different types of finite elements, so the original plan of using different pieces of software in an operator splitting approach was dropped.

In addition, Dr. Griesse has initiated a cooperation with Prof. A.J. Meir (Auburn University, USA) concerning the modeling of free surface problems arising in MHD, which led to the joint publication [10].

#### Preconditioning of KKT Systems arising in PDE-Constrained Optimization

Dr. Griesse has started research activities concerning the efficient iterative solution of Karush-Kuhn-Tucker (KKT) systems arising in PDE-constrained optimization. He has written a joint paper with Jun.-Prof. Andrea Walther [4] describing the preconditioning of KKT systems by a geometric multi-grid algorithm. This algorithm employs only matrix-vector products, and derivatives are generated by Automatic Differentiation (AD). Moreover, Dr. Griesse has given a talk in a seminar series on "Preconditioning of KKT Systems" during the Special Semester on Computational Mechanics at RICAM.

#### Robustness of Optimal Solutions in PDE-Constrained Optimization

Dr. Griesse has written a joint paper [12] with Dr. Boris Vexler on the sensitivity analysis of the quantity of interest in PDE-constrained optimization, which extends his previous research efforts in the area of parametric sensitivity analysis. In addition, Dr. Griesse has supervised the master's thesis of Dipl.-Math. Kerstin Brandes (University of Bayreuth, Germany), titled "Robustness of Optimal Solutions in Optimal Control of PDEs".

#### Relationship of Interior Point Approximations and Parametric Sensitivities in Optimal Control

Dr. Griesse has written a joint paper [9] with Dr. Martin Weiser (ZIB Berlin, Germany) concerning the approximation of parametric sensitivity derivatives in optimal control of PDEs, using interior point methods. Convergence orders of these quantities in terms of the path-following parameter were proved and confirmed numerically.

Within the special semester on computational mechanics, Dr. Griesse organized two workshops together with Dr. Boris Vexler, Prof. Dr. Karl. Kunisch, and Prof. Dr. Ekkehard Sachs:

- 1) Workshop "Control of complex fluids" held at RICAM, Linz, October 10-13, 2005
- 2) Workshop "Efficient methods for time-dependent optimal control: preconditioning, reduced order modelling and feedback control" held at RICAM, Linz, November 21-24, 2005

### **Scientific Cooperations**

#### Internal

Prof. Dr. Karl Kunisch, Research Group "Optimization and Control", RICAM  
 Dr. Boris Vexler, Research Group "Optimization and Control", RICAM  
 Dr. Marco Discacciati, Research Group "Computational Methods for Direct Field Problems", RICAM  
 PD Dr. Arnd Rösch, Research Group "Inverse Problems", RICAM

#### External

Dr. Juan Carlos de los Reyes, Berlin University of Technology, Germany  
 Dipl.-Math. Daniel Wachsmuth, Berlin University of Technology, Germany  
 Jun.-Prof. Andrea Walther, Dresden University of Technology, Germany  
 Prof. A.J. Meir, Auburn University, USA  
 Dr. Martin Weiser, ZIB Berlin, Germany  
 Dr. Moritz Diehl, University of Heidelberg, Germany  
 Ao. Prof. Stefan Volkwein, University of Graz, Austria

Dr. Axel Voigt, Caesar Bonn, Germany  
 Ao. Prof. Alfio Borzi, University of Graz, Austria  
 Ao. Prof. Michael Hintermüller, University of Graz, Austria  
 Prof. Michael Hinze, Dresden University of Technology, Germany

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

#### Conferences

- |  |  |
|--|--|
| <ul style="list-style-type: none"> <li>▪ March 28-April 1, 2005</li> <li>▪ April 11-13, 2005</li> <li>▪ April 18-23, 2005</li> <li>▪ May 16-20, 2005</li> <li>▪ July 18-22, 2005</li> <li>▪ September 19-23, 2005</li> <li>▪ September 26-28, 2005</li> <li>▪ October 10-13, 2005</li> <li>▪ November 21-25, 2005</li> </ul> | GAMM Luxemburg<br>Workshop on “Inverse Problems” and 1 <sup>st</sup> Austrian Numerical Analysis Day, Obergurgl, Austria<br>Workshop on “Optimal Control of Coupled PDE Systems”, Oberwolfach, Germany<br>SIAM Conference on Control, Stockholm, Sweden<br>IFIP TC 7, Turin, Italy<br>ÖMG/DMV/SIAM Conference, Klagenfurt, Austria<br>Workshop on “Trends in Simulation and Control of Coupled PDE Systems”, WIAS Berlin, Germany<br>Workshop on “Control of Complex Fluids”, RICAM Linz, Austria<br>Workshop on “Efficient Methods for Time-Dependent Optimal Control”, RICAM Linz, Austria |
|--|--|

#### Activities as Organizer

- |  |  |
|--|--|
| <ul style="list-style-type: none"> <li>▪ March 28-April 1, 2005</li> <li>▪ May 16-20, 2005</li> <li>▪ October 10-13, 2005</li> <li>▪ November 21-25, 2005</li> </ul> | Organization of a Young Researchers’ minisymposium, GAMM Luxemburg (jointly with Jun.-Prof. Andrea Walther, TU Dresden, Germany)<br>Organization of a minisymposium on “Numerical Methods for PDE-Constrained Optimization”, SIAM Conference on Optimization, Stockholm, Sweden (jointly with Prof. Stefan Volkwein, Graz, Austria)<br>Workshop on “Control of Complex Fluids”, RICAM Linz, Austria (jointly with Dr. Boris Vexler, Prof. Karl Kunisch and Prof. Ekkehard Sachs)<br>Workshop on “Efficient Methods for Time-Dependent Optimal Control”, RICAM Linz, Austria (jointly with Dr. Boris Vexler, Prof. Karl Kunisch and Prof. Ekkehard Sachs) |
|--|--|

#### Scientific Visits

- |                      |   |
|----------------------|---|
| February 14-18, 2005 | Dresden University of Technology, Germany (cooperation with Jun.-Prof. Andrea Walther)  |
| February 21-25, 2005 | Zuse Institute Berlin, Germany (invited by Dr. Martin Weiser; cooperation with Dr. Martin Weiser and Dr. Moritz Diehl)  |
| September 5-9, 2005  | Berlin University of Technology, Germany (invited by Prof. Fredi Tröltzscher; cooperation with Dr. Juan Carlos de los Reyes and Dipl.-Math. Daniel Wachsmuth) |

#### Scientific Talks

- “Towards Simulation and Control in Magnetohydrodynamics” (RICAM group seminar)
- “Parametric Sensitivity Analysis for 3D Reaction-Diffusion Control Problems” (ZIB Berlin, Germany)
- “Matrix-Free AD-Based Preconditioning of KKT Systems” (GAMM Luxemburg)

- “Parametric Sensitivity Analysis and Applications” (Workshop Obergurgl, Austria)
- “Optimal Control in Magnetohydrodynamics” (Workshop Oberwolfach, Germany)
- “Optimal Control in Magnetohydrodynamics” (IFIP TC 7, Turin, Italy)
- “Preconditioning of Linear Systems in PDE-Constrained Optimization” (RICAM group seminar)
- “Optimal Control in Magnetohydrodynamics” (Klagenfurt, Austria)
- “Modeling and Optimal Control in Magnetohydrodynamics” (TU Berlin, Germany)
- “Optimal Control in Magnetohydrodynamics” (WIAS Berlin, Germany)
- “Modeling and Optimal Control in Instationary Magnetohydrodynamics” (Workshop “Control of Complex Fluids, RICAM” )
- “Analysis, Numerical Simulation and Optimal Control of Coupled PDE Systems” (University of Münster, Germany)
- “A Stokes-MHD Problem” (RICAM group seminar)

**Publications 2005**Appeared

1. A. Borzi and R. Griesse: “Experiences with a Space-Time Multigrid Method for the Optimal Control of a Chemical Turbulence Model”, *International Journal for Numerical Methods in Fluids* 47(8-9), pp. 879-885, 2005
2. R. Griesse, M. Hintermüller and M. Hinze: “Differential Stability of Control-Constrained Optimal Control Problems for the Navier-Stokes Equations”, *Numerical Functional Analysis and Optimization* 26(7-8), pp. 829-850, 2005
3. R. Griesse and S. Volkwein: “A Primal-Dual Active Set Strategy for Optimal Boundary Control of a Reaction-Diffusion System”, *SIAM Journal on Control and Optimization* 44(2), pp. 467-494, 2005
4. R. Griesse and A. Walther: “Towards Matrix-Free AD-Based Preconditioning of KKT Systems in PDE-Constrained Optimization”, *PAMM* 5(1), pp. 47-50, 2005

Accepted

5. A. Borzi and R. Griesse: “Distributed Optimal Control of Lambda-Omega Systems”, *Journal of Numerical Mathematics*, to appear
6. R. Griesse: “Lipschitz Stability of Solutions to Some State-Constrained Elliptic Optimal Control Problems”, *Journal of Analysis and its Applications*, to appear
7. C. Büskens and R. Griesse: “Computational Parametric Sensitivity Analysis of Perturbed PDE Optimal Control Problems with State and Control Constraints”, *Journal of Optimization Theory and Applications*, to appear
8. R. Griesse and S. Volkwein: “Parametric Sensitivity Analysis for Optimal Boundary Control of a 3D Reaction-Diffusion System”, in: *Nonconvex Optimization and its Applications* 83 (edited by G. Di Pillo and M. Roma), to appear

Submitted

9. R. Griesse and M. Weiser: “On the Interplay Between Interior Point Approximations and Parametric Sensitivities in Optimal Control”, submitted, 2005
10. R. Griesse and A.J. Meir: “Modeling of an MHD Free Surface Problem Arising in CZ Crystal Growth”, submitted, 2005
11. J.C. de los Reyes and R. Griesse: “State-Constrained Optimal Control of the Stationary Navier-Stokes Equations”, submitted, 2005
12. R. Griesse and B. Vexler: “Numerical Sensitivity Analysis for the Quantity of Interest in PDE-Constrained Optimization”, in revision, 2005
13. R. Griesse and K. Kunisch: “Optimal Control for a Stationary MHD System in Velocity-Current Formulation”, in revision, 2005

**Nataliya Metla**

See the presentation of the group 2.2. "Inverse Problems".

**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 2005**

In 2004, Dr. Vexler has worked on the following topics:

- 1) Adaptive space-time finite element methods for parabolic optimization problems (in cooperation with D. Meidner). We developed a-posteriori error estimates for space-time finite element discretization of parabolic optimization problems. The provided error estimates assess the discretization error with respect to a given quantity of interest and separate the influence of different parts of the discretization (time, space, and control discretization). This allows to set up an efficient adaptive algorithm which successively improves the accuracy of the computed solution by construction of locally refined meshes for time and space discretizations. The corresponding publication is in preparation.
- 2) Optimal Vortex Reduction for Instationary Flows Based on Translation Invariant Cost Functionals (in cooperation with Prof. Dr. K. Kunisch). We developed a new optimal control formulation for vortex reduction problems in unsteady flows described by the Navier-Stokes equations. This formulation is based on the introduction of an objective cost functional, which is directly related to a physically correct definition of a vortex. In paper [8] we presented the analysis as well as an efficient numerical realization of this concept.
- 3) Superconvergence in Finite Element Methods for the Optimal Control Problem of the Stokes Equations (in cooperation with PD Dr. A. Rösch). We investigated a priori error analysis for finite element discretization of an optimal control problem for 2-d and 3-d Stokes equations with pointwise control constraints. We suggested a superconvergence based post-processing, which allows for significant improvement of the accuracy, see [6].
- 4) Numerical Sensitivity Analysis for the Quantity of Interest in PDE-Constrained Optimization (in cooperation with Dr. R. Griesse). We analysed the dependence of solutions of PDE-Constrained optimization problems subject to perturbations in the data. In paper [7] we devised an efficient procedure for the evaluation of the sensitivity derivatives of a given quantity of interest with respect to perturbation parameters.
- 5) Finite Element Approximation of Elliptic Dirichlet Optimal Control Problems.  
We presented a numerical discretization scheme for finite element Galerkin discretization of elliptic Dirichlet optimal control problems with finite dimensional control space. In [9] we proved the optimal order of convergence for this discretization.

Dr. B. Vexler was nominated as a finalist for ``ECCOMAS award for the best PhD thesis 2004'' by Gesellschaft für Angewandte Mathematik und Mechanik (GAMM)

Within special semester on computational mechanics, Dr. B. Vexler organized two workshops together with Dr. R. Griesse, Prof. Dr. K. Kunisch, and Prof. Dr. E. Sachs:

- Workshop "Control of complex fluids" held at RICAM, Linz, October 10 - 14, 2005
- Workshop "Efficient methods for time-dependent optimal control: preconditioning, reduced order modelling and feedback control" held at RICAM, Linz, November 21 - 24, 2005

### **Scientific Cooperations**

#### Internal

Prof. Dr. Karl Kunisch, Research Group "Optimization and Control", RICAM  
 Dr. Roland Griesse, Research Group "Optimization and Control", RICAM  
 Dr. Samuel Amstutz, Research Group "Optimization and Control", RICAM  
 PD Dr. Arnd Rösch, Research Group "Inverse Problems", RICAM

#### External

- Prof. Dr. Rolf Rannacher, University of Heidelberg, Germany
- Prof. Dr. Roland Becker, University of Pau, France
- Prof. Dr. Thomas Apel, Universität der Bundeswehr München, Germany
- Dr. Malte Braack, University of Heidelberg, Germany
- Dipl. Math. Dominik Meidner, University of Heidelberg, Germany
- Dipl. Math. Michael Schmich, University of Heidelberg, Germany
- Dr. Takeo Takahashi, Université Henri Poincaré Nancy, France

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

#### Conferences

|                        |   |
|------------------------|---|
| April 11-13, 2005      | Workshop on Inverse Problems, Obergurgl, Austria  |
| April 26-29, 2005      | Workshop "Optimal Control of Coupled Systems of PDE", Oberwolfach, Germany  |
| July 17-23, 2005       | 22nd IFIP TC 7 Conference on System Modeling and Optimization , Turin, Italy  |
| July 18-22, 2005       | Workshop on PDE Constrained Optimization, Tomar, Portugal   |
| September 11-14, 2005  | Evolutionary and Deterministic Methods for Design, Optimisation and Control with Applications to Industrial and Societal Problems (EUROGEN 2005), Munich, Germany |
| October 10 - 14, 2005  | Workshop "Control of complex fluids", Linz, Austria   |
| November 15, 2005      | Miniworkshop "Error-Estimates", Linz, Austria   |
| November 21 - 24, 2005 | Workshop "Efficient methods for time-dependent optimal control", Linz, Austria  |
| December 5 – 6, 2005   | Miniworkshop "Variational Multiscale Methods and Stabilized Finite Elements", Heidelberg, Germany   |

#### Scientific Visits

January 3 – 7, 2005 University of Heidelberg, Germany  
 December 7 – 9, 2005 University of Heidelberg, Germany

#### Scientific Talks

- 1) Parameter Estimation and Sensitivity Analysis with Adaptive Finite Elements (Workshop on Inverse Problems, Obergurgl, Austria)

- 2) Adaptive Finite Element Methods for Optimization Problems (Workshop "Optimal Control of Coupled Systems of PDE", Oberwolfach, Germany)
- 3) Optimal Vortex Reduction for Instationary Flows (22nd IFIP TC 7 Conference on System Modeling and Optimization , Turin, Italy)
- 4) Finite Element Discretization of Dirichlet Optimal Control Problems (Workshop on PDE Constrained Optimization, Tomar, Portugal)
- 5) Optimal Vortex Reduction for Instationary Flows (EUROGEN 2005, Munich, Germany)
- 6) Optimal Vortex Reduction for Instationary Flows (Workshop "Control of complex fluids", Linz, Austria)
- 7) Adaptive Space-Time Finite Element Methods for Parabolic Optimization Problems (Minisymposium "Error-Estimates", Linz, Austria)
- 8) Adaptive Space-Time Finite Element Methods for Parabolic Optimization Problems (Workshop "Efficient methods for time-dependent optimal control", Linz, Austria)
- 9) Discretization of Optimal Control Problems by Stabilized Finite Element Methods (Minisymposium "Variational Multiscale Methods and Stabilized Finite Elements", Heidelberg, Germany)

## Publications 2005

### Appeared

1. R. Rannacher and B. Vexler "A priori error estimates for the finite element discretization of elliptic parameter identification problems with pointwise measurements", *SIAM Journal on Control and Optimization*, Vol. 44(5):1844-1863, 2005
2. R. Becker, M. Braack and B. Vexler "Parameter Identification for Chemical Models in Combustion Problems", *Applied Numerical Mathematics*, Vol. 54(3-4), 519 - 536, 2005
3. R. Becker and B. Vexler "Mesh Refinement and Numerical Sensitivity Analysis for Parameter Calibration of Partial Differential Equations", *Journal of Computational Physics*, Vol. 206(1), 95 - 110, 2005
4. B. Vexler "Adaptive Finite Elements for Output-Oriented Model Calibration" in Proc. of International Conference on High Performance Scientific Computing, Hanoi, March 10-14, pp. 523-538, Springer Berlin, Heidelberg, 2005.

### Submitted

5. R. Becker, D. Meidner and B. Vexler "Efficient Numerical Solution of Parabolic Optimization Problems by Finite Element Methods", submitted, 2005.
6. A. Rösch and B. Vexler "Superconvergence in Finite Element Methods for the Optimal Control Problem of the Stokes Equations", submitted, 2005
7. R. Griesse and B. Vexler "Numerical Sensitivity Analysis for the Quantity of Interest in PDE-Constrained Optimization", submitted, 2005
8. K. Kunisch and B. Vexler "Optimal Vortex Reduction for Instationary Flows Based on Translation Invariant Cost Functionals", submitted, 2005
9. B. Vexler "Finite Element Approximation of Elliptic Dirichlet Optimal Control Problems", submitted, 2005
10. R. Becker, D. Meidner, R. Rannacher and B. Vexler "Adaptive Finite Element Methods for PDE-Constrained Optimal Control Problems" in Reactive Flows, Diffusion and Transport, R. Rannacher et. al. (eds.), Springer Verlag, Berlin, to appear, 2005.

### 3. SPECIAL SEMESTER, CONFERENCES, COLLOQUIA

#### 3.1. OVERVIEW

As in the previous years, the institute had many external visitors, most (but not all) of them also gave talks. It is important for RICAM scientists to attend such talks, but their number has grown too much for the scientists to be able to attend all talks. Therefore, the talks have been structured into 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 at least two groups in RICAM and should therefore be attended by all RICAM scientists.

##### Radon-Group-Seminars:

These are specialized talks by internal and external scientists intended mostly for members of the organizing group(s), although, of course, members of other groups are also welcome.

In 2005, the following talks were given in these three groups:

#### *Radon Colloquia*

|   |
|---|
| <b>Prof. Henrik Shahgholian</b><br>Department of Mathematics, KTH Stockholm<br>Wednesday, January 12, 16:00, HF 136   |
| Title: A Catalog of Free Boundary Problems  |
| Abstract: We discuss several free boundary problems of obstacle type<br>$Lu = f(u)$<br>where, L is an elliptic/parabolic operator and $f(u)$ is in general in, and it has discontinuity along<br>Other type of $f$ maybe considered as well.  |
| <b>Prof. Dr. Rainer Blatt</b> in association with Johannes Kepler Symposium (JKU & ÖMG)<br>Institut f. Experimentalphysik, Universität Innsbruck und<br>Institut f. Quantenoptik und Quanteninformation der ÖAW<br>Wednesday, January 19, 17:15, HS2  |
| Title: Quantum Computer – Dream and Realization<br>Abstract: Computational operations always rely on real physical processes, which are data input, data representation in a memory, data manipulation using algorithms and finally, the data output. With conventional computers all the processes are classical processes and can be described accordingly. Theoretically, it is known for several years now that certain computations could be processed much more efficiently using quantum mechanical operations. Therefore, there it would be desirable to build a quantum computer. This requires the implementation of quantum bits (qubits), quantum registers and quantum gates and the development of quantum algorithms. In this talk, several techniques for the implementation of a quantum computer will be presented and compared. Special emphasis will be given to the ion storage and laser cooling techniques which are currently investigated for an application with quantum computers. Experimental realizations of quantum registers and quantum gate operations using strings of trapped ions in a linear Paul trap will be discussed. With a small ion-trap quantum computer based on two and three trapped |

$\text{Ca}^+$  ions as qubits we have generated in a pre-programmed way specific quantum states. In particular, entangled states of two particles, i.e. Bell states, and of three particles, i.e. GHZ and W states, were generated using an algorithmic procedure. With a tomographic method, these states were subsequently analysed and the respective entanglement was characterized using various entanglement measures. With Bell states as a resource, entangled states were applied for teleportation and improved precision measurements.

**Prof. Dr. Tautenhahn**

Hochschule Zittau/Görlitz

Wednesday, February 2, 17:15, K033C

Title: Regularization and Parameter Choice for Ill-Posed Problems

Abstract: Linear and nonlinear ill-posed problems arise in different applications in science and engineering. For their stable solution regularization methods are required. In this talk we discuss questions of optimal and order optimal recovery and regularization. We provide order optimal error bounds for regularized approximations in cases of proper a priori and a posteriori parameter choice. We distinguish our studies into (i) the Classical Theory and (ii) the Hilbert Scale Theory. The results cover the special case of finitely smoothing operators and extend recent results for infinitely smoothing operators.

**Prof. Thomas Apel**

Bundeswehruniversität München

Wednesday, March 2, 17:15, HF9901

Title: Anisotropic finite elements for resolving edge singularities and boundary layers

Abstract: Anisotropic finite element meshes are characterized by elements with a large or even asymptotically unbounded aspect ratio. Such meshes are known to be particularly effective for the resolution of directional features of the solution. In the talk, we characterize suitable anisotropic meshes for approximating edge singularities in various elliptic problems and boundary layers in singularly perturbed problems.

Modern discretization methods do not work on one fixed mesh but adapt it iteratively to the solution. Besides reliable and efficient a-posteriori error estimators, further information like the desired stretching direction and the appropriate aspect ratio of the elements are necessary to obtain for the adaptive refinement. The optimal reconstruction of the mesh is one of the current challenges. In the talk we discuss all these ingredients.

In solving the Stokes or Navier-Stokes problem the question arises which pairs of elements are stable independent of the aspect ratio of the elements. For several pairs of elements positive and negative results are given.

**Prof. Franco Brezzi**

Università degli Studi di Pavia

Friday, April 8, 15:00, HS12

Title: Mimetic finite differences for diffusion problems

Abstract:

**Prof. Axel Klar**

TU Kaiserslautern; Fraunhofer ITWM Kaiserslautern

Thursday, April 21, 18:00, BA9911

Title: Modelling and optimization of traffic flow on road networks

Abstract: The talk gives a survey of dynamic traffic flow models. Different models based on ordinary and partial differential equations are discussed. Simplified models using nonlinear algebraic relations or linear programmes are derived from the detailed dynamics. In particular, we discuss the development of traffic jams and the description of traffic flow on road networks. Moreover, traffic management problems, i.e. control problems in networks are considered. Optimal control methods adapted to the above hierarchy of models like adjoint methods or MIP solvers are investigated. Finally, a comparison of the different methods is given.

**Prof. Dr. Willi Freeden**

Universität Kaiserslautern

Wednesday, June 1, 18:00, HS 8

Title: Wavelet Generated by Layer Potentials

Abstract: By means of the limit and jump relations of classical potential theory with respect to the Helm-

holtz equation a wavelet approach is established on a regular surface. A multiscale procedure is constructed in such a way that the emerging potential kernels act as scaling functions, wavelets are defined via a canonical refinement equation. A tree algorithm for fast computation of a function discretely given on a regular surface is developed based on numerical integration rules. By virtue of the tree algorithm, an efficient numerical method for the (regularized) solution of Fredholm integral equations involving boundary-value problems of the Helmholtz equation corresponding to a (general) regular (boundary) surface is discussed in more detail.

### **Dr. Karsten Wolters**

Institute for Biomagnetism and Biosignalanalysis, University of Münster

Monday, June 27, 15:30, K 269D

Title: EEG and MEG based Source Reconstruction in the Human Brain: A Simulation and Visualization Study using a High Resolution Anisotropic Finite Element Headmodel.

Abstract: The inverse problem in Electro- and Magneto-EncephaloGraphy (EEG/MEG) aims at reconstructing the underlying current distribution in the human brain using potential differences and/or magnetic fluxes that are measured non-invasively directly, or at a close distance, from the head surface. The solution requires repeated computation of the forward problem, i.e., the simulation of EEG and MEG fields for a given dipolar source in the brain using a volume-conduction model of the head. The associated differential equations are derived from the Maxwell equations.

Not only do various head tissues exhibit different conductivities, some of them are also anisotropic conductors as, e.g., skull, brain white and also gray matter. To our knowledge, previous work has not extensively investigated the impact of modeling tissue anisotropy on source reconstruction.

Currently, there are no readily available methods that allow direct conductivity measurements. Furthermore, there is still a lack of sufficiently powerful software packages that would yield significant reduction of the computation time involved in such complex models hence satisfying the time-restrictions for the solution of the inverse problem.

In my talk, techniques of multimodal Magnetic Resonance Imaging (MRI) are presented in order to generate high-resolution realistically shaped anisotropic volume conductor models. One focus is the presentation of an improved segmentation of the skull by means of a bimodal T1/PD-MRI approach. The eigenvectors of the conductivity tensors in anisotropic white matter are determined using whole head Diffusion-Tensor-MRI. The Finite Element

(FE) method in combination with an EEG and MEG lead field basis approach and a parallel algebraic multigrid solver with simultaneous treatment of multiple right hand sides yields a highly efficient solution of the anisotropic forward problem.

I then study the sensitivity to anisotropy of the EEG/MEG forward problem for deep and eccentric sources with differing orientation components.

The influence of anisotropy will be presented by high resolution visualization of field distribution, isopotential-surfaces and return current flow and by topography and magnitude error measures.

The combination of simulation and visualization provides a deep insight into the effect of head tissue conductivity anisotropy.

It was found that for EEG, the presence of tissue anisotropy both for the skull and white matter compartment substantially compromises the forward potential computation and therefore the inverse source reconstruction.

Skull anisotropy has a smearing effect on the forward potential computation and it has no effect on the MEG. For the MEG, only the anisotropy of the white matter compartment has an effect. The deeper the source and the more it is surrounded by anisotropic fiber bundles, the larger the effect is.

In the first instance, the return currents tend to compensate the primary current, but in the second instance the anisotropic geometry influences the flow in the way that, driven by the higher conductivity, the secondary currents tend to flow parallel to the white matter fiber tracts.

Furthermore, the degree of error resulting from the uncompensated presence of tissue anisotropy depended strongly on the proximity of the anisotropy to the source, remote anisotropy had a much weaker influence than anisotropic tissue that included the source.

In summary, high-resolution anisotropic FE forward modeling is crucial for an accurate solution of the inverse problem in EEG and MEG.

|   |
|---|
| <p><b>Prof. James Bramble</b><br/> Texas A&amp;M University<br/> Tuesday, October 11, 17:15, HF 9901</p> <p>Title: Analysis of a finite PML approximation for the three dimensional time-harmonic maxwell and acoustic scattering problems</p>  |
| <p>Abstract: We consider the approximation of the frequency domain three dimensional Maxwell scattering problem using a truncated domain perfectly matched layer (PML). We also treat the time-harmonic PML approximation to the acoustic scattering problem. A transitional layer based on spherical geometry is defined which results in a constant coefficient problem outside the transition. A truncated (computational) domain is then defined which covers the transition region. The truncated domain need only have a minimally smooth outer boundary (e.g., Lipschitz continuous). We consider the truncated PML problem which results when a perfectly conducting boundary condition is imposed on the outer boundary of the truncated domain. The existence and uniqueness of solutions to the truncated PML problem will be shown provided that the truncated domain is sufficiently large, e.g., contains a sphere of radius <math>R_t</math>. We also show exponential (in the parameter <math>R_t</math>) convergence of the truncated PML solution to the solution of the original scattering problem inside the transition layer. Our results are important in that they are the first which show that the truncated PML problem can be posed on a domain with non-smooth outer boundary. This allows the use of approximation based on polygonal meshes. In addition, even though the transition coefficients depend on spherical geometry, they can be made arbitrarily smooth and hence the resulting problems are amenable to numerical quadrature. Approximation schemes based on our analysis are the focus of future research.</p>   |
| <p><b>Univ.-Prof. em. Dr.-Ing. habil. Dr.-Ing. E.h. Dr. h.c. mult. Erwin Stein</b><br/> Institute of Mechanics and Computational Mechanics, University of Hannover<br/> Thursday, November 10, 19:00, Room: HS 10</p>   |
| <p>Title: Gottfried Wilhelm Leibniz- far ahead of his time</p> <p>Abstract: The design and research for our (so far seven) Hannover Leibniz Exhibitions since 1990, entitled “Gottfried Wilhelm Leibniz (1646-1716): Philosopher, Mathematician, Physicist, Engineer, ...”, follows the intention “Leibniz for touching and understanding” by presenting the key ideas of his multi-ingenious intellectual achievements in the so-called ‘Leibniz worlds’ with his postulates “Theoria cum Praxi” and “Commune Bonum” and showing new fully functional and vivid models of his technical inventions, especially his calculating machines, in the second half of the 17th century which is often called ‘the cradle of modern natural sciences and engineering technology’.</p> <p>After an introduction into Leibniz’ guidelines of thinking in humanities as well as the key points of his inventions in mathematics and physics, a major part of the lecture treats the history of his decimal “Four-Function-Calculating Machines” from 1673 and 1693-1695 and of the “Machina Arithmeticae Dyadicae”, the binary calculating machine, described in 1679. Special attention is given to the principal and technical insufficiencies of Leibniz’ machines, furthermore J. T. Lehmann’s replicas of the “large” decimal Four-Function Machine, built in Dresden in the 80th of last century, and L. von Mackensen’s first design of Leibniz’ binary machine for adding and multiplying from 1969 in Munich, built by the Deutsches Museum München in 1971, as well as our new-designed models which overcome the shortcomings of the originals and the former replicas in regard of the authenticity with the original machines to the greatest possible extend.</p> <p>Also Leibniz’ major technical developments for mining in the Harz mountains with the goals of saving human efforts and energy are outlined by Powerpoint pictures.</p> <p>The lecture ends with considerations on his philosophical concepts and with reflections on the restless personality of this so-called last universal scholar.</p> <p>References:</p> <ul style="list-style-type: none"> <li>[1] Popp, Karl and Stein, Erwin, (eds.): Gottfried Wilhelm Leibniz: Philosoph, Mathematiker, Physiker, Techniker, Instruction Book to the Leibniz Exhibition 2000 in Hannover, seperated into (a) German and (b) English language, Schlütersche, Universität Hannover, (2000)</li> <li>[2] Stein, Erwin: Gottfried Wilhelm Leibniz, seiner Zeit weit voraus als Philosoph, Mathematiker, Physiker, Techniker ... – ein Extrakt der gleichnamigen Ausstellungen –, in: Abhandlungen der Braunschweigischen Wissenschaftlichen Gesellschaft (BWG), Vol. 54, 131-171, (2005)</li> </ul> |

[3] Kopp, Franz-Otto, Stein, Erwin und Popp, Karl: Neue Forschungsergebnisse und Nachbauten zu den Leibnizschen Rechenmaschinen, submitted for publication in ‘*Studia Leibniziana*’ of the Leibniz-Gesellschaft Hannover in 2005

**Prof. Robert Anderssen**

CSIRO Mathematical and Information Sciences, Australia

Monday, November 14, 14:00, Bruckner-Privatuniversität, Göttinger Saal  
a cooperation with the Anton Bruckner University

Title: A New Music Aesthetic for Piano Sound - The Stuart & Sons Pianos

Abstract: To establish a new musical aesthetic, one must create a significantly new and special sound that catches the attention of the general public as well as musicians and composers. In general, this will only occur when something truly novel and innovative is achieved. For piano sound, this is the situation for the Stuart / Sons pianos manufactured by Piano Australia. The innovation is the replacement of the traditional horizontal zig-zag clamping of the strings on the bridge on the soundboard by a vertical zig-zag clamping. To understand the relevance and significance of this achievement, it is first necessary to review the history of the development of the piano, as well as understand the role played by aesthetics in achieving stability of sound for composers, musicians and audiences. To explain why the Stuart & Sons pianos appear to have an enhanced singing sound, one must turn to a discussion of the psychoacoustics of hearing along with the some facts about the nature of the vibration of piano strings. Scientifically, the proof is simple, just play C two octaves above (or below) middle C on different pianos and listen to the differences. Musically, it is not only a matter of adapting the performance practice of the music of the composers of the past to the new genre, but also composing music, with new sound effects, that cannot be produced on traditional instruments and which catches the attention of composers, musicians and audiences.

**Radon Seminars**

Dr. Georg Regensburger

RICAM/Gruppe: Symbolic Computation

Tuesday, February 1, 13:30, HF 136

Title: Parametrized Wavelets

Abstract: Wavelets have become a fundamental tool in many areas of applied mathematics and engineering over the last two decades. The new image coding format JPEG 2000 for example uses wavelet transforms. In this talk, we first discuss the construction of wavelets based on scaling functions. A scaling function satisfies a functional equation given by a linear combination of filter coefficients and dilated and translated versions of the scaling function. We consider the related multiresolution analysis and the fast wavelet transform. Then we show how symbolic methods, in particular Groebner bases, can be used to construct parametrized families of filter coefficients and wavelets. Finally, we present examples and some applications of parametrized wavelets.

Dr. Willem De Graaf

RICAM/Gruppe: Symbolic Computation

Monday, February 7, 15:30, HF 136

Title: Classifying solvable Lie algebras

Abstract: In this talk I will describe a method for obtaining the classification of small-dimensional solvable Lie algebras. One of the main ingredients is a method for finding isomorphisms of Lie algebras, using the theory of Groebner bases. The method has been applied to find the classification of solvable Lie algebras of dimension not exceeding 4.

Sergei Perverzev

ITWM – Kaiserslautern

Monday, February 14, 15:30, HF 136

Title: Regularized Fixed-Point Iteration for Nonlinear Ill-Posed Problems

Abstract: Standard methods for solving nonlinear inverse problems involve knowledge of Frechet derivative. Its computation is time consuming especially in multidimensional problems. Therefore one tries to avoid it. We consider the situation when nonlinear operator is split into some linear and nonlinear parts. Such splitting suggests a

fixed-point-like iteration, however each iteration is ill-posed and need to be regularized. We derive conditions on linear and nonlinear parts, which guarantee stable behavior of the method with respect to the number of iterations. Application of the technique is considered to the initial temperature reconstruction for the nonlinear heat equation which describes glass cooling.

Hend Benmeur

Ecole Nationale d'Ingenieurs de Tunis

Monday, February 14, 13:30, HF 136

Title: Refinement indicators: Theory and applications

Abstract: An important step in the resolution of inverse problems is the choice of a parametrization of the unknown quantity that we have to identify. The idea of using refinement and coarsening indicators to define an adaptive progressing parametrization was first applied to identify hydraulic transmissivity in porous media. This technique can be applied in the general case where we want to locate discontinuities of some parameters. In a current work, this technique is applied for image segmentation, the obtained results are promising.

Prof. Dr. Sergej Rjasanow

Universitaet des Saarlandes

Tuesday, March 1, 15:30, HF136

Title: The Boltzmann Equations: Theory and Numerics

Marco Di Francesco

RICAM – Group: Analysis of Partial Differential Equations

Monday, March 21, 15:30, HF 136

Title: Time dependent rescalings and intermediate asymptotics for nonlinear diffusion equations

Abstract: We are interested in the mathematical theory of nonlinear diffusion equations. We shall first recall some existence theory and qualitative properties of nonnegative solutions to the initial value problem for nonlinear diffusion equations, posed in the euclidean space  $R^d$ . If the nonlinearity function is a power law (porous medium equation or fast diffusion equation), then the equation enjoys several useful scaling invariance properties, which imply the existence of special 'self-similar' solutions called Barenblatt-Pattle solutions. Such solutions are known to approximate (in some sense) any nonnegative solution with initial datum in  $L^1$  as time tends to infinity. We propose a new approach to detect a typical asymptotic profile when the nonlinearity is not a power law. Our method relies in the so-called 'optimal mass transfer' or 'Monge-Kantorovich' problem.

Prof. Dr. Hans Josef Pesch

Universität Bayreuth

Wednesday, March 23, 10:00, HF 136

Title: On PDE Constrained Optimal Control --- An Application Oriented Approach

Abstract: By means of two difficult examples from engineering applications, approaches are outlined how to handle PDE-constrained optimization problems in real life applications. The first problem is concerned with the optimal control of a molten carbonate fuel cell modelled by 28 partial differential algebraic equations of different type and with nonstandard boundary conditions. Objectives are optimized load changes or optimal efficiency. The second problem is concerned with a parameter optimization problem in laser welding which can be done by a combination of analytical and numerical methods. Here, the objective is to avoid hot cracks.

Dr. Yasmin Dolak

RICAM – Analysis of Partial Differential Equations

Thursday, April 7, 18:00, BA9910

Title: The Keller-Segel Model for Chemotaxis: Parameter Identification and Small Diffusion

Abstract: Chemotaxis is the oriented movement of cells towards or away from chemical gradients.

In this talk, we will focus on the classical model for chemotaxis, the so-called Keller-Segel model, which is a drift-diffusion equation for the cell density coupled with an elliptic equation describing the evolution of the chemoattractant. Based on this model, we will first study the parameter identification of quantities like the chemotactic sensitivity using data describing the evolution of the cell density in time.

Then, we will study a special case of the Keller-Segel model, where a nonlinear advection term turns off the chemotactic response at high cell densities. If the diffusivity of the cells is small enough, plateau-like

solutions are formed, showing an interesting long-time behavior. We investigate the asymptotic behavior of these solutions in one and two space dimensions both analytically and numerically. In one space dimension, a system of ordinary differential equations describing the slow motion of internal layers is derived.

Prof. Dr. Josef Schicho

RICAM – Symbolic Computation, Computational Algebra

Thursday, April 7, 18:30, BA9910

Title: Algebraic Subproblems in Multigrid Methods

Dr. Joachim Schöberl

RICAM – Computational Methods for Direct Field Problems

Thursday, April 7, 19:00, BA9910

Title: Finite Element Maxwell Solvers: Theory and Applications

Prof. Simeon Reich

Department of Mathematics

The Technion - Israel Institute of Technology

Wednesday, April 27, 13:30, HF136

Title: Nonlinear semigroups, inverse problems, and delay equations

Abstract: In the first part of this talk I intend to discuss an inverse problem in nonlinear semigroup theory. This problem is related to the equivalence between resolvent consistency and convergence. The second part of the talk will be devoted to approximation methods for parameter identification in a class of nonautonomous nonlinear evolution equations with delay.

Dr. Hansjörg Albrecher

Department of Mathematical Sciences, University of Aarhus

Friday, May 13, 14:00, HF 136

Title: On Static Hedging of Asian Options under General Market Models

Abstract: We discuss the importance of the availability of (quasi-)static hedging strategies for exotic options in incomplete markets and present a static superhedging strategy for the payoff of an arithmetic Asian option in terms of a portfolio of European options. The obtained hedge is applicable under general stock price models and can be optimized using comonotonicity theory. Numerical illustrations of the hedging performance are given for various Lévy models calibrated to market data.

Prof. Kazufumi Ito

North Carolina State University

Monday, May 30, 15:30, HF 136

Title: Preconditioned Iterative Methods on Sparse Subspaces and Applications

Abstract: When some rows of the system matrix and a preconditioner coincide preconditioned iterations can be reduced to a sparse subspace.

Taking an advantage of this property can lead to considerable memory and computational savings. This is particularly useful with the GMRES method. We consider the iterative solution of discretized partial differential equation on this sparse subspace. With a domain decomposition method and a domain embedding method the subspace corresponds a small neighborhood of an interface. As numerical examples we solve the Helmholtz equation using a domain decomposition method and an elliptic equation with jump in the diffusion coefficient using a separable preconditioner.

Prof. Victor Isakov

Wichita State University

Monday, June 13, 12:45, HF 136

Title: Increased stability in the uniqueness of the continuation and detection by waves

Abstract: We discuss stability in the (lateral) Cauchy problems for the Helmholtz and wave equations. We show that under some convexity conditions on the surface with the Cauchy data stability is increasing with growing frequency and that the lateral Cauchy problem is Lipschitz stable for the wave equation. On the other hand, in different geometry stability deteriorates with increased frequency. We outline proofs based on Fourier analysis and Carleman estimates.

We discuss generalization to variable coefficients and to thier identification, as well as to parabolic equa-

|   |
|---|
| tions   |
| Prof. Peter Markowich<br>TU Wien / RICAM<br>within the DGL-Seminar<br>Tuesday, June 21, 11:00, HF136  |
| Dr. Hanna Katriina Pikkarainen<br>Institute of Mathematics, Helsinki University of Technology<br>Thursday, June 23, 13:30, HF 136   |
| Title: A mathematical model for electrical impedance process tomography   |
| Abstract: We consider the process tomography problem of the following kind: based on electromagnetic measurements on the surface of a pipe, describe the concentration distribution of a given substance in a fluid moving in the pipeline. We view the problem as a state estimation problem. The concentration distribution is treated as a stochastic process satisfying a stochastic differential equation referred to as the state evolution equation. The measurements are described in terms of an observation equation containing the measurement noise. The time evolution is modelled by a stochastic convection-diffusion equation. The measurement situation is represented by the most realistic model for electrical impedance tomography, the complete electrode model. We give the mathematical formulation of the state evolution and observation equations and then we derive the time discrete infinite dimensional state estimation system. |
| Since our motive is to monitor the flow in the pipeline in real time, we are dealing with a filtering problem in which the estimator is based on the current history of the measurement process. For computational reasons we present a discretized state estimation system where the discretization error is taken into account. The discretized filtering problem is solved by the Bayesian filtering method.   |
| Dr. Axel Voigt<br>Caesar Institut<br>Tuesday, July 26, 10:00, HF136   |
| Title: Surface evolution on the nanometer scale   |
| Abstract: Approaching smaller and smaller length scales dramatically changes the properties of materials, which is due to an increasing influence of surface effects. A detailed description of such surfaces is therefore of utmost importance in many materials science applications. We investigate higher order anisotropic geometric evolution laws by different numerical methods, such as front tracking, phase field and level sets.  |

### **Group Seminars**

|   |
|---|
| <b>GROUP: Inverse Problems and Optimization and Optimal Control</b>   |
| <b>Daniel Wachsmuth</b>   |
| TU Berlin   |
| Tuesday, January 18, 13:45, HF 136  |
| Title: Numerical solution of optimal flow control problems  |
| Abstract: Active control of flows is a recent research topic in both engineering and mathematics. Design goals are for instance the improvement of the lift-drag ratio of aircrafts or reduction of noise emission. Since numerical methods are available to compute the flow reaction to control actions, one is interested in optimizing the flow actuation.  |
| In the talk we will consider numerical methods to solve optimal flow control problems. The flow is governed by the instationary incompressible Navier-Stokes equations. The control is brought in the system as Dirichlet boundary or distributed control. It has to obey pointwise convex constraints. The presented methods include SQP techniques to tackle the nonlinear optimization problem and active set methods to cope with the control constraints. Numerical results show the efficiency of the proposed methods. |
| <b>GROUP: Optimization and Optimal Control &amp; Computational Methods for Direct Field Problems</b>  |
| <b>Dr. Roland Griesse (RICAM)</b>   |
| Monday, February 28, 11:00, HF 136  |
| Title: Towards Simulation and Control in Magnetohydrodynamics   |

|  |
|--|
| <p><b>Abstract:</b></p> <p><b>GROUP: Computational Logic – Theorema</b></p> <p><b>Dr. Christian Urban</b></p> <p>Thursday, March 3, 16:00, HF 136</p> <p><b>Title:</b> Nominal Reasoning Techniques in the Theorem Prover Isabelle</p>   |
| <p>Abstract: The handling of variable binding in lambda-terms is a recognised challenge in formal proofs. I will describe how informal proofs about the lambda-calculus can be formalised with ease in Isabelle/HOL using a variant of Pitts' nominal logic work. I will first present an inductive definition for alpha-equated lambda-terms (having names) and then a strong induction principle, which looks very much like the Bar-endregt variable convention. I applied these results and formalised proof for Church-Rosser and strong-normalisation.</p>   |
| <p><b>GROUP: Computational Methods for Direct Field Problems</b></p> <p><b>Dirk Langemann</b></p> <p>Universität Rostock - Institute for Mathematics</p> <p>Monday, March 14, 15:30, HF 136</p> <p><b>Title:</b> Numerical simulation of the deformation and the motion of a water droplet in an electric field</p>  |
| <p>Abstract: Water droplets on outdoor insulators of high-voltage equipment influence strongly the aging process and thus the insulating and hydrophobic properties of the material. The investigation of the behaviour of a single water droplet in a strong electric field leads to a coupled problem. The mechanical deformation of the droplet depends on the ponderomotoric force density acting on the droplet surface and vice versa. We get a free boundary value problem for the electric potential with the free droplet surface. This surface is described by a boundary value problem itself. The feed-back loop is numerically decoupled by an iteration over both the sub-problems. Modelling the deformation of the droplet and its interaction with the electric field is an essential part of the work. Particular questions are the dependency of the contact angle and of the growth of the ponderomotoric force density near the triple line on the electric field. We use dissipative pseudo-transient processes for solving the non-linear mechanical sub-problem as well as for discussing the convergence of the iteration mentioned above. The electric sub-problem consists in a 3d elliptic problem with material interfaces. After a restriction to a bounded domain, it is solved by finite elements on an adapted triangular mesh designed for the needs of the coupled problem. We present 2d and 3d results of the deformation of dielectric and conductive droplets. Finally, it is shown that the total ponderomotoric force acting on an uncharged body is not vanishing in general. A method to approximate the motion of uncharged droplets in an electric field is given. We show a sample droplet moving on the surface of an insulator. Such droplets leave dry bands and water films which further the development of undesired electric currents or flash-overs.</p> |
| <p><b>GROUP: Groups: Inverse Problems, Optimization and Optimal Control and Computational Methods for Direct Field Problems</b></p> <p><b>Gunter Winkler</b></p> <p>Bundeswehruniversität München</p> <p>Wednesday, March 2, 15:15, HF 136</p> <p><b>Title:</b> "The Order of Convergence of an Optimal Control Problem on non-convex Domains"</p>   |
| <p>Abstract: The talk presents an optimal control problem with pointwise control constraints governed by an elliptic partial differential equation. The domain may exhibit reentrant corners. The resulting singularities of the state function are treated by apriori mesh grading near these corners.</p>  |
| <p><b>GROUP: Computational Methods for Direct Field Problems</b></p> <p><b>Ronan Perrussel</b></p> <p>Electrical Engineering Center of Lyon, FRANCE</p> <p>Monday, April 11, 15:30, HF 136</p> <p><b>Title:</b> Compatible coarse nodal and edge elements through energy functionals</p>   |
| <p>Abstract: Our aim is to define an algebraic multilevel method for solving Maxwell's equations discretized by edge elements. The first principles have been presented by Reitzinger and Schöberl to solve this class of problems; some improvements have also been introduced by Bochev et al. We propose another approach coming from the construction of coarse nodal elements by using a minimisation problem based on an energy norm; this idea has been proposed by Wan, Chan and Smith. We will review this technique in</p>   |

the nodal element case and we will extend this method to the construction of coupled coarse nodal and edge elements; the important details of the approach will be explained and numerical results on structured and unstructured meshes, in two and three dimensions, will be presented.

#### **GROUP: Computational Methods for Direct Field Problems**

##### **DI DI Martin Ludwig Zitzmann**

BMW AG, München

Wednesday, April 14, 14:00, HF 136

Title: Fast and iterative solution techniques for PEEC modeling in automotive EMC simulation

Abstract: New highly sophisticated automotive electronic systems combined with high operating frequencies lead to an increased risk in terms of problems in the field of electromagnetic compatibility (EMC). Mastering potential EMC problems in the early design phase of cars is a main technical issue for automotive manufacturers. Even if all sub-systems fulfill the given EMC standards a combined integration into the car result in electromagnetic interferences within the total system. Using measurement techniques only this disturbances can not be detected before the first complete prototype is available. At this late stage modifications are usually complex and expensive to execute.

Numerical simulation techniques are an important key to predict the system EMC quality in the early design phase. A numerical simulation method suitable for automotive EMC simulation ist the partial element equivalent circuit method (PEEC). The PEEC method transforms a 3D complex conducting object to a equivalent linear network with basic electrical elements. The electrical behaviour of this circuit can be evaluated by conventional circuit simulators (e.g. SPICE) based on the solution of linear equations. System matrices for realistic problems in the PEEC approach are of dimension 105 - 108 which results in enormous complexity and storage demands. Moreover the density of the system matrices makes this approach improper for iterative solving methods.

By using sophisticated matrix sparsification techniques in conjunction with the well known nodal-analysis (NA) formulation it is possible to obtain a sparse symmetric system of linear equations suitable for iterative solvers.

#### **GROUP: Analysis of Partial Differential Equations**

##### **Dr. Shun-Yin Chu, RICAM**

Monday, May 23, 15:00, HF136

Title: Some introduction and progress of Cahn-Hilliard equations

Abstract:

#### **GROUP: Optimization and Optimal Control & Computational Methods for Direct Field Problems**

##### **Juan Carlos de los Reyes**

TU Berlin

Tuesday, May 24, 10:00, HF 136

Title: "Analysis and numerical solution of the state-constrained optimal control problem governed by the Navier-Stokes equations

Abstract: The optimal control problem of the Navier-Stokes equations in presence of pointwise state constraints is studied. Besides existence and first order optimality conditions, a semi-smooth Newton method is applied for the numerical solution.

#### **GROUP: Financial Mathematics**

##### **Wolfgang Putschögl**

RICAM

Thursday, June 9, 10:00, HF136

Title: Flexible complete models with stochastic volatility generalising Hobson-Rogers

#### **GROUP: Financial Mathematics**

##### **Dr. Jörn Saß**

RICAM

Thursday, June 9, 11:00, HF136

Title: The minimal variance portfolio in markets driven by Levy processes

**GROUP: Financial Mathematics****Dr. Klaus Scheicher**

RICAM

Thursday, June 9, 12:00, HF136

Title: Efficient simulation of the Levy area.

**Group: Computational Logic – Theorema; Group Leader: Professor B. Buchberger****Alberto Damiano**

George Mason University

Wednesday, Juni 15, 13:30, HF 136

Title: COMPUTATIONAL ASPECTS OF SOME PROBLEMS IN ALGEBRAIC ANALYSIS

Abstract: In this talk I introduce some methods used for the algebraic analysis of linear constant coefficient systems of partial differential equations. Examples come from the theory of Dirac operators on Clifford Algebras, which include the Cauchy-Fueter operator acting on functions of (several) quaternionic variables. The main object of study is the symbol matrix  $P$  of the system and the module generated by its rows. I will focus on the computational aspects of this topic, highlighting the use of Groebner Basis techniques whenever possible. I will try to show how Groebner Bases helped in both the experimental phase of the research and in the proof of some results. Some ideas on how to exploit the block matrix structure of  $P$  without the use of Groebner Basis methods are also presented. An alternative, non commutative approach is also discussed using particular differential forms defined "ad hoc" for the Dirac operator. If time permits, I will also briefly talk about the construction of the so called Noetherian Operators which appear in an integro-differential formula for the general solution of linear constant coefficient systems of PDEs.

**GROUP: Optimization and Optimal Control****Samuel Amstutz**

Fraunhofer Institut

Monday, June 20, 11:45, HF136

Title: On the topological sensitivity analysis: some theoretical and numerical aspects

**GROUP: Analysis of Partial Differential Equations****Prof. Corrado Lattanzio, University of L'Aquila**

Tuesday, June 21, 15:30, HF136

Title: Diffusive relaxation limit for hyperbolic systems

Abstract: Our aim is to study the relaxation limits of several hyperbolic systems of balance laws with singular non-homogeneous terms, which lead to parabolic equilibrium systems. In particular, we will discuss the case of strongly parabolic equilibrium systems, either via BGK approximations in the case of weak solutions, by means of compensated compactness techniques, and in the case of Sobolev solutions, by means of singular perturbations techniques. Moreover, we will study the case of semilinear relaxation approximations to incomplete hyperbolic-parabolic equilibrium system, with applications to viscoelasticity, in the case of classical solutions in one or several space variables. The latter case will be discussed by using standard and modulated relative energy estimates.

**GROUP: Analysis of Partial Differential Equations and Inverse Problems****Prof. Jorge Zubelli**

IMPA Rio de Janeiro

Friday, July 1, 10:00, HF 136

Title: On the identification problem of doping profiles in semi-conductors

Abstract: In this talk we will briefly review the identification problem for doping profiles in semiconductors using the voltage to current map. We will show its connection with a local version of the electrical impedance tomography problem and describe some preliminary theoretical as well as numerical results.

This is joint research with Antonio Leitao (UFSC-Brazil) and Peter Markowich (Vienna).

**GROUP: Analysis of Partial Differential Equations****Lukas Neumann**

Universität Wien

Friday, July 1, 11:15, HF 136

Title: Convergence to equilibrium for linear collisional kinetic equations

Abstract: This talk is based on a joint work with Clément Mouhot.

Many kinetic equations feature a collision operator that admits a spectral gap in velocity but due to the degeneracy in space it is impossible to derive convergence to equilibrium in phase space directly. We use the transport term to overcome this difficulty and prove (for a large class of linear collision operators) an exponential decay estimate on the semi-group associated to the non homogeneous problem. Important physical models, like the linearized Boltzmann equation for hard spheres, are covered by our method. The result can be extended to nonlinear equations near equilibrium.

**GROUP: Financial Mathematics****Dr. Klaus Scheicher**

RICAM

Thursday, June 9, 12:00, HF136

GROUP: Financial Mathematics

Dr. Gottlieb Pirsic

RICAM

Thursday, July 8, 10:00, HF136

Title: A Brownian Path construction by Walsh functions

**GROUP: Financial Mathematics****DI Markus Hahn**

RICAM

Thursday, July 8, 11:00, HF136

Title: Optimal trading under partial information

**GROUP: Computational Methods for Direct Field Problems****Dr. Satyendra Tomar**

RICAM

Thursday, July 14, 13:00, HF 136

Title: A study of discontinuous Galerkin methods for water waves simulation

Abstract: A discontinuous Galerkin finite element method for the numerical simulation of water waves will be presented. An accurate representation of the nonlinear waves with a significant amplitude gives rise to the deforming elements and it is well known that the standard

finite element techniques with asymmetric spatial discretization lead to instabilities in the numerical solution of such problems. To overcome this problem, among the practically successful techniques are, the addition of the viscosity terms to the free surface (FS), and

the finite difference (FD) reconstruction of the FS. However, both of these approaches have their own limitations, the viscosity approach unnecessarily damps the wave amplitude, and the FD approach is not attractive in general geometries and for hp- adaptation. In this talk two approaches will be discussed: (1) using the coupled form of the FS equations and implicit time discretizations, and (2) treating the FS equations in decoupled form and explicit time schemes.

A detailed semi-discrete stability analysis, followed by a fully discrete stability analysis of RK4 scheme of the second approach will be presented. Further, to improve the accuracy of the computed velocity field a superconvergent gradient recovery technique based on L2 projections has been employed and the supporting results from the stability analysis will be presented.

**GROUP: Computational Methods for Direct Field Problems****A.o. Univ.-Prof. Dr. Michael Hintermueller**

K.F. Universitaet Graz

Monday, August 1, 14:00, HF 9904

Title: Semismooth Newton Methods: Theory, Numerics, and Applications

**Abstract:**

Recently it was found that semismooth Newton methods are highly efficient numerical solution techniques for certain classes of complementarity and variational inequality problems in function space.

Particular realizations can be easily implemented as primal-dual active set strategies, and they are widely applicable in practice.

The aim of this talk is to discuss the state-of-the-art in semismooth Newton methods for function space problems. Among others, the main topics that will be addressed are finite vs. infinite dimensional methods and a suitable generalized differential, convergence theory -- fast local convergence and rate of convergence, mesh independence, special problem classes yielding global convergence, path-following semismooth Newton concepts in case of low regularity, full multigrid acceleration, and applications ranging from optimal control of partial differential equations, obstacle problems, over contact and crack problems to problems in image restoration.

**GROUP: Computational Methods for Direct Field Problems****Dr. Andrea Cangiani**

University of Pavia

Thursday, Sept. 1, 11:00, HF 9904

Title: Stabilized FEM's and residual-free bubbles for convection diffusion problems:  
Anisotropic meshes and adaptivity

Abstract: The theory of stabilized methods (e.g. SUPG, GLS) for the numerical solution of linear convection-diffusion problems is well established.

Recently, attempts have been made to derive stabilized methods from fundamental principles to better understand their stabilization mechanisms and possible generalizations.

This goal led to the development of the residual-free bubble (RFB) method.

This is based on the

idea of enriching the finite element space and is justified by the fact that the solution of convection-dominated-diffusion problems present multi-scale behaviour (e.g. thin layers).

We shall present our work on the analysis of the RFB method concentrating on anisotropic meshes and mesh adaptivity.

As a byproduct of such analyses, we derived a theoretically optimal value for the SUPG stabilization parameter on anisotropic meshes and obtained a new local indicator that detects in which portions of the mesh stabilization is really necessary.

Finally, we shall present a new algorithm (RFBe) based on combining RFB with exponential fitting techniques.

**GROUP: Computational Logic – Theorema****Manfred Minimair**

Seton Hall University, South Orange, New Jersey, USA

Friday, September 2, 10:00, HF 136

Title: Dixon resultant of Multi-Univariate Composed Polynomials

Abstract: The behavior of Cayley-Dixon resultant construction is analyzed for composed polynomial systems constructed from a multivariate system in which each variable is substituted by a univariate polynomial in a distinct variable. It is shown that the resultant of the composed system can be expressed as a power of the resultant of the outer polynomial system multiplied by powers of the leading coefficients of the univariate polynomials substituted for variables in the outer system. The derivation of the resultant formula for the composed system unifies all the known related results in the literature. Furthermore, it demonstrates that the resultant of a composed system can be effectively calculated by considering only the resultant of the outer system. Since the complexity of resultant computation is typically determined by the degree (and support) of the polynomial system, resultants of a composed system can be computed much faster by focussing only on the outer system.

**GROUP: Computational Methods for Direct Field Problems****Andrew Knyazev**

Department of Mathematics, University of Colorado at Denver

Monday, September 5, 14:00, HF 136

Title: Locally Optimal Block Preconditioned Conjugate Gradient method

**Abstract:** We present the Locally Optimal Block Preconditioned Conjugate Gradient (LOBPCG) method for symmetric eigenvalue problems and discuss its implementation in the software package Block Locally Optimal Preconditioned Eigenvalue Xolvers (BLOPEX). The LOBPCG method, suggested and developed by Andrew Knyazev [1] in the past decade, recently attracts an increasing attention as a potential alternative to the shift-and-invert Lanczos and preconditioned Davidson methods due to its simplicity robustness and fast convergence. Several MATLAB, C, C++ and FORTRAN implementations of the LOBPCG are developed by different groups, e. g., for such applications areas as electromagnetics, structured mechanics and electronic structure calculations.

[1] A.V. Knyazev, "Toward the Optimal Preconditioned Eigensolver: Locally Optimal Block Preconditioned Conjugate Gradient Method."

SIAM Journal on Scientific Computing 23 (2001), no. 2, pp. 517-541.

**GROUP: Inverse Problems**

**Richard Tsai**

University of Texas, Austin

Montag, September 12, 14:00, HF136

Title: Visibility Optimizations

**Abstract:** In this talk, we present our ideas for the search of a path in R2 or R3 that maximizes certain optimality conditions involving visibility. The visibility is defined as the solution of a watered down high frequency wave propagation problem in the presence of occluders with complicated geometry.

Related applications include certain types of path-planning and pursuer-evader problems.

This framework uses a function that encodes visibility information in a continuous way. This continuity allows for powerful techniques to be used in the discrete setting for interpolation, integration, differentiation, and set operations. Using these tools, we are able to limit the scope of search and produce locally optimized solutions. We will also discuss the related control and game formulations.

This is joint work with LT Cheng

**GROUP: Inverse Problems**

**Hend Ben Ameur**

Faculty of Sciences Bizerte, University of Tunis, Tunisia

Dienstag, September 20, 10:30, HF136

Title: Inclusions identification in linear elasticity and thermoelasticity

**Abstract:** We study identifiability and Local Lipschitz stability for the geometric inverse problem of inclusions identification from over specified data.

The normal component of the stress tensor satisfies a homogeneous boundary condition on the unknown geometry. The overspecified data are boundary measurements of the displacement in the case we consider the linear elastic problem and both displacement and temperature in the thermoelastic case.

**GROUP: Optimization and Optimal Control**

**Uwe Prüfert**

TU Berlin

Wednesday, October 5, 14:00, HF136

Title: Interior Point Methods for Optimal Control with Mixed Control-State Constraints

Abstract:

**GROUP: Symbolic Computation – Computational Algebra**

**Prof. Josef Schicho**

RICAM

Wednesday, October 12, 13:30, AS 50

Title: The Markov Equation

Abstract:

**GROUP: Inverse Problems**

**Christina Stöcker**

Caesar Institut

Tuesday, October 18, 11:00, UC 5

Title: Anisotropic mean curvature flow and surface diffusion - numerical solution with level set methods

**Abstract:** Geometric evolution equations are a quite interesting research field, not only from the geometric perspective, but particularly for many modern applications, for example crystal growth. In this talk the evolution laws for anisotropic mean curvature flow and surface diffusion will be presented and a numerical treatment with level set methods and finite elements will be given. A physical application of anisotropic mean curvature flow which has been analyzed already in many scientific papers, is the effect of thermal faceting. Here a non-convex anisotropy function is used leading to backward parabolic equations which are unstable. Regularization of the anisotropy function helps out, and a level set formulation for the regularization will be derived. Another important topic in the level set context is the need of redistancing or reinitialization. In our implementations we make use of a method based on the Hopf-Lax formula which is easy to implement on unstructured grids. An outline of this approach will be given.

**GROUP: Computational Algebra & Financial Mathematics**

**Dr. Klaus Scheicher**

RICAM

Friday, October 21, 10:00, HF136

**Title:** There are strong connections between number systems and fractal tilings of the n-dimensional space.

**Abstract:** In this talk, I will present some results concerning the so called fundamental domain of canonical number systems. Furthermore, I will discuss some related results for algebraic function fields. These results emerge from a collaboration with T. Beck.

**GROUP: Optimization by PDEs**

**Dr. Friedemann Leibfritz**

Tuesday, October 25, 16:00, HF136

**Title:** "Nonlinear semidefinite programs arising in feedback control design for PDE systems"

**Abstract:**

**GROUP: Computational Algebra**

**Dr. Oliver Labs**

RICAM

Tuesday, November 8, 10:15, HF136

**Title:** Hypersurfaces with many singularities

**Abstract:**

**GROUP: Inverse Problems**

**Prof. Alfredo Iusem**

IMPA, Brasil

Tuesday, November 15, 14:15, HF136

**Title:** Inexact versions of proximal point and augmented Lagrangian algorithms in Banach spaces

**Abstract:** We generalize a proximal-like method for finding zeroes of maximal monotone operators in Hilbert spaces with quadratic regularization due to Solodov and Svaiter, making it possible the use of other kind of regularizations and extending it to Banach spaces. In particular, we introduce an appropriate error criterium to obtain an inexact proximal iteration based on Bregman functions and construct a hyperplane which strictly separates the current iterate from the solution set. A Bregman projection onto this hyperplane is then used to obtain the next iterate. Boundedness of the sequence and optimality of the weak accumulation points are established under suitable assumptions on the regularizing function, which hold for any power greater than 1 of the norm of any uniformly smooth and uniformly convex Banach space, without any assumption on the operator other than than existence of zeroes. These assumptions let us, also, obtain similar results in Banach spaces for the Hybrid Extragradient-Generalized Proximal Point method, proposed by Solodov and Svaiter for finite dimensional spaces. We then transpose such methods to generate augmented Lagrangian methdos for Lp-constrained convex optimization problems in Banach spaces, obtaining two alternative procedures which allow for inexact solutions of the primal subproblems. Boundedness of both the primal and the dual sequences, and optimality of primal and dual weak accumulation points, are then established, assuming only existence of Karush-Kuhn-Tucker pairs.

|   |
|---|
| <b>GROUP: Financial Mathematics</b>   |
| <b>Abdelali Gabih</b>   |
| Universität Leipzig   |
| Tuesday, November 15, 12:30, HF136  |
| Title: Portfolio optimization with bounded shortfall risks.   |
| Abstract: We focus on modeling portfolio managers as expected utility maximizers, who derive utility from wealth at some horizon and who must comply with different risk constraints imposed at that horizon, requiring that the wealth may decrease below a given floor. Using the Black-Scholes model of a complete financial market with full information and applying martingale duality methods, analytic expressions for the optimal terminal wealth and the optimal portfolio strategies are given. In a second part we consider a multi-stock market model where the instantaneous rates of return are modeled as an unobservable continuous time, finite state Markov chain. For investment decisions only the prices are available. We combine filtering results with Malliavin calculus to derive the optimal trading strategy in terms of observable processes. |
| <b>GROUP: Financial Mathematics / Forschungsseminar des Instituts für angewandte Statistik</b>  |
| <b>Dr. Gernot Müller</b>  |
| TU München  |
| Thursday, November 24, 15.30, K 224B  |
| Title: Estimation of the COGARCH(1,1) model   |
| Abstract: This talk is about estimation procedures for the COGARCH(1,1) model which is a continuous-time GARCH model introduced by Klüppelberg, Lindner and Maller (2004). We restrict to the case where the driving Levy process is a compound Poisson process. After summarizing some theoretical results for the COGARCH(1,1) model we consider the estimation by the method of moments. This method is applicable only under some restrictive assumptions, e.g. that the observations are equally spaced. To get rid of this assumption we derive a Markov chain Monte Carlo estimation procedure. This procedure can also be used to get volatility estimates for the COGARCH process.   |
| Reference:  |
| Klüppelberg, C., Lindner, A., Maller, R. (2004).<br>A continuous time GARCH process driven by a Levy process:<br>stationarity and second order behaviour.<br><i>J. Appl. Prob.</i> 41, no. 3, 601-622.  |
| <b>GROUP: Computational Algebra &amp; Financial Mathematics</b>   |
| <b>Christiaan van de Woestijne</b>  |
| RICAM   |
| Thursday, November 24, 10:15, AS50  |
| Title: Deterministic equation solving over finite fields  |
| Abstract: Taking of roots in finite fields and, more generally, factoring polynomials over them is usually only efficient if one uses probabilistic algorithms, like the Tonelli-Shanks square root algorithm. In my talk, I'll explain the (?) reason for this, and also I'll give some results from my PhD project, which show that in some cases efficient deterministic algorithms do exist. This is notably the case for quadrics, for diagonal varieties whose degree is less than their dimension, and for elliptic curves.  |
| <b>GROUP: Financial Mathematics</b>   |
| <b>Dr. Gottlieb Pirsic</b>  |
| RICAM   |
| Monday, December 5, 16:15, HF 136   |
| Title: A Malliavin calculus for the discrete time setting   |
| Abstract: Subject of this talk is a paper by Leitz-Martini, where the attempt is made to transport several definitions and theorems of the usual continuous Malliavin calculus to the finite horizon discrete time setting. A crucial tool in this approach is the use of Walsh functions. The Wiener-Ito expansion, Skorohod integral and Malliavin derivative can be defined such that analogous  |

results to the continuous case are obtained. Also, a Clark-Ocone formula can be achieved.

### **GROUP WORKSHOP: Inverse Problems and Financial Mathematics**

RICAM

Tuesday, December 6, 16:00 -18:30, HF136

Talks: 16.00: H. Engl: "Introduction into regularization methods for nonlinear inverse problems"

17.00: H. Egger: "Some aspects of parameter identification problems in computational finance"

17.30: J. Sass: "Hidden Markov and Markov switching models in finance"

18.00: M. Hahn: "Parameter estimation for Markov switching models with Markov Chain Monte Carlo"

18:30: J. Maruhn: "A Semi-Infinite Programming Approach to Robust Static Super-Replication of Barrier Options"

### **GROUP: Computational Algebra**

**Janka Pilnikova**

RICAM

Thursday, Dec. 1, 10:15, AS50

Title: Splitting central simple algebras over the rational numbers.

Abstract: I will present algorithms for finding an isomorphism between a given central simple algebra up to degree 4 over  $\mathbb{Q}$ , and a full matrix algebra, provided it exists. In the talk I will focus on algebras of degree 4 and explain how can the proposed problem be reduced to solving a relative norm equation. Alternative approaches will also be mentioned.

### **GROUP: Financial Mathematics**

**Dr. Juri Hinz**

Institute of Operations Research, ETH Zuerich

Thursday, December 15, 9:15, HF 136

Title: Gas as a flow commodity with implications for pricing and hedging

Abstract: In this talk, we elaborate on valuation of energy--related financial contracts written on prices of flow commodities (such as natural gas, oil, and electrical power). The pricing methodology for such options is not obvious and so the correct valuation is still under lively debate.

We follow an axiomatic setting where a minimal set of reasonable assumptions provides a connection to interest rate theory whose toolkit we utilize to consistently price several option types like caps, floors and collars and cross commodity spreads.

### **GROUP: Computational Algebra**

**Dr. Natee Tongsiri**

Univ. Linz, RISC.

Thursday, Dec. 15, 10:15, AS50

Title: Configuration Space Approach to Piano Mover's Problem

Abstract: One major approach to solve spatial planning problems is to use the concept of Configuration Space. These configuration spaces can be regarded as geometric objects, representable by using semi-algebraic representation.

I will first present the general idea of Configuration Space to the Mover's problem. I will also discuss some ideas and results from my previous work of utilising quantifier elimination, spatial sub-division and pruning to speed up some Mover's problem with both translational and rotational movements.

### **GROUP: Computational Algebra**

**Prof. Josef Schicho**

RICAM

Thursday, Dec. 22, 10:15, AS50

Title: Finding a Point on a Del Pezzo Surface of Degree 6

Abstract: The Lie algebra method was introduced by Willem de Graaf, Michael Harrison, Janka Pilnikova and myself in order to solve systems of algebraic equations with many symmetries, over the field of rational numbers. In this talk we describe a variant solving a case where the Lie algebra is trivial.

***Conferences co-organized by RICAM*****Workshop on “Level Set Methods for Direct and Inverse Problems”  
Linz, September 14 - 16, 2005**Speakers

Gregoire Allaire (Ecole Polytechnique, Paris, France)  
 Luis Caffarelli (University of Texas, Austin, USA)  
 Antonin Chambolle (Ecole Polytechnique, Paris, France)  
 Gerhard Dziuk (University Freiburg, Germany)  
 Michael Hintermüller (University Graz, Austria)  
 Stanley Osher (University of California, Los Angeles, USA)  
 Martin Rumpf (University Bonn, Germany)  
 Fadil Santosa (University of Minnesota, Minneapolis, USA)  
 Otmar Scherzer (University Innsbruck, Austria)  
 Yen-Hsi Richard Tsai (University of Texas, Austin, USA)  
 Hongkai Zhao (University of California, Irvine, USA)  
 Jean-Paul Zolesio (INRIA, Sophia Antipolis, France)

Sponsors

SFB F013 Numerical and Symbolic Scientific Computing, FWF Austrian Science Foundation  
 Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences  
 Government of Upper Austria  
 City of Linz

**Workshop "Inverse Problems"  
in Trippstadt (Germany) from November,24 to November,25, 2005.**Speakers

Bauer Frank (Universität Göttingen )  
 Becker Matthias (TU Darmstadt )  
 Burger Martin (Johannes-Kepler Universität)  
 Constantinescu Dragos (TU Braunschweig)  
 Flury Jacob (TU München)  
 Glaßmeier Karl-Heinz (TU Braunschweig)  
 Grafarend E.W. (Universität Stuttgart)  
 Groten Erwin Heck Bruno (Universität Karlsruhe)  
 Hofmann Bernd (TU Chemnitz)  
 Hohage Thorsten (Universität Göttingen)  
 Jacoby Wolf (Universität Mainz)  
 Kaltenbacher Barbara (Friedrich-Alexander-Universität)  
 Keiner Jens (Medizinische Universität Lübeck)  
 Keller Wolfgang (Universität Stuttgart)  
 Kügler Philipp (Johannes-Kepler Universität)  
 Kusche Jürgen Delft (University of Technology)  
 Maaß Peter (Universität Bremen)  
 Mathe Peter (Weierstraß-Institut für Angew. Analysis und Stochastik)  
 Nashed Zuhair (University of Central Florida)  
 Prestin Jürgen (Medizinische Universität Lübeck)  
 Pereverzev Sergei (RICAM)

Peters Thomas (TU München)  
Rieder Andreas (Universität Karlsruhe)  
Rummel Reiner (TU München)  
Rundell William (Texas A&M University)  
Schreiner Michael (Interstaatliche Hochschule für Technik Buchs NTB)  
Simons F.J. (UCL Earth Sciences)  
Sneeuw Nico (Universität Stuttgart)  
Tautenhahn Ulrich (Hochschule Zittau/Görlitz (FH))  
Xu Peiliang (Kyoto University)

**Workshop on Cell Motility and Cytoskeletal Dynamics**  
**WPI, Wien, Nov. 10 - Nov 12, 2005**

Organizers:

Y. Dolak (RICAM, Linz)  
C. Schmeiser (University of Vienna, RICAM)  
V. Small (IMBA, Vienna)

**Workshop "Control of Complex Fluids"**  
**Workshop, Linz, October 10-14, 2005**  
within the Special Semester on Computational Mechanics

Speakers

Marek Behr (RWTH Aachen and Rice University)  
Martin Berggren (Uppsala University)  
Thomas Bewley (UCSD)  
Malte Braack (University of Heidelberg)  
Nicolas Gauger (DLR Braunschweig and HU Berlin)  
Omar Ghattas (University of Texas at Austin)  
George Haller (MIT)  
Matthias Heinkenschloss (Rice University)  
Vincent Heuveline (University of Karlsruhe)  
Amnon Meir (Auburn University)  
Volker Schulz (University of Trier)  
Nicholas Zabaras (Cornell University)

**MEGA 2005 (Effective Methods in Algebraic Geometry)**  
in Alghero, Italien.

MEGA is a series of roughly biannual conferences on computational and application aspects of algebraic geometry and related topics with very high standards.

In 2005, MEGA was organized by:

Patrizia Gianni (Pisa, Italy), chairman  
Alicia Dickenstein (Buenos Aires, Argentina)  
Andre Galligo (Nice, France) Marc Giusti (Palaiseau, France)  
Teo Mora (Genova, Italy)  
Tomas Recio (Santander, Spain)  
Josef Schicho (Linz, Austria)

**Computational Mechanics Challenges Day**  
**Linz, October 21, 2005**  
within the Special Semester on Computational Mechanics

Workshop Topics

The purpose of this one-day event on October 21, 2005 during the Special Radon Semester 2005 was the promotion of new computational techniques for mechanical problems.

We invited scientists from Austrian universities as well as other Austrian research institutions to present and discuss challenging problems in mechanics, for which computational techniques are not yet available or, if available, require significant further development.

The framework of the special semester with the presence of a large group of international experts gives the unique opportunity to discuss possible novel strategies for tackling these problems in a highly competent forum of scientists in computational mathematics and mechanics.

Speakers

Hartmut Bremer (Johannes Kepler University of Linz, Austria)

Helmut Ennsbrunner and Kurt Schlacher (Johannes Kepler University of Linz, Austria)

Alexander Kainz (Johannes Kepler University of Linz, Austria)

Franz Dieter Fischer (University of Leoben, Austria)

Sergei Repin (Steklov Institute of Mathematics at St. Petersburg, Russia)

Markus Schoeberl and Kurt Schlacher (Johannes Kepler University of Linz, Austria)

Klaus Zeman and Konrad Krimpelstaetter (Johannes Kepler University of Linz, Austria)

**International Workshop on  
"Direct and Inverse Field Computations in Mechanics"**  
**Workshop, Linz, November 7 - 11, 2005**  
within the Special Semester on Computational Mechanics

Workshop Topics

Computational Methods in Non-linear Mechanics

Computational Structural Mechanics

Mixed and Nonstandard FEM

Domain and Hybrid Decomposition Methods

Topology Optimization and Optimal Design in Mechanics

Optimal Control in Mechanics

Inverse Problems in Mechanics

Speakers

Mark Ainsworth (Strathclyde University, Glasgow, Scotland)

Bob Anderssen (CSIRO, Australia)

Martin P. Bendsoe (Technical University of Denmark, Denmark)

Edgar Bertotí (University of Miskolc, Hungary)

Manfred Bischoff (TU München)

Hans Georg Bock (University of Heidelberg)

Marc Bonnet (Ecole Polytechnique, Paris, France)

Blaise Bourdin (Louisiana State University)

Zdenek Dostál (Technical University of Ostrava, Czech Republic)

Pierre Duysinx (University of Liège, Belgium)

Alexandra Gaevskaya

Ville Havu (Helsinki University of Technology, Finland)

Michael Hintermueller (University of Graz, Austria)  
Thorsten Hohage (University of Göttingen, Germany)  
Axel Klawonn (University of Essen, Germany)  
Michal Kocvara (Academy of Sciences of the Czech Republic, Prague)  
Vadim G. Korneev (St. Petersburg, Russia)  
Günter Leugering (University of Erlangen-Nuremberg, Germany)  
Alfred Louis (Saarland University, Germany)  
Yvon Maday  
Joyce R McLaughlin (Rensselaer Polytechnic Institute, New York, USA)  
Arnd Meyer (Technical University of Chemnitz, Germany)  
Gen Nakamura (Hokkaido University, Japan)  
Sergei Nepomnyaschikh (Academie of Science, Novosibirsk, Russia)  
Günter Of (University of Stuttgart, Germany)  
Joseph E. Pasciak (Texas A & M University, USA)  
Daya Reddy (University of Cape Town, South Africa)  
Sergei Repin (Steklov Institute of Mathematics at St. Petersburg, Russia)  
Joachim Schöberl (Johann Radon Institute, Austria)  
Roman Stainko (SFB F013, University of Linz, Austria)  
Rolf Stenberg (Helsinki University of Technology, Finland)  
Mathias Stolpe (Technical University of Denmark, Denmark)  
Emilio Turco (University of Sassari, Italy)  
Jan Valdman (SFB F013, University of Linz, Austria)  
Ragnar Winther (University of Oslo, Norway)  
Barbara Wohlmuth (University of Stuttgart, Germany)

### **Block Lectures**

**"Conversion from imperfection-sensitive into imperfection-insensitive elastic structures"**  
**by Herbert Mang** (President, ÖAW, Vienna University of Technology, Austria),  
October 17, 2005  
within the Special Semester on Computational Mechanics

**Workshop "Efficient methods for time-dependent optimal control: preconditioning, reduced order modelling and feedback control"**

**Workshop, Linz, November 21 - 24, 2005**  
within the Special Semester on Computational Mechanics

### Workshop Topics and Scope

Time dependent optimal control problems require special attention in various aspects to achieve an efficient numerical solution. The themes of this workshop were grouped around issues of preconditioning, use of reduced order models and design of feedback controllers. The workshop consisted of lectures by experts in the field and informal plenary and non-plenary discussion periods.

### Speakers

Peter Benner (TU Chemnitz)  
George Biros (University of Pennsylvania)  
Lars Grasedyck (Max Planck Institut Leipzig)  
Michael Hinze (TU Dresden)  
Angela Kunoth (University of Bonn)  
Friedemann Leibfritz (University of Trier)

Rainer Tichatschke (RICAM)  
 Michael Ulbrich (University of Trier)  
 Stefan Ulbrich (TU Darmstadt)  
 Stefan Volkwein (University of Graz)  
 Andy Wathen (Oxford University)  
 Karen Willcox (Massachusetts Institute of Technology)  
 Walter Zulehner (Johannes Kepler Universität Linz)

### **3.2. SPECIAL SEMESTER ON COMPUTATIONAL MECHANICS**

#### ***Overview by Prof. Ulrich Langer***

The Special Semester on “Computational Mechanics” was held at RICAM in Linz, October 3 – December 16, 2005. Nine long-term visitors agreed to organise lectures, seminars, workshops and mini-workshops on the following topics:

#### **Novel Discretization and Solver Techniques in Mechanics:**

Discontinuous Galerkin methods:

Organizer: Raytcho Lazarov (TAMU, USA)  
 Co-organizer: Satyendra Tomar (RICAM, Austria)

Non-standard mixed FE-techniques:

Organizer: Dietrich Braess (University of Bochum, Germany)  
 Co-organizer: Joachim Schoeberl (RICAM, Austria), Walter Zulehner (JKU, Austria)

hp-techniques in mechanics:

Organizer: Alexander Duester (TU Munich, Germany)  
 Co-organizer: Joachim Schoeberl (RICAM, Austria)

A posteriori estimates and adaptivity in solid mechanics:

Organizer: Sergei Repin (Steklov Institute of Mathematics at St. Petersburg, Russia)  
 Co-organizer: Jan Valdman (SFB013, Austria)

H-matrix techniques:

Organizer: Wolfgang Hackbusch (MPI, Leipzig, Germany)  
 Co-organizer: David Pusch (JKU, Austria)

Robust parallel algebraic multigrid and multilevel techniques:

Organizer: Svetozar Margenov (BAS, Bulgaria)  
 Co-organizer: Johannes Kraus (RICAM, Austria)

Domain Decomposition Methods:

Organizer: Sergei Nepomnyaschikh (Academy of Science, Novosibirsk, Russia)  
 Co-organizer: Sven Beuchler (JKU, Austria)

Numerical simulation of coupled fields:

Organizer: Manfred Kaltenbacher (University Erlangen, Germany)  
 Co-organizer: Marco Discacciati (RICAM, Austria)

#### **Inverse, Control, and Optimization Problems in Mechanics:**

Inverse problems and model identification in mechanics:

Organizer: Barbara Kaltenbacher (Uni Erlangen, Germany)  
 Co-organizer: Martin Burger (JKU, Austria)

Control and optimization problems in mechanics:

Organizer: Ekkehard Sachs (Uni Trier, Germany)  
 Co-organizer: Roland Griesse (RICAM, Austria), Karl Kunisch (RICAM, Austria)

Conversion from imperfection-sensitive into imperfection-insensitive elastic structures  
Organizer: Herbert Mang (Vienna University of Technology and ÖAW, Austria)  
Co-organizer: Roman Stainko (SFB F013, Austria)

There were several block lectures and talks on challenging problems in Mechanics delivered by distinguished scientists in mechanical engineering (see chapter 3.1 Conferences co-organized by RICAM). The highlights of the special semester were the special events organized by the long-term visitors and by local people. The complete list of the special events can be found on the home page

<http://www.RICAM.oeaw.ac.at/sscm/>

of the special semester, where you can also find the complete programme and further information about the special semester. We would like to mention here only three special events which had a great impact on the research activities of the participants and on the public:

International Workshop on "Direct and Inverse Field Computations in Mechanics"  
held at RICAM, November 7 - 11, 2005: The sessions of this workshop were devoted to the following topics:

Computational Methods in Non-linear Mechanics,  
Computational Structural Mechanics,  
Mixed and Non-standard FEM,  
Domain and Hybrid Decomposition Methods,  
Topology Optimization and Optimal Design in Mechanics,  
Optimal Control in Mechanics,  
Inverse Problems in Mechanics.

More than 30 scientists from all over the world presented their newest research results.

See [http://www.RICAM.oeaw.ac.at/sscm/srs\\_ev/difcome/](http://www.RICAM.oeaw.ac.at/sscm/srs_ev/difcome/) or more information, see also chapter 3.1 Conferences co-organized by RICAM.

Computational Mechanics Challenges Day held at RICAM on October 21, 2005:

The purpose of this one-day event was the promotion of new computational techniques for mechanical problems. The framework of the special semester with the presence of a large group of international experts provided the unique opportunity to discuss possible novel strategies for tackling these problems in a highly competent forum of scientists in computational mathematics and mechanics.

See [http://www.RICAM.oeaw.ac.at/sscm/srs\\_ev/challenge/](http://www.RICAM.oeaw.ac.at/sscm/srs_ev/challenge/) for more information, see also chapter 3.1 Conferences co-organized by RICAM.

Public Lecture on "Gottfried Wilhelm Leibniz - far ahead of his time"

by Erwin Stein (University of Hanover, Germany), November 10, 2005: This lecture attracted much public attention of the media and resulted also in radio and TV broadcasts.

See [http://www.numa.uni-linz.ac.at/Board/jks\\_2005/stein.html](http://www.numa.uni-linz.ac.at/Board/jks_2005/stein.html) for more information.

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 will result in joint publications, in improved or new software packages, in joint presentations on conferences, in joint organizations of conferences, workshops, minisymposia etc. Therefore, the follow-up phase will show the long-term impact of this special semester on the scientific community. We will provide more information about this follow-up phase on the home page of the special semester. A detailed description of the activities during the special semester and a first estimation of the output in form of publications etc. and of the impact on the scientific community will be given in a special report that is in progress.

All participants of the special semester who stayed for some extended period were asked to fill in an evaluation form. Out of 117, 31 returned the form. We now give an overview over the questions and over the number of replies in each category:

|   |  |  |
|---|--|--|
| How many days were you in residence at RICAM?   | up to 7 days<br>1 to 6 weeks<br>more than 6 weeks  | 11 participants<br>4<br>16                               |
| Please give your current position   | Graduate<br>Student<br>post-doctoral<br>other  | 8<br>3<br>6<br>13  |
| Overall, how useful did you find this Special Semester?   | very useful<br>moderately useful<br>not useful   | 27<br>2<br>2   |
| Overall, did you find that the lectures assumed a level of knowledge that was ...                     | High<br>Medium<br>Low  | 22<br>9<br>0   |
| Overall, what level of interest were the topics to you personally                                     | High<br>Medium<br>Low  | 22<br>9<br>0   |
| Please indicate the items you found particularly useful in connection with the Special Radon Semester | Website<br>Social Activities<br>Organisation<br>Lecture Rooms<br>Staff<br>Info Folder<br>Computer Facilities<br>Accommodation<br>Workspace<br>Location               | 25<br>12<br>18<br>20<br>23<br>12<br>16<br>26<br>12<br>12 |
| How would you rate the overall educational value or merit of the program?                             | Exceptional Opportunity<br>Worthwhile Experience<br>Generally not too useful, might help some<br>Probably of no merit  | 21<br>10<br>0<br>0                                       |
| How would you rate the overall scientific quality of the program?                                     | Excellent<br>Very good<br>Somewhat good<br>Poor  | 22<br>10<br>0<br>0                                       |
| Has the experience you've had at RICAM been useful training for your intended career?                 | very useful<br>moderately useful<br>not useful<br>does not apply   | 18<br>8<br>0<br>5  |
| How would you describe the attitude of the directors and other senior participants to you?            | Encouraged spirit of inquiry, helpful<br>Willing, but did not go out of their way<br>Discouraging, not helpful<br>Does not apply                                     | 22<br>5<br>0<br>4  |
| How would you describe the opportunity you had to relate to fellow participants and visitors?         | Open, friendly supportive atmosphere<br>Permitted but not encouraged<br>Generally unfriendly, closely-knit group<br>Discouraging, unfriendly place<br>Does not apply | 28<br>3<br>0<br>0<br>0                                   |

|   |   |                         |
|---|---|-------------------------|
| How would you rate the overall quality of the tutorials and workshops organized by RICAM? | Excellent<br>Very good<br>Generally average<br>Poor overall<br>Does not apply | 14<br>13<br>4<br>0<br>1 |
| How would you rate the opportunity you had to develop your own workgroups, seminars etc.? | Excellent<br>Good<br>Poor<br>Does not apply                                   | 11<br>6<br>4<br>10      |
| Speaking personally, in terms of productivity, how would you describe your time at RICAM? | Very productive<br>Moderately productive<br>Not productive<br>Does not apply  | 21<br>8<br>1<br>1       |

Comments

- All went very smoothly, nice job.
- Please think carefully about the group, the Special Semester is addressed to. If one writes „Computational Mechanics“ for „young PhDs“ there won‘t only be mathematicians.
- It would have been helpful if there had been more tutorials and extra courses for beginners. In all: I very much liked the organization and program of the Special Semester, thank you very much!
- Very good workshop, great atmosphere!
- Some of the lectures were not as well prepared as the others.
- Directors and senior participants strongly support any new ideas!
- The topics were not directly linked with my work, but it is always useful to have some general background knowledge.
- I would like to thank very sincerely the whole RICAM staff involved in the organisation of the Special Semester. I hope to see you again!
- One form of scientific work was not enough presented: it is Round Table, Open Discussions on a particular area.
- For me the contact with other researchers was comparably more valuable than the lectures itself.
- Introduction of new areas of knowledge: It could not have been better in this respect!
- The lectures were a pleasure!
- RICAM is a great and inspiring place to visit!
- Directors and senior participants: extremely engaged – thanks!
- The Raab-Heim was a good choice due to its good location to university, friendly staff, nice rooms
- Organization and information in advance: Everything perfect, compliments to M. Fuchs, A. Weihs and J. Kraus!!
- Thanks further for all generous activities besides, like the day trip to Wachau, coffee during breaks, conference dinners ...
- Maybe keep one day a week free of lectures ... for workshops and further special events.
- If the time allows it, a presentation of some people of RICAM would be interesting as well ...

**3.3. FURTHER PLANS FOR SPECIAL SEMESTERS**

The Special Semester on Groebner Bases and Related Methods takes place in Linz from February to July 2006. It is organized by RICAM in close cooperation with RISC. It is directed by Bruno Buchberger (RICAM and RISC) and Heinz Engl (RICAM) with the help of Alexander Zapletal and Magdalena Fuchs.

The special semester brings together researchers from all over the world for joint research on Groebner bases and related theories and methods. Also, through the special semester, knowledge on these theories should be made available and disseminated in a new way that uses both recent advances in formalized mathematics as well as web technology. Both established researchers as well as junior researchers, post docs, and PhD students are welcome to participate in the activities of the special semester.

The Special Semester has 4 major research focus lines:

- Groebner Bases Theory and Applications in Algebraic Geometry
- Computations of Groebner Bases
- Formal Groebner Bases Theory
- Recent Applications of Groebner Bases

For each of these focus lines one or more workshops are organized. Altogether, 8 workshops will be held. Each of it lasts for several days or one or two weeks and has one or more chairmen. Most of them are world leading experts in their field of research. In the following table, one can find all workshops and their chairmen:

|  |  |
|--|--|
| A, Groebner Bases Theory and Applications in Algebraic Geometry                | Gert-Martin Greuel<br>Gerhard Pfister                        |
| B1, Approximate Commutative Algebra  | Lorenzo Robbiano   |
| B2, Efficient Computation of Groebner Bases                                    | Jean-Charles Faugère<br>Viktor Levandovskyy<br>Quoc-Nam Tran |
| C, Formal Groebner Bases Theory  | Bruno Buchberger   |
| D1, Groebner Bases in Cryptography, Coding Theory, and Algebraic Combinatorics | Mikhail Klin<br>Ludovic Perret<br>Max Sala                   |
| D2, Groebner Bases in Symbolic Analysis  | Peter Paule<br>Dongming Wang<br>Markus Rosenkranz            |
| D3, Groebner Bases in Control Theory and Signal Processing                     | Hyungju Park   |
| D4, Groebner Bases in Life Sciences  | (under negotiation)  |

The participants of the special semester come from all over the world, like Canada, Iran, Kenya, Japan, Germany, France, Italy, Russia, Argentina etc. Most of them will stay at RICAM for one or two workshops. Among all these guests there are well-known experts like Sergey A. Abramov, N.K. Bose, Hans-Gert Gräbe, Herwig Hauser, Erich Kaltofen, Theo Mora, Marko Petkovsek, Dana Scott, Michael Singer, Hans J. Stetter, Carlo Traverso, Mark van Hoeij and many more.

Additionally, there are several young PhD students who come for a longer period of time to participate in several workshops.

Altogether, more than 200 visitors will come to RICAM during this special semester.

All information concerning the special semester can be found on  
<http://www.RICAM.oeaw.ac.at/srs/groeb/>

### **3.4. SPECIAL SEMESTER ON MATHEMATICS IN LIFE SCIENCES**

This special semester, for which a precise name still has to be found, will take place approximately from October 2007 through January 2008. Organizers include Robert Aderessen (Canberra), Martin Burger (Linz), Vincenzo Capasso (Milano), Robert Eisenberg (Rush University Chicago), Heinz Engl (RICAM), Philipp Kugler (Linz), Peter Markowich (RICAM), Peter Pohl (Biophysics, Linz), Otmar Scherzer (Innsbruck), Christian Schmeiser (RICAM), Peter Schuster (Vienna). Heinz Engl is currently chairing the activities.

The current planning is as follows:

First week: tutorials, setting the stage for the main topics, interlaced talks on bio topics and on mathematical methods.

During the semester: 2 longer periods of workshops connected to each other (timing and precise setup still to be discussed).

Culminating workshop end of January 2008 (in Obergurgl, Tyrol).

In between: a lot of ad-hoc-organized internal events, not too many formal events. Smaller specialized workshops possible. But: enough time for starting cooperations is needed, not too many formal events!

Participants on 3 time scales: whole semester (mainly postdocs, if possible also from biosciences, doctoral students, hopefully some senior persons); several weeks; workshop participants.

Desired outcome:

Long term cooperations between bioscientists and mathematicians in and around RICAM

Joint publications, survey papers e.g. in EJAM, one or more books with longer survey articles in the Radon series (de Gruyter)

Software for some special tasks (proposed by Schmeiser), semester should clarify if this is feasible, for which tasks, with which requirements

Main topics (to be covered both in tutorials and by major workshops):

Biomechanics of cells: Schmeiser, Markowich, Small(?)

Chemotaxis (emphasis on mathematical aspects): Markowich

Pattern formation (stochastic models, pde aspects, multiscale analysis, use of neighborhood relations and heuristic models): Capasso, Schuster, Burger, Anderssen

Bioimaging: Scherzer, Markowich, Seidler (?)

Systems biology (mainly ODE aspects, forward and inverse): Engl, Kugler, Schuster

Membranes and channels: Eisenberg, Pohl, Burger

The names mentioned are those who contributed to the discussion and are not meant exclusive; (?) indicates that those have not been asked yet.

Organizing committees should be not too large and with clear responsibilities!

Possible additional topics (e.g., for smaller workshops): bio (e.g. blood) flow (Kunisch, Canic, Quarterni), mathematical models in food production (Anderssen), tumor growth (Friedman), "silicon cell" (Schmeiser), discrete aspects (?), symbolic methods.

Topics which we do NOT cover either due to the lack of expertise and/or since they are well studied elsewhere include folding and bioinformatics topics like data mining.

### **3.5. SPECIAL SEMESTER – PUBLICATIONS**

Of course, most of the results obtained in the special semesters will be published as regular journal papers. But, in addition, we plan two edit books containing longer survey papers originating from the courses given in the special semester. The first such book (originating from the special semester on Computational Mechanics) is already in a concrete planning stage. The outlet for these books will be most likely a

“Radon Series for Computational and Applied Mathematics”

to be published by de Gruyter. The tentative editorial board will include:

Hansjörg Albrecher, Heinz W. Engl (Editor-in-Chief), Ronald Hoppe, Karl Kunisch, Ulrich Langer, Harald Niederreiter, Christian Schmeiser