AUSTRIAN ACADEMY OF SCIENCES

ANNUAL REPORT 2004

Johann Radon Institute for Computational and Applied Mathematics

PERIOD:	1.1.2004- 31.12.2004
DIRECTOR:	Prof. Heinz W. Engl
ADDRESS:	Altenbergerstr. 69 A-4040 Linz

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 employees individually.

1.) The Development of the Institute in General: Personnel, Infrastructure

The Institute started its operation officially on January 1, 2003, the official opening ceremony took place in Linz on March 28, 2003. According to the Mission Statement approved by the Board at its first meeting, the Institute plans to

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

The year 2004 was the first year where the Institute, though still in its development and build-up phase, was fully operational. At the end of 2003, the Institute had employed 14 scientists in five working groups. In 2004, while a few scientists left the Institute again, e.g. to accept permanent positions, we succeeded in attracting further promising young scientists both as PostDocs and, via external funding, as doctoral students. We will report about this aspect below.

The first year was dedicated to building up the infrastructure and to attract scientists that will enable us to achieve these goals; as we hope this report will show, we are well under way, and also, the scientific achievements obtained in the short period that the scientists we could attract were in residence so far conform to high international standards. It is a priority to encourage collaborations between the groups at the Institute, and to this end, we started with internal and external seminars as soon as the first scientists had started to work in Linz (for details see below). First plans for Special Semesters were formulated; their realization will be started as soon as the budget figures for 2004 and 2005 are known.

The Institute could move into its offices in the "Hochschulfondsgebäude" at the campus of the Johannes Kepler Universität Linz in late August of 2003. We currently have 14 rooms (including our own seminar and lecture room) totaling 327 m². Already now, the offices are very crowded, we need more space. Fortunately, the university is able to rent some space in the immediate neighborhood of the campus and will sublet about 300 m² to the Academy for the use of RICAM. These new offices will have to undergo some renovation and will have to be furnished, we hope to be able to move into these offices gradually from March 2005. The full use of these additional offices will be absolutely necessary for our first Special Semester in the fall of 2005 (see below). It is not an ideal situation that we will now have two separate sets of offices in different locations, but this is the only option currently available, and a walk between these two locations takes only five minutes. In about three years, there will be the option to move the whole Institute into the "Science Park" next to the university campus; it will have to be decided then if this is feasible. Currently, the Institute has its offices in the same building as the Industrial Mathematics Institute of the University of Linz, the Industrial Mathematics Competence Center (which are also headed by the Institute Director Heinz W. Engl) and part of the FWF Special Research Area SFB013 "Numerical and Symbolic Scientific Computing", other university institutes which cooperate closely with RICAM via their heads are in the next building (with the only exception of RISC – the Research of Symbolic Computation, which is located in nearby Hagenberg). This close proximity of a large number of applied mathematicians in different institutions provides ample opportunities for cooperation, and this fact will have to be weighed against the opportunity to bring the whole Institute back together into one location when this decision will have to be taken.

In 2004, the computing infrastructure had to be expanded; in 2005, another major expansion will have to take place due to the fact that the Institute will have a second location. In addition to Florian Tischler (who works half time as software engineer at RICAM and is also employed half time at the Industrial Mathematics Institute of Linz University, which provides a lot of synergies), we hired a second computer engineer (Wolfgang Forsthuber), who will mainly be in charge of the computer infrastructure at the second location and also handle all computer and WWW-needs for the Special Semesters.

We give a short overview over what was bought in 2004 and what is planned for 2005:

IT-Infrastructure:

2004

Clients:

Laptops:

Acer Travelmate 8003 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 each scientific employee. 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 programmed applications or with the application transparent cluster software Mosix. As scientific mathematics software Matlab, Mathematica and Maple are installed as needed.

Servers:

Communication server:

The server provides the RICAM webpage including database access, email access through pop3 and imap, spam and virusfilter for email services, webmail access, groupware scheduler, mailing list manager and cvs repository. Operating System is Linux with extra access control kernel patches to add an extra security layer. All used software (except for virus scanner) is open source and free for use. In 2004 a self written content management system for our publications database and the events page was added and the users got the possibility to train our spamfilter through copying unrecognized messages to a special "learn-folder"

Fileserver:
The Fileserver allows centalized user management and data storage for Windows and Linux Clients. Each user can access his 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 Johannes Kepler University of Linz. 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 2004 customised scripts for easy user management where added.

Terminal server:
The terminal server allows access to Windows applications on linux through the rdesktop client. Operating system is Windows2003 Server with Terminal Services licensed. No changes to the configuration where made in 2004 as everything is working well.

Peripheral devices:

24 port 1000Mbit switch:
We got a 24 port 1000Mbit switch from Austrian Academy of Sciences computer center for the fileserver and the workstations cluster enabled workstations.

Video projector:
A fixed video projector for the presentation room was bought.

Plans for 2005

Clients:

More PC architecture based dual processor workstations will be bought to provide a workstation for each employee. As operating systems Linux will be installed to expand our cluster. Only if requested a dual boot configuration with both Linux and Windows will be 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 programmed applications or with the application transparent cluster software Mosix. As scientific mathematics software Matlab, Mathematica and Maple will be installed as needed.

Servers:

Depends on the requirements of the scientific employees. Currently there are no plans to buy additional servers.

Peripheral devices:

Hardware firewall:
The for 2004 planned firewall will be bought soon. The delay was caused by temporary budgetary situation.

Printer:
A color laser printer and 4 small black&white laser printers will be bought for the new premises.

Network at the new premises:

The new premises will be connected by a 10Mbit leased line. The same network subsegment will be used in both locations to provide access between all computers. The firewall will also protect all computers at the new premises.

The crucial step in the development of the Institute was of course the process of hiring scientific employees. We continued to recruit internationally and to hire only PostDocs (or even more senior scientists) from the basic funds (ÖAW / Land Oberösterreich) who should then, in due course, bring in external funds via FWF and similar projects for hiring PhD students. Some have already succeeded in doing so, and more have either already submitted project proposals for external funding (mainly to FWF) or will do so in the near future. In addition to scientific achievements (with special emphasis on inter-disciplinary cooperations), success in acquiring external funds will be a criterion for extensions of employment contracts.

Of those 14 scientists employed by RICAM at the end of 2003, the following ones left in 2004:

Name	Employed until	Left to	Position
Antonio Leitao	April 2004	Federal University of Santa Catarina	Associate Professor
Christian Schmeiser	October 2004	University of Technology in Vienna	Professor at the University of Technology, Vienna
Mircea Marin	October 2004	University of Tsukuba	Tenured Research Scientist
Sven Beuchler	September 2004	University of Linz	University Assistent

It should be noted that it was the intention from the outset that the half-time employment of Christian Schmeiser at RICAM should last only for one year to help build up the institute; since October 2004, Schmeiser is again full-time with the University of Technology in Vienna, but is co-leader of the group “Analysis of Partial Differential Equations” and is regularly present in Linz (as most of the other external group leaders).

In 2004, the following additional PostDocs were hired:

Name	At RICAM since	Doctorate: year, institution	Came to RICAM from
Henry Chu	01.05.2004	2003, The Chinese University of Hong Kong	The Chinese University of Hong Kong
Willem De Graaf	01.10.2004	1997, University of Eindhoven	The University of Sydney
Yasmin Dolak	01.09.2004	2004, Vienna University of Technology	Vienna Univ. of Technology
Roland Griese	15.07.2004	2003, University of Bayreuth	Karl-Franzens University, Graz
Karel Janecek	01.10.2004	2004, Carnegie Mellon University, Pittsburgh	Carnegie Mellon University
Stefan Müller	01.11.2004	1999, University of Vienna	University of Vienna
Florina Piroi	01.10.2004	2004, University of Linz	RISC, University Linz
Elena Resmerita	01.03.2004	2003, University of Haifa, Israel	UCLA
Markus Rosenkranz	01.07.2004	2003, University of Linz	University of LInz
Joachim Schöberl	01.09.2004	1999, University of Linz	University of Linz
Boris Vexler	01.10.2004	2004, University of Heidelberg	University of Heidelberg

All these persons are funded via basic funds from ÖAW/Land Oberösterreich. In addition, Dipl.-Ing. Alexander Zapletal was hired via these basic funds for the task of scientific planning (under the direction of Bruno Buchberger) of the Special Semester on Gröbner Bases, planned for the fall of 2006.

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

Name	At RICAM since	Doctorate: year, institution	Poject: agency/number/leader
Nicoleta Bila	01.04.2004	1999, University of Bucharest	FWF, F1308, Engl
Pavel Chalmoviansky	01.04.2004	2002, University of Bratislava	FWF, F1315, Schicho
Wilfried Meidl	01.09.2004	1998, University of Klagenfurt	FWF, S8313, Winterhof
Georg Regensburger	01.11.2004	2004, University of Innsbruck	FWF, F1322, Buchberger

Name	At RICAM since	Diploma: year, institution	Poject: agency/number/leader
Almedin Becirovic	01.11.2004	2002, University of Linz	FWF, Y192, Schöberl
Tobias Beck	01.04.2004	2002, University of Erlangen	FWF, F1303, Schicho
Nina Brandstätter	01.04.2004	2004, University of Vienna	FWF, S8313, Winterhof
Hui Cao	01.08.2004	2004, University of Beijing	FWF, P17251-N12, Pereveryzev
Herbert Egger	01.04.2004	2002, University of Linz	FWF, F1308, Engl
Robert Gaisbauer	01.11.2004	2002, University of Linz	FWF, Y192, Schöberl
Benjamin Hackl	01.10.2004	2000, University of Linz	FWF, F1308, Engl
Andreas Hofinger	01.04.2004	2003, University of Linz	FWF, F1308, Engl
Shuai Lu	01.08.2004	2004, Fudan University, Shanghai	FWF, P17251-N12, Pereveryzev
Janka Pilnikova	01.04.2004	1999, Comenuis University, Slovakia	FWF, F1303, Schicho
Ibolya Szilagyi	01.04.2004	2000, University of Debrecen	FWF, F1303, Schicho
Sabine Zaglmayr	01.11.2004	2002, University of Linz	FWF, Y192, Schöberl

Thus, at the end of 2004, there were as many externally funded scientists as there are Post-Docs financed via the basic funds. Also, there were as many Austrians as there are foreigners, although this distinction is not completely informative: There are both Austrians who joined RICAM coming from abroad and foreign nationals who did their prior work at other institutions in Austria.

In 2004, a sixth working group was added: Optimization and Optimal Control, led by Prof. Karl Kunisch (Universität Graz). The procedure for adding a working group, which will also be followed in the future, was to have a proposal reviewed by the Board (Kuratorium), on whose recommendation the Institute Director established the group. In the future, we hope to be able to add a group on Mathematical Aspects of Computer Science headed by the Wittgenstein Prize winner Prof. Georg Gottlob (TU Vienna), which would fit into the Institute quite well scientifically. Prof. Gottlob, who is interested in this option, will be invited to submit a proposal as soon as it becomes clear that the long-term budget of the Institute will allow the establishment of this group. A pre-proposal outlining his general ideas is the following:

Hypergraph-Based Methods for Problem-Solving

Many computational problems are difficult to solve because they are NP-hard, which means that they have most likely no polynomial-time solution algorithm. Among these problems are a large number of problems of high industrial relevance, such as scheduling, sequencing, and various other optimization problems. Note that NP-hardness refers to the worst-case complexity of problems. Recognizing problem instances that easier than these "worst cases" is a rewarding task given that better algorithms can be used for these easy cases.

The NP hardness of a problem is often due to the intricate and highly cyclic structure of the graphs or hypergraphs representing the hardest instances. For a large class of problems, instances having an associated graph or hypergraph of low cyclicity are solvable in polynomial time (and often even in linear time). One of the best measures of the "degree of cyclicity" of a graph is Robertson's and Seymour's notion of treewidth [1]. Many NP-hard problems become polynomially solvable on instances of bounded treewidth. There are, however, problems whose structure is better descibed by hypergraphs than by graphs, cf. [3]. Consequently, various cyclicity measures for hypergraphs have been developed, among which the notion of "hypertree width" [2], based on "hypertree decompositions" which is more general than other measures published so far, and has the advantage that hypergraphs of bounded hypertree width can be recognized in polynomial time [2]. Briefly, such decompositions specify how a problem should be decomposed in order to be solvable by polynomial-time divide-and-conquer algorithms. Problems of bounded hypertree width can, morover, be solved by highly parallel algorithms [4]

So far, hypertree decompositions have beeen applied to various problems in the database domain (e.g., conjuntive query optimization) [2]and in AI (constraint satisfaction problems) [3]. It was, moreover, shown that sparse integer programs of bounded hypertree width can be solved in polynomial time. However, many research problems related to hypertree decompositions are left for future research [2,5,6]. For example, some important generalizations of hypertree-width are known, that also lead to polynomial problem-solving in case of bounded width. However, it is currently not known whether hypergraphs of bounded width relative to these notions can be recognized in polynomial time, and whether suitable hypergraph-decompositions can be constructed in polynomial time. On the more applied side, it would be interesting to apply graph and hypergraph decomposition methods to problems in new domains such as e.g. biocomputing and genetic string analysis. Finally, the current algorithms of computing hypertree decompositions should be improved for obtaining faster decomposition methods.

Another important computational problem related to hypergraphs is computing hypergraph transversals [7-9]. While this problem is relevant to a large number of industrial applications (testing of Boolean circuits, database design, etc., cf. [7]), its complexity is currently unknown. Fredman and Khachiyan have shown that the problem is solvable in quasipolynomial time, more specifically, in n^{O(log n)}. More recently, large classes of polynomially solvable cases were identified [9], in particular, the case of bounded treewidth. Moreover, it was shown that the problem can be solved in polynomial time with O(log^2) nondeterministic bits [9]. Investigating the complexity of the transversal problem, finding new tractable cases and better algorithms, and establishing better links between this problem and the theory of hypergraph decompositions are important and practically relevant research goals.

[1] Neil Robertson and Paul D. Seymour, Graph minors. II. Algorithmic aspects of tree-width. J. Algorithms 7 (1986), no. 3, 309--322.

[2]Georg Gottlob, Nicola Leone, Francesco Scarcello: Hypertree Decompositions and Tractable Queries. J. Comput. Syst. Sci. 64(3): 579-627 (2002)

[3] Georg Gottlob, Nicola Leone, Francesco Scarcello: A comparison of structural CSP decomposition methods. Artif. Intell. 124(2): 243-282 (2000)

[4] Georg Gottlob, Nicola Leone, Francesco Scarcello: The complexity of acyclic conjunctive queries. J. ACM 48(3): 431-498 (2001)

[5] Georg Gottlob, Nicola Leone, Francesco Scarcello: Robbers, marshals, and guards: game theoretic and logical characterizations of hypertree width. J. Comput. Syst. Sci. 66(4): 775-808 (2003)

[6] Georg Gottlob, Reinhard Pichler: Hypergraphs in Model Checking: Acyclicity and Hypertree-Width versus Clique-Width. SIAM J.Comput. 33(2): 351-378 (2004)

[7]Thomas Eiter, Georg Gottlob: Identifying the Minimal Transversals of a Hypergraph and Related Problems. SIAM J. Comput. 24(6): 1278-1304 (1995)

[8] Michael L. Fredman, Leonid Khachiyan: On the Complexity of Dualization of Monotone Disjunctive Normal Forms. J. Algorithms 21(3): 618-628 (1996)

[9] Thomas Eiter, Georg Gottlob, and Kazuhisa Makino New Results on Monotone Dualization and Generating Hypergraph Transversals SIAM J.Computing 32:2, pp. 514 - 537, (2003)

In addition to doing their own research, the scientists and the group leaders should collaborate between different groups (and, of course, also with groups outside RICAM). The reports about scientific achievements below will show that a lot of such cooperations have actually started and are showing first results. The first step to initiate this process is of course that everybody has to get to know everybody else scientifically and personally. To achieve this, we continued

- Radon Seminars, which are mainly talks by RICAM members and other scientists from Linz on their work, and
- Radon Colloquia, where scientists from other institutions speak;

all these talks should be such that they are understandable to non-specialists.

This is the theory; in practice, we also had (maybe too many) outside speakers in Radon Seminars, and many of the talks were too specialized to be understandable to members of other groups. For this reason, we introduced Group Seminars, which can be specialized and need to be attended only by members of the specific organizing group. We hope that in 2005, the Seminars and Colloquia will really be what they were intended to be and will be attended by all Institute members.

A list of these Radon Colloquia, Radon Seminars and Group Seminars held in 2004 follows:

Radon Colloquia:

Prof. Dr. Jürgen Sprekels Weierstrass Institute for Applied Analysis and Stochastics Wednesday, March 3, 5 p.m., HS 16
Title: Phasenfeld-Modelle und Hysterese-Operatoren
Abstract: Phasenfeldmodelle zur Beschreibung von Phasenübergängen führen in natürlicher Weise auf gekoppelte Systeme nichtlinearer partieller Differentialgleichungen, in denen so genannte "Hysterese-Operatoren" an mehreren Stellen auftreten, unter anderem auch unter partiellen Ableitungen. Im Vortrag, der auch auf Fragen der thermodynamischen Modellierung eingeht und die Grundlagen der mathematischen Theorie der Hysterese-Operatoren bereit stellt, werden derartige Systeme gekoppelter nichtlinearer partieller Differentialgleichungen behandelt. Eine besondere Schwierigkeit für die Analysis besteht darin, dass Hysterese-Operatoren keine Differenzierbarkeitseigenschaften besitzen und bezüglich der Zeitvariablen ein nichtlokales Gedächtnis haben. Hieraus resultieren schlechte Kompaktheitseigenschaften, die in der Existenztheorie kompensiert werden müssen. Es stellt sich heraus, dass die natürlichen Dissipationsmechanismen der Hysterese (genauer, energetische "Kettenregelungleichungen") hierfür den Schlüssel darstellen.
Prof. Dr. Bernd Hofmann TU Chemnitz, Fakultät für Mathematik Wednesday, March 10, 5 p.m., HS 10
Title: On the ill-posedness nature of some nonlinear inverse problems and its consequences
Abstract: This talk deals with phenomena and situations of ill-posedness for some nonlinear inverse problems and consequences of the specific ill-posedness nature for chances and limitations of regularization approaches. In particular, the role of source conditions with respect to different local degrees of ill-posedness is studied. As one of the benchmark problems the talk considers the calibration of a time-dependent volatility function from the term-structure of prices for options with a fixed strike in spaces of continuous and power-integrable functions. The explicitly available structure of the forward operator as a composition of an inner linear convolution operator and an outer nonlinear Nemytskii operator allows analyzing in detail the ill-posedness phenomena and ways of regularization. For the outer problem treated in a C-space setting the use of arbitrage-free data acts as a specific regularizer. To overcome the local ill-posedness of the complete inverse problem, Tikhonov regularization in $L2$ and maximum entropy regularization in $L1$ are applicable, convergence rates can be proven and source conditions can be evaluated and interpreted. The occurring structure of the Fréchet derivative of the forward operator can be found also in other applications of natural sciences and engineering. It is pointed out that at-the-money options represent a singular situation, in which instability effects occurring for small times in the

cases of in-the-money and out-of-the-money options may disappear and properties of the forward operator may degenerate. The talk is partially based on collaboration with Torsten Hein, Romy Krämer, Dana Düvelmeyer and Gunter Fleischer.
Prof. Dr. Harald Niederreiter National University of Singapore Thursday, April 1, 5 p.m., HF9901
Title: Large Digital Nets and Coding Theory
Abstract: Applications in multidimensional numerical integration have led to the development of the theory of digital nets, which are point sets in unit cubes of arbitrary dimension with strong uniformity properties. Recent research has established close links between digital nets and coding theory. In fact, the problem of constructing good digital nets can now be viewed as the problem of constructing good linear codes in metric spaces that are more general than Hamming spaces. In this talk we will report on the fascinating connections between digital nets and codes. In particular, we will describe some code constructions that can be extended to constructions of digital nets. Further topics include the duality theory for digital nets and the asymptotics of digital-net parameters. A very recent result that we present is the improvement on a famous bound in coding theory, the Tsfasman-Vladut-Zink bound, by means of ideas stemming from the theory of digital nets.
Prof. Dr. William Rundell Texas A&M University Thursday, April 1, 5 p.m., HF9901
Title: Inverse eigenvalue problems: from vibrating strings to the interiors of stars
Abstract: More than 50 years ago Krein asked whether one could determine the density of a string from knowledge of its vibrational modes. More recently, helioseismologists seek to determine the composition of the interior of the sun (and along the way verify or refute various fundamental questions in physics). These are both examples of inverse eigenvalue problems and the issues of uniqueness, stability and constructibility will form the subject of the talk.
Prof. Dr.-Ing. Dr. h.c. Wolfgang L. Wendland Institut für Angewandte Analysis und numerische Simulation, Lehrstuhl für Angewandte Mathematik University of Stuttgart Thursday, April 29, 5:15 p.m., BA9910
Title: Radons Konvergenzbeweis der Neumannschen Methode für Dipolpotentiale
Abstract: In den 80er und 90er Jahren des 19. Jahrhunderts bewies Carl Neumann die Existenz harmonischer Lösungen von zwei- und dreidimensionalen Dirichlet- und Neumann-Problemen in allgemeinen konvexen Gebieten. 1919 hat Johann Radon in zwei Abhandlungen mit Hilfe des Spektrums des Doppelschichtpotentials zum Laplace-Operator Neumanns Methode auf beliebige auch nicht konvexe Gebiete mit C2-Rändern erweitert und mit ihnen sowohl die Funktionalanalysis signierter Radon-Maße als auch des Funktionalkalküls holomorpher Operatorfamilien begründet. Insbesondere konnte J. Radon einen auf Joseph Plemelj zurückgehenden Zusammenhang zwischen Spektrum und Energien von Potentialfeldern sicherstellen, den man auf Lipschitz-Gebiete übertragen kann. Hiermit wurde es jetzt möglich, die Konvergenz der Neumannschen Methode für allgemeine formal positiv elliptische selbstadjungierte Differentialgleichungssysteme zweiter Ordnung und Innen- sowie Außenraumaufgaben mit Lipschitz-Rändern sicherzustellen. Dies ermöglicht die Stabilitäts- und Konvergenzanalysis von Randelementmethoden, Gebietszerlegungsalgorithmen und der zugehörigen Steklov-Poincaré-Operatoren sowie von effizienten Lösungsalgorithmen und a posteriori Fehlerschätzern.
Prof. Dr. Michael Drmota TU Wien Thursday, May 6, 4:15 p.m., BA9911
Title: Statistische Eigenschaften von Ziffernentwicklungen
Abstract: Die Binärdarstellug von ganzen Zahlen spielt nicht nur bei allen numerischen Algorithmen eine große Rolle. Sie wird z.B. auch zur Konstruktion von Pseudo-Zufallszahlen (Van-der-Corput-Folge, Netzfolgen, ...) verwendet und taucht in verschiedenen Zusammenhängen in der Analyse von kombinatorischen Algorithmen auf. Zur Analyse dieser Verfahren ist es daher notwendig, das "durchschnittliche" Verhalten von Ziffernentwicklungen zu kennen.

Dieser Vortrag wird sich im wesentlichen auf die Ziffernsumme konzentrieren, deren "statistisches Verhalten" durch einen zentralen Grenzwertsatz beschrieben werden kann. Ausgehend von der "klassischen" Fragestellung werden verschiedene Verallgemeinerungen behandelt, wie z.B. die gemeinsame Verteilung verschiedener Ziffernentwicklungen und die Ziffernentwicklung von Quadratzahlen. In allen Fällen kann ein zentraler Grenzwertsatz formuliert werden.

PD Dr. Ronny Ramlau

Zentrum für Technomathematik University of Bremen

Wednesday, May 26, 5:15 p.m., HF 9904

Title: Effiziente Verfahren zur Regularisierung nichtlinearer Gleichungen

Abstract: In den letzten 15 Jahren wurden viele der ursprünglich für lineare schlecht gestellte Probleme entwickelten Verfahren auch für nichtlineare Gleichungen verallgemeinert. Tikhonov-Regularisierung spielt dabei eine besondere Rolle, da hier Konvergenz und Konvergenzraten unter relativ schwachen Vorraussetzungen an den nichtlinearen Operator gezeigt werden konnten. Im Gegensatz dazu gestaltet sich eine Konvergenzanalyse für iterative Verfahren oft schwieriger, Konvergenzaussagen konnten oft nur unter starken Einschränkungen an den Operator getroffen werden. Ein möglicher Ausweg besteht darin, Regularisierungsverfahren über eine Kombination der Tikhonov-Regularisierung mit einem iterativen Optimierungsalgorithmus zu definieren. Verwendet man als Optimierungsalgorithmus zum Beispiel ein Gradientenverfahren, so konnten für den resultierenden TIGRA (Tikhonov-Gradienten) Algorithmus Konvergenzraten unter schwachen Bedingungen an den Operator gezeigt werden. Obwohl der Algorithmus sehr stabil ist, konvergiert er doch oft recht langsam, was vor allem an der Verwendung des Gradientenverfahrens liegt. Im Vortrag soll deshalb vor allem auf die Frage eingegangen werden, inwieweit man das Gradientenverfahren durch eine schneller konvergente Fixpunktiteration ersetzen kann. Für die entwickelten Algorithmen werden Konvergenzresultate und numerische Ergebnisse vorgestellt.

Panayot S. Vassilevski

Center for Applied Scientific Computing, UC Lawrence Livermore National Laboratory

Wednesday, June 2, 5:15 p.m., HF 9904

Title: A general framework for algebraic multigrid

Abstract: This presentation deals with the construction of efficient iterative methods for solving linear systems of algebraic equations that typically arise in (finite element) discretizations of (elliptic) partial differential equations (or PDEs). The traditional iterative methods, such as Richardson or Gauss--Seidel, i.e., those that update a current iterate at a given node based on the values of the iterate at neighboring nodes converge very slow. The most efficient iterative methods in practice exploit a second (coarse) discretization, or even a sequence of coarse discretizations. A typical two--grid method in addition to a traditional iteration process exploits updates based on coarse grid problems. The traditional iterations (like Jacobi, Richardson, Gauss--Seidel) turn out to be efficient only on the highly oscillating components of the error. That is why they are often called "smoothers''. Thus, what is left out, after the smoothing, is the smooth component of the error which can be well approximated on coarse grid(s). This is the fundamental principle of the popular multigrid methods. This talk will deal with the construction of two--grid methods without the availability of (geometric) coarse grid(s). A typical practical situation is the discretization of PDEs on general unstructured meshes. Thus, one has access only to a given matrix A (coming from a single grid). The matrix A is assumed to be symmetric positive definite (or s.p.d.) and all reMayning tools, the coarse grid and the transfer of data between the grids based on an interpolation matrix P, have to be constructed by algebraic means, i.e., based on A and the fixed smoother. We present necessary and sufficient conditions for guaranteed optimal convergence of two-grid algebraic multigrid based on a given sparse s.p.d. matrix A and a fixed general smoother. First, we present a sharp convergence estimate of the method and then formulate two important corollaries which appear also to be sufficient conditions for the convergence. The latter corollaries offer also a variety of algorithms to select the coarse grid and to build the interpolation matrix P.

Prof. A. Kaveh

Iran University of Science and Technology

Friday, September 17, 1:00 p.m., HF 9904

Title: Topological Transformations in Structural Mechanics

Abstract: In this lecture a number of topological transformations are proposed for simplifying certain problems in mechanics of structures. For each case, the Mayn problem is stated and then the transformation is established. Once the required topological analysis is completed, a back transformation results in the solution for the Mayn problem. Expedient transformations studied here employ (1) models drawn on lower dimensional spaces, (2) models embedded onto higher dimensional spaces, (3) interchange models defined which have more suitable connectivity properties than the corresponding original structural model, (4) models studied by their essential components such as their generators. The aim of the present talk is two fold. In one hand it shows to mathematicians how the apparently pure mathematical concepts can be applied to the efficient solution of problems in structural mechanics. In the other hand it illustrates to engineers the important role of mathematical concepts for the solution of engineering problems.

Karol Mikula

Department of Mathematics, Slovak University of Technology, Bratislava

Wednesday, November 3, 5:15 p.m., TNF HS14

Title: Mathematical models and computational methods in image analysis

Abstract: In many applications computers analyse images or image sequences quality of which can be poor, e.g., they are contaminated by a noise and/or boundaries of image objects are partly missing (e.g. in medical imaging, in scene with occlusions or ilusory contours). We will discuss how nonlinear partial differential equations can be used to denoise and segment such images, complete the missing boundaries, etc. Dicretizations by the variational methods of the geometrical image selective smoothing and segmentation equations (Riemannian mean curvature flow and Perona-Malik problem) will be presented. The computational results in bio-medical image processing and subjective contours extraction will be given.

Prof. Albrecht Irle

Mathematisches Seminar, Christian-Albrechts-University of zu Kiel

Tuesday, November 9, 3:30 p.m., HS 5

Title: Optimal Stopping Problems in Mathematical Finance

Abstract: Optimal stopping theory has again become an active area of research, one of the reasons being their importance for pricing American options. In this talk two new methods for finding optimal stopping rules are described. The first method is discrete in nature and may be used to construct algorithms of simulation type. The second method pertains to diffusion processes and uses suitable martingales. Applications to mathematical finance are described.

Prof. Igor Shparlinski

Macquarie University, Sydney

Friday, December 17, 10:15 a.m., HS 6

Title: Spherical configurations, exponential sums, and quantum computation

Abstract: We describe two types of vector systems on the n-dimensional sphere over C, which are useful for quantum computation. For one type, such configurations can be obtained from Gaussian sums for every prime n. Configurations of the other type are not known to exist for infinitely many n. We show that using bounds of exponential sums with polynomials one can achieve certain approximate solutions. The results are based on both the Weil and Weyl bounds and also the result of Baker-Harman-Pintz about gaps between consecutive primes.

Radon Seminars:

Dr. Klaus Scheicher

RICAM/Gruppe: Financial Mathematics

Monday, January 12, 3:30 p.m., HF 136

Title: On the Efficiency of the Brownian Bridge Algrithm

DI Michael Gee

University of Stuttgart, Institut für Baustatik

Tuesday, January 13, 3:30 p.m, HF 136

Title: Ein Paralleler Multilevel Lösungsansatz für lineare Gleichungssysteme nichtlinearer Schalenprobleme

Abstract: Dünnwandige Schalen, die mit der Methode der Finiten Elemente diskretisiert werden, führen zu schlecht konditionierten linearen Gleichungssystemen. Wendet man iterative Lösungsstrategien auf

solche Gleichungssysteme an, so ist deren Konvergenzrate im Allgemeinen niedrig, wenn überhaupt eine Konvergenz erzielt werden kann. Die Ausgangslage verschlechtert sich noch deutlich, wenn eine dreidimensionale Schalenformulierung verwendet wird, die die Dickenänderung der Schale berücksichtigt. Ein paralleler Vorkonditionierer für eine solche Schalenformulierung wird hier vorgestellt, der zwei unterschiedliche Ansätze miteinander kombiniert. Der erste Ansatz ist eine mechanisch motivierte Verbesserung der Kondition der resultierenden Steifigkeitsmatrizen, die in der Lage ist, die Kondition auf das Niveau "klassischer" Schalenformulierungen ohne Berücksichtigung der Dickenänderung zu heben. Der zweite Ansatz ist ein paralleler semi-algebraischer Multilevel-Vorkonditionierer auf der Basis Schwarz'scher Gebietszerlegungsmethoden. Es wird gezeigt, dass die beiden Ansätze sich gut ergänzen. Der konvergenz- und geschwindigkeitssteigernde Effekt dieses kombinierten Vorkonditionierers wird anhand von Beispielen demonstriert.

Dr. Karsten Eppler

TU Berlin, Institute for Mathematics

Monday, January 19, 3:30 p.m, HF 136

Title: Potential methods for elliptic shape optimization problems

Abstract: The talk deals with the application of potential theory and BIE-methods both for developing a differential calculus as well as for the numerical solution of constrained 2D-elliptic shape optimization problems. The complete boundary integral representation of the shape gradient and Hessian for a boundary variational approach is addressed in the first part. A wavelet-Galerkin BEM is used for the computation of related quantities in optimization algorithms. At the end, results for several applications are presented.

Dr. Laurent Gosse

University of Bari

Tuesday, January 20, 10 a.m., HF 136

Title: Multiphase Approximation of 1D Schrödinger Equation via WKB Techniques

Nguyen Chanh Dinh

University of Augsburg, Institute for Mathematics

Monday, February 2, 10 a.m., HF 136

Title: Level Set Methods for Nonlinear Deposition

Abstract: This work aims to provide a level set method for solving an equation which describes the evolution of hypersurfaces by deposition process. Such kinds of equations occur, for instance, in the processes which model the microscopic growth of vapor-deposited amorphous $Zr_{65}Al_{7.5}Cu_{27,5}$ on silicon substrates. In this case, the growth process is determined by curvature-included surface diffusion, adatom concentration triggered surface diffusion, and geometrical effects.

PD Dr. Olaf Steinbach

Institut für Angewandte und Numerische Simulation, University of Stuttgart

Monday, March 1, 3:30 p.m, HF 136

Title: Tearing and Interconnecting DoMayn Decomposition Methods

Abstract: DoMayn decomposition methods are a well established tool for the approximation of coupled field problems using different discretization schemes such as finite and boundary elements. Here we present an unified framework of non-overlapping doMayn decomposition methods which are based on the solution of local subproblems. Using a tearing and interconnecting idea one is able to construct efficient preconditioned iterative solvers.

Dr. Manfred Trummer

Department of Mathematics Simon Fraser University and Pacific Institute for the Mathematical Sciences

Monday, March 15, 3:30 p.m, HF 136

Title: Spectral Differencing with a Twist

Abstract: Spectral collocation methods have become very useful in providing highly accurate solutions to differential equations. A straightforward implementation of these methods involves the use of spectral differentiation matrices. To obtain optimal accuracy these matrices must be computed carefully. We demonstrate that naive algorithms for computing these matrices suffer from severe loss of accuracy due to roundoff errors. Several improvements are analyzed and compared. A number of numerical examples are provided, demonstrating significant differences between the sensitivity of the forward problem and inverse problem.

Konstantinos Chrysafinos

Carnegie Mellon University, Department of Mathematical Sciences

Monday, March 22, 3:30 p.m, HF 136

Title: Analysis and finite element approximations of oprimal flow control problems.

Abstract: We present several results related to optimal control problems for Navier-Stokes flows. In particular, we develop and analyze the velocity tracking problem based on the artificial compressibility formulation. Using the artificially compressible Navier-Stokes equations we are able to derive semi-discrete finite element error estimates for the corresponding optimality system. In addition, we discuss several analytical and numerical issues related to the finite element approximation of optimal boundary control problmes. Finally, we propose an alternative approach based on moving-mesh finite element methods for distributed optimal control problems.

Boris Vexler

Institute of Applied Mathematics, University of Heidelberg

Monday, March 29, 3:30 p.m, HF 136

Title: Adaptive Finite Element Methods for Parameter Identification Problems

Abstract: We consider parameter identification problems involving partial differential equations with finite number of unknown parameters. We present an a posteriori error estimator, which aims to control the error in the parameters due to discretization by finite elements. This question is treated in a general setting exploiting the special structure of the parameter identification problem. This allows us to derive an error estimator which is cheap in comparison to the optimization algorithm. Several applications, including parameter identification in CFD problems and estimation of chemical models in reactive flows, illustrate the behavior of an adaptive mesh refinement algorithm based on our error estimator.

Prof. Dr. Jorge P. Zubelli

IMPA, Brazil

Monday, March 29, 10 a.m., HF 136

Title: Three-Dimensional Reconstruction by Chahine's Method from Projections Corrupted by Electron Microscope Aberrations

Abstract: This work is motivated by electron microscopy imaging of macromolecules from biological specimens. A projection image obtained by an electron microscope can be conceived of as an "ideal" projection subjected to a contrast transfer function (CTF), which eliminates some frequencies and reverses the phase of others. The aberration caused by the CTF makes the problem of reconstruction from such data difficult, especially at light of the low signal-to-noise ratio in the data. We reformulate the problem so that Chahine's method becomes applicable to it. We substantiate our results with ample numerical evidence using both simulated and actual electron microscopy data.

Frank Bauer

University of Kaiserslautern, Institut für Mathematik

Monday, April 19, 3:30 p.m, HF 136

Title: Auto-Regularization for Inverse Problems in Satellite Geodesy

Abstract:

DI Jürgen Hartinger

TU Graz

Thursday, April 19, 17:00, HF 136

Title: On dividends and the discounted penalty function in a risk model with linear barrier

Abstract: The distributions of the time of and deficit at ruin were thouroughly studied in the past decades. In dividend barrier endowed risk models these characteristics may be used to consider optimization critera more general than expected dividends. The aim of this talk is to generalize recent results on the time of, the deficit at ruin and the moments of the discounted dividends from models with constant barriers to linear barrier models.

Jamel Ferchichi

Optimierung und Kontrolle, Karl-Franzens-Universitat, Graz

Monday, May 24, 3:30 p.m, HF 136

Title: Shape Sensitivity for the Laplace-Beltrami Operator with Singularities

Abstract: We present in this paper a shape sensitivity analysis result for the Neumann tangential problem formulated on a two dimension manifold with a fracture. We characterize the shape derivative of a quadratic functional as a distributed gradient supported on the manifold's boundary, a limit of a “jump” through the crack plus a Dirac measures at the crack extremities. That is why we introduce a family of envelopes surrounding the fracture which enable us to relax certain terms and to overcome the lack of regularity which results from the presence of the fracture. We use the min-max derivation in order to avoid differentiating the state equation and to manage the crack's singularities. Therefore, we write the functional in a min-max formulation on a space undertaking the hidden boundary regularity established by the tangential extractor method. Finally, we provide the existence of an optimal doMayn by using, basically, the Kuratowski continuity of Sobolev spaces.

Cristina Sebu

Laboratoire de Physique Mathématique, Université Montpellier

Monday, June 7, 3:30 p.m, HF 136

Title: An integral equation method for the inverse conductivity problem

Abstract: I present an image reconstruction algorithm for the Inverse Conductivity Problem based on reformulating the problem in terms of integral equations. I use as data the values of injected electric currents and of the corresponding induced boundary potentials, as well as the boundary values of the electrical conductivity. A priori information is used to find a regularized conductivity distribution by first solving a Fredholm integral equation of the second kind for the Laplacian of the potential, and then by solving a first order partial differential equation for the regularized conductivity itself. Many of the calculations involved in the method can be achieved analytically using the eigenfunctions of an integral operator.

Tolga Guyer

Universitesi Gazi

Monday, June 14, 3:30 p.m, HF 136

Title: A Symbolic Computation Approach to a Dirichlet-Type Problem Reduced from an Inverse Problem

Abstract: This study presents a symbolic algorithm for computing an approximated analytic solution to a Dirichlet-type problem for the third order partial differential equations based on Galerkin method.

Henry Chu

RICAM – Analysis of Partial Differential Equations

Monday, June 28, 12:45 a.m., HF 136

Title: Some progress on Prandtl's system

Abstract: We consider unsteady boundary layer problem of three dimensional axisymmetric viscous flows over upper half space, with both cases of no swirls and having swirls. We are interested in the case that the separation of the boundary layer does not occur so that the problem is governed by the Prandtl's system. We use the splitting method developed by Xin and Zhang to show the existence of global weak solution of unsteady boundary layer problem of three dimensional axisymmetric Prandtl's system with no swirls.

Furthermore, we generalize the problem to the axisymmetric Prandtl's system with nonvanishing swirls which has been considered to be very important yet difficult. We formalize the definition of weak solution of the case of ignoring the effect of radial variable and show the existence of weak solution to the three dimensional axisymmetric Prandtl's system with positive swirls. The problem can be reduced into a system of degenerated porus-medium type equations. The keys to our analysis are some new a-priori estimates derived by comparison arguments, energy-estimates, and the Nash-Moser iterations.

Roman Heizle University of Innsbruck Institut für Technische Mathematik, Geometrie und Bauinformatik Monday, June 28, 3:30 p.m, HF 136
Title: Numerische Behandlung von DAE Systemen mit Unstetigkeiten und Anwendung auf die dynamsiche Kraftwerkssimulation
Abstract: Bei der Simulation von Gas- und Dampfkraftwerken sowie in vielen anderen praktischen Anwendungen müssen Systeme von differentiellen und algebraischen Gleichungen, sogenannte DAE-Systeme, mittels numerischer Integrationsverfahren gelöst werden. Das Auftreten von Unstetigkeiten in diesen Gleichungen kann den Integrator stark verlangsamen oder zu ungenauen Resultaten führen, weshalb eine spezielle Behandlung von Unstetigkeiten sehr sinnvoll erscheint. Die Grundidee hierfür ist die kontinuierliche Integration über die unstetige Stelle mit Hilfe einer modifizierten Fehlerschätzung bzw. Schrittweitensteuerung. Diese Methode wurde an zahlreichen Modellprobleme und Testbeispielen zurSimulation von Gas- und Dampfkraftwerken ausprobiert. In allen Fällen zeigte sich eine deutliche Verbesserung der Genauigkeit des Resultats und zugleich eine Steigerung der Effizienz.
Prof. Andrzej Kisielewicz University of Wroclaw Friday, July 2, 1 p.m., HF 136
Title: A new approach to permutation groups
Abstract: In the talk a new way to classify permutation groups by means of certain graphical structures will be presented. We introduce elementary concepts of a supergraph and graphical complexity of a permutation group, present basic results, and discuss some natural research problems. Our new approach is justified by applications in various areas of mathematics and computer science.
Dr. Klaus Johannsen University of Heidelberg, Interdisciplinary Center for Scientific Computing (IWR) Friday, July 16, 9 a.m., HF 136
Title: Numerical Aspects of Density Driven Flow in Porous Media
Abstract: The analysis as well as the numerical simulation of density driven flow in porous media is still a challenging task. Whereas thorough theoretical investigations are limited to special situations, the numerical treatment, especially of real-world problems, requires special numerical techniques. In this talk we focus on two aspects, which are relevant in this context. The first deals with the design of robust multigrid solvers for problems with high spatial anisotropies. In the second part, we investigate the structure of the steady state solutions for a special model problem. The results shed some light on the difficulties arising in the analysis of the underlying mathematical problem.
PD Dr. Nicolas Neuß University of Heidelberg, Interdisciplinary Center for Scientific Computing (IWR) Monday, November 8, 3:30 p.m, HF136
Title: Numerics of Multiscale Problems
Abstract: Many problems in applications have multiscale character, that is, processes on several scales have to be taken into account for understanding and simulating the observed phenomena. In this talk, we consider Maynly flow in porous media, where small-scale heterogeneities in the medium often lead to difficulties in both analysis and numerical simulation. We will look at two specific situations. First, if the heterogeneities are periodic, it is possible to derive effective laws and to calculate constants appearing in those laws with high accuracy. Second, if the heterogeneities are not periodic, for example, if they are locally periodic or of stochastic nature, it is still possible to take into account the multiscale nature for deriving coarse-scale approximations and effective solvers.
Ibolya Szilagyi RICAM – Symbolic Computation Monday, November 15, 3:30 p.m, HF136
Title: Numerical stability of surface implicitization
Abstract: For a numerically given parametrization we cannot compute an exact_ implicit equation, just an approximate one. We introduce a condition number to measure the worst effect on the solution when the input data is perturbed by a small amount. Using this_ condition number the perturbation behaviour

of various implicitization methods can be analyzed.
Romy Krämer TU-Chemnitz Monday, November 15, 1:30 p.m., HF136
Title: The Inverse Problem of Parameter Estimation in a Generalized Ornstein-Uhlenbeck model
Abstract: Parameter calibration in financial mathematical models is a notorious instable or ill-posed problem. We consider a generalization of the bivariate Ornstein-Uhlenbeck model introduced by Lo, Wang (The Journal of Finace, 1995). Our aim is to calibrate a time depending volatility function sigma(t) and the other unknown (real-valued) parameters in the model. As data we use observed vanilla call option prices and some emipirical moments of the logarithmic returns. After formulating the inverse problem in form of a nonlinear operator equation we discuss properties of the forward operator as well as uniqueness, solvability and ill-posedness of the inverse problem. Based on these properties we apply the theory of Engl, Hanke, Neubauer concerning Tikhonov regularization to the nonlinear inverse problem. Particularly, we show convergence of the regularized solution to the true data and study the form of source conditions which ensure convergence rates. Finally we illustrate some of the above mentioned theoretical results by numerical case studies.
PD Dr. Peter Mathé Weierstraß-Institut für Angewandte Analysis und Stochastik Wednesday, November 17, 11 a.m., HF136
Title: "Parameter choice principles under general source conditions "
Abstract:
Dr. Roland Griesse RICAM – Optimization and Optimal Control Monday, November 22, 3:30 p.m, HF136
Title: "Sensitivity Analysis for Constrained Optimization Problems"
Abstract: In the presentation we consider constrained optimization problems: Minimize f(x) subject to g(x)=0 and h(x)<=0, where the functions f,g and h may depend on a parameter p. The central question is: How does a solution of the optimization problem depend on changes in the parameter p? Some known and new results will be presented, together with illustrative numerical examples.
Prof. Josef Schicho und Dr. Johannes Kraus RICAM – Symbolic Computation und Computational Methods for Direct Field Problems Monday, December 6, 1:30 p.m., HF136
Title: Algebraic construction of edge matrices with application to AMG
Abstract: In the first part of this talk we consider the problem of splitting a symmetric positive definite (SPD) stiffness matrix A arising from finite element discretization into a sum of edge matrices thereby assuming that A is given as a sum of symmetric positive semidefinite (SPSD) element matrices. We give necessary and sufficient conditions for the existence of a decomposition into SPSD edge matrices and provide a feasible algorithm for the computation of edge matrices in case of general SPSD element matrices. In the second part of the talk, we focus on a new approach in algebraic multigrid (AMG): Based on the knowledge of edge matrices, we discuss how to alter the concept of 'strong' and 'weak' connections, as it is used for coarse-grid selection in classical AMG. We further derive interpolation from a local energy minimization rule: the 'computational molecules' involved in this process are assembled from edge matrices. Numerical tests show the robustness of the new method, which we refer to as AMGm (Algebraic MultiGrid based on computational molecules).
Prof. Vincenzo Capasso Milan Research Centre for Industrial and Applied Mathematics (MIRIAM) Monday, December 6, 3:30 p.m, HF136
Title: Stochastic geometries in birth-and-growth processes
Abstract: Scope of stochastic geometry is the mathematical analysis of the spatial structure of patterns which are random in location and shape. In this context the mathematical interest is in spatial occupation, so that geometric measure theory is involved in presence of stochastic fluctuations. Examples are provided by forest growth, tumor growth, crystallization processes in sea shells, etc. In a more detailed

description, all these rocesses are birth-and-growth processes. In forest growth, births start from seeds randomly dispersed in a region of interest, and growth is due to nutrients in the soil that may be randomly distributed themselves or driven by a fertilization procedur; in tumor growth abnormal cells are randomly activated and develop thanks to a nutritional underlying field driven by blood circulation (angiogenesis); in crystallization processes as in sea shells, nucleation and growth may be due to a biochemical underlying field, to temperature, etc. All this kind of phenomena are subject to random fluctuations, as the same underlying field, because of intrinsic reasons or because of a strong coupling with the growth process itself. A possible characterization of the final spatial pattern may be given in terms of mean densities of interfaces of the random decomposition of space (tessellation), at different Hausdorff dimensions (n-facets: cells, faces, edges, vertices), with respect to the usual Lebesgue measure. Evolution equations of the above spatial densities are presented here in terms of the kinetic parameters of a typical birth-and-growth process coupled with the evolution equations of the underlying field. Problems of multiple scales may arise, so that homogenization at the larger scale may be carried out, leading to simplified approximating hybridmodels. Of great interest in this context are control problems.

Dr. Alexandru Tamasan

University of Toronto

Monday, December 6, 5:00 p.m., HF136

Title: On the Fluorescence Problem

Abstract: In the fluorescence problem the goal is to determine the source of radiation passing through an absorbing and scattering tissue, from far away radiation or, equivalently, from boundary measurements. In the high energy case, when absorption and scattering effects are negligible this problem was long solved by J. Radon in 1917. In the case of single photon emission or positron emission, the attenuation effect can not be neglected. Mathematically the problem reduces to the inversion of the attenuated X-ray transform. This problem was independently solved by A.L. Bukhgeim in 1989 and R.G. Novikov in 2001. In a joint work with G. Bal, we consider the case when scattering cannot be neglected. For sufficiently small anisotropic part of scattering, finding the source is still possible. I will present a converging iterative algorithm. Counter-intuitive, for three dimensional models, only scattering in the directions parallel to a fixed plane need to be small.

Yasmin Dolak

RICAM – Analysis of Partial Differential Equations

Monday, December 12, 3:30 p.m, HF136

Title: Advection-dominated models for chemotaxis

Abstract: Chemotaxis - the biased migration towards or away from chemical gradients - is a fundamental mechanism cells have developed to find food or to avoid toxic substances. In the first part of my talk, we will derive kinetic models for chemotaxis, incorporating the ability of cells to assess temporal changes of the chemoattractant concentration as well as its spatial variations. A formal hyperbolic limit leads to a drift equation with a diffusion term as a higher order correction. As an application, we will study aggregation of the slime mold Dictyostelium discoideum and perform numerical experiments. In the second part of the talk, we will study 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. We consider the case of small diffusivity and investigate the limit as the diffusion coefficient goes to zero. Considering a model where the drift term vanishes at high cell densities leads to a nonlinear equation which allows the formation of shocks in the limit. Moreover, we look at the long term behaviour of solutions.

Gergana Bencheva

Institute for Parallel Processing, Bulgarian Academy of Sciences

Monday, December 20, 3:30 p.m, HF 136

Title: Parallel Algorithms for Separation of Variables and Sparse Matrices Factorization

Abstract: The appearance of parallel architectures and the recent progress in computational technologies has inspired quite a lot of interest in development of efficient parallel algorithms for solution of problems
in almost all nowadays scientific areas. Presented dissertation is devoted to construction and analysis of parallel methods. Subject of investigations in the thesis are numerical methods for solution of large systems of linear algebraic equations obtained after discretization of a second order elliptic boundary value problems. Two approximation approaches are considered: a) by finite differences with five-point stencil for a separable problem; b) by rotated bilinear nonconforming finite elements (NFE) for a problem in a

general form. The Mayn results, obtained in the thesis, are constructive. They are presented in three chapters. A theoretical and experimental comparative analysis of five separable solvers is made in the first part. Namely, the attention is focused on the standard (SV) and the fast (FASV) algorithm for separation of variables as well as on the standard (SM) and two variants (GMF and GMS) of the generalized marching algorithm. The proposed original modification GMS of GMF simplifies the structure of the generalized marching algorithm and has advantages with respect to parallel implementation. An almost optimal separable preconditioner for anisotropic elliptic boundary value problems discretized by rotated bilinear NFE is proposed and investigated theoretically and experimentally. A characterization of the anisotropy coefficient influence on the efficiency of the preconditioner is obtained. The second part deals with parallel direct solvers. New parallel implementations of the algorithms FASV, GMF and GMS are proposed and a theoretical comparative analysis of their properties is derived. The third part is devoted to parallel iterative methods. A new parallel preconditioner for anisotropic elliptic boundary value problems, discretized by rotated bilinear NFE is proposed. The modified incomplete Cholesky factorization is applied to a locally constructed approximation of the stiffness matrix. Uniform estimates for the condition number are obtained with respect to the problem size and coefficient jumps. A characterization for the parallel efficiency of the constructed direct and iterative solvers is obtained for classes of distributed memory parallel computing systems. An experimental comparative analysis of the behaviour of each of the proposed parallel solvers on distributed systems with different characteristics is made.

Group Seminars:

GROUP: Computational Methods for Direct Field Problems

Dr. Andrea Toselli

Seminar for Applied Mathematics, ETH Zürich

Tuesday, July 13, 2004, 3:30 p.m., HF 136

Title: Domain decomposition preconditioners of Neumann-Neumann and FETI type for *hp* approximations on highly anisotropic meshes

Abstract: Solutions of elliptic boundary value problems in polyhedral domains have corner and edge singularities. Singularities may also arise at material interfaces. In addition, boundary layers often arise in flows with moderate or high Reynolds numbers and in conductor materials with very large conductivity jumps, at faces, edges, corners, and material interfaces. Suitably graded anisotropic meshes, geometrically refined toward corners, edges, faces, and/or interfaces, allow to achieve an exponential rate of convergence of hp finite element approximations. In many practical applications, it is not merely a matter of speeding up convergence, but of making computations possible, since simple h or p approximations ion isotropic meshes would require a prohibitively large number of unknowns.
The bottleneck for computations involving such problems is often the solution of the corresponding algebraic systems, which have huge condition numbers due to the simultaneous effect of the large number of unknowns, the large coefficient jumps, the huge aspect ratios of the mesh, and small parameters. Robust preconditioning is mandatory.

In the last years, we have been able to devise a successful robust domain decomposition preconditioning strategy for some hp approximations of scalar problems on highly anisotropic two and three dimensional meshes. More recently, this strategy has been extended to some edge element approximations of electromagnetic problems. Thanks to a particular choice of the sub domains and of the coarse solvers, our preconditioners ensure quasioptimality, scalability, robustness with respect to coefficient jumps and huge aspect ratios of the meshes. We will illustrate these features through numerical tests.

GROUP: Symbolic Computation

Prof. Kisielewicz

Friday July 23, 2004, 11:00 a.m., HF 136

Title: Equational logic in semigroups

expository talk with Andrzej Kisielewicz followed by questions and discussions

GROUP: Computational Methods for Direct Field Problems

Dr. Satyendra Tomar

Department of Applied Mathematics, University of Twente

Monday, September 27., 2004, 1:00 p.m., HF 136

Title: Numerical simulation of linear water waves using discontinuous Galerkin method

Key Words: Discontinuous Galerkin method, water waves, free surface, non-uniform mesh, velcity reconstruction, unstructured mesh, symmetric positive definite system, preconditioned conjugate gradient method, adaptive techniques, parallelization.

GROUP: Computational Methods for Direct Field Problems

Dr. Satyendra Tomar

Department of Applied Mathematics, University of Twente

Monday, September 27, 2004, 4:00 p.m., HF 136

Title: An exponentially accurate parallel *h-p* spectral element method for elliptic problems on non-smooth domains

Key Words: Elliptic problem, non-smooth domain, corner singularity geometric mesh, Direchlet and mixed boundary conditions, least-squares approach, Schur complement, poly-logarithmic condition number, exponential accuracy.

GROUP: Computational Methods for Direct Field Problems

Tino Eibner

TU Chemnitz

Tuesday, October 12, 2004, 1:45 p.m., HF136

Title: Boundary concentrated finite element methods

Abstract: The boundary concentrated finite element method is a version of the hp-fem particularly suited for solving elliptic boundary value problems with analytic coefficients on the one hand and boundary conditions with low
regularity or non-smooth geometries on the other hand.

In this talk we will consider different aspects of the boundary concentrated fem, such as basic properties and local error analysis as well as a fast and efficient method for setting up the stiffness matrix in hp-fem on triangular/tetrahedral meshes.

GROUP: Computational Methods for Direct Field Problems

DI Günther OF - Universität Stuttgart

Prof. Dr. Olaf Steinbach - TU Graz

Friday, October 29, 2004, 13:00, HF136

Title: Efficient iterative solvers for Boundary Element Tearing and Interconnecting Method

Abstract:

GROUP: Computational Methods for Direct Field Problems

Dr. Zhenyu Liu

IMTEK - Institute for Microsystem Technology, University of Freiburg, Germany

Dienstag, November 16, 2004, 1:45 p.m., T112

Title: Structure Topology Optimization: New progress and application for MEMS design

Abstract: Structure topology optimization method has gained much attention in the design of mechanisms, functional materials and MEMS. To date, there are several approaches which can be used to implement topology optimization. We will first review the basic procedure to implement structure topology optimization by the element-density design variable method, and then introduce some progresses by the point-density design variable method and the level set method. Some examples, such as compliance minimization structure, compliance mechanism, electro-mechanic coupled problem, are presented to illustrate the performance of structure topology optimization in MEMS design.

GROUP: Computational Methods for Direct Field Problems

Dipl.-Math. Jens Breuer

Institut für Angewandte Analysis und Numerische Simulation Universität Stuttgart

Dienstag, November 23, 2004, 1:45 p.m., HF136

Title: Fast boundary elements for the simulation of eddy currents and their heat production and cooling

Abstract:

Group: Analysis of Partial Differential Equations

Dezsö Boda

University of Veszprém (Hungary), Department of Physical Chemistry

Tuesday, November 23, 2004, 1:45 p.m., HF136

Title: Modeling and simulating complex ionic systems in the presence of dielectric inhomogeneities

Abstract: In coarse-grained models of systems containing ions and molecules carrying partial charges, the most significant degrees of freedom are treated explicitly, while others are described as a macroscopic continuum. One type of coarse-graining replaces the fast atomic and molecular motions by a macroscopic dielectric response that is summarized by a spatially varying dielectric coefficient. Examples include calculations of electrochemical interfaces, electron-hole plasmas at semiconductor junctions, the solvation DNA and proteins, or the physiologically crucial problem of membrane proteins, and specifically, ion channels.

Computer simulation techniques, such as Monte Carlo or molecular dynamics simulation methods, provide a powerfool tool to study such models. If the system contains source charges moving in an inhomogeneous dielectric environment, the energy of the system has to be calculated in accordance with the laws of electrostatics, namely, the polarization charges induced by the source charges on the dielectric interfaces have to be calculated.

We present the Induced Charge Computation (ICC) method for the calculation of the polarization charges [Boda et al. Phys. Rev. E 69 Art. No. 046702 (2004)]. The method results in an integral equation that turns into a matrix equation after discretization. The induced charges are directly calculated by solving the linear matrix equation Ah =c, where h contains the discretized induced charge density, c depends only on the source charges - the ions moved in the simulation - and the matrix A depends on the geometry of the dielectrics, which is assumed to be unchanged during the simulation.

We verify the efficiency and accuracy of the method by means of Monte Carlo simulations of hard sphere ions moving near sharp dielectric interfaces of various geometries. Results for curved interfaces, where the matrix is need be computed with extra care, are given. Present and future efforts are made on the development of the method by including the possibility to impose certain boundary conditions on the boundaries confining the simulation cell.

GROUP: Computational Methods for Direct Field Problems

Marco Discacciati

EPFL - Swiss Federal Institute of Technology

Monday, December20, 9:30 a.m., HF 136

Title: Domain decomposition methods for the coupling of surface and groundwater flows

Abstract: This presentation concerns the study of mathematical and numerical models for simulating incompressible fluid flows through heterogeneous media. In particular, we consider the case of free fluids which can filtrate through a porous medium occupying a neighbouring domain to the fluid one. This topic has many important applications, among which we recall the hydrological environmental ones and mass transfer in biomechanics. In this talk we outline the mathematical and numerical analysis of a coupled Navier-Stokes/Darcy problem. In particular, by adopting the Beavers and Joseph interface conditions, we will assess the well-posedness of the global problem, and we will introduce a suitable Galerkin finite element approximation. Then, we will focus our attention on iterative substructuring methods inspired by domain decomposition theory which allows to solve the global problem through the independent solution of both the fluid and the porous media subproblems in each subdomain. Through the analysis of suitable Steklov-Poincar´e interface operators, we can characterize optimal preconditioners to solve the discrete algebraic problem, which can be applied in the framework of Krylov type methods. The effectiveness of the computational methods that we have introduced will be shown on some test cases, with particular concern on the dependence of these methods on the gris size and on the most relevant physical parameters which characterize the filtration problem.

Co-organized Conferences by RICAM

➢ AISC 2004 - 7th International Conference on

Theory, Implementations and Applications
September 22 - 24, 2004

General Chair: Prof. Bruno Buchberger

Artificial Intelligence and Symbolic Computation are two views and approaches for automating problem solving, in particular mathematical problem solving. The two approaches are based on heuristics and on mathematical algorithmics, respectively. Artificial Intelligence can be applied to Symbolic Computation and Symbolic Computation can be applied to Artificial Intelligence. Hence, a wealth of challenges, ideas, theoretical insights and results, methods and algorithms arise in the interaction of the two fields and research communities. Advanced tools of software technology and system design are needed and a broad spectrum of applications is possible by the combined problem solving power of the two fields.

Hence, the conference was in the center of interest and interaction for various research communities:

- artificial intelligence,
- symbolic computation,
- computer algebra,
- automated theorem proving,
- automated reasoning,
- formal mathematics,
- mathematical knowledge management,
- algorithmic invention and learning,
- logic,
- software technology,
- language and system design,
- implementation and performance issues,
- semantic web technology,
- computer-based math teaching and didactics,
- computer-supported publishing,
- language and system design,
- implementation and performance issues,
- any topics related to the above.

Invited Speakers

- Alan Bundy (University of Edinburgh, UK)
- Markus Rosenkranz (RICAM Institute, Austrian Academy of Sciences, Linz, Austria)
- Helmut Schwichtenberg (Ludwig-Maximilian University, Munich, Germany)
- Zbigniew Stachniak (York University, Toronto, Canada)

Proceedings:
B. Buchberger, J. Campbell (eds.)

➢ Numbertheoretic Algorithms and Related Topics

September 27 - October 1, Strobl, Austria
Prof. Gerhard Larcher and Dr. Arne Winterhof were involded (Program committee)

The workshop was supported by the Austrian Science Foundation FWF via a "Forschungsschwerpunkt" (FSP) devoted to Number Theoretic Algorithms and Their Applications. The aim of the workshop was to bring together internationally renowned specialists on related areas with the Austrian research groups of the FSP, in particular with the rising generation.

Of particular interest were the following topics:

- Diophantine Analysis
- Enumeration Systems
- Coding theory and Cryptography
- Pseudorandomness and Quasi Monte Carlo Methods
- Discrepancy
- Ergodic Theory and Dynamical Systems
- Fractals

Plenary Speakers

- Valérie Berthé
- Vitaly Bergelson
- Harald Niederreiter
- Attila Pethö
- Gerald Tenenbaum
- Robert Tijdeman

➢ <u>Workshop on complexity and discrepancy</u>

October, 4-5, 2004
Organisation: Prof. Gerhald Larcher

➢ <u>ISSAC 2004</u>

International Symposium on Symbolic and Algebraic Computation
hosted by the University of Cantabria Santander, Spain, July 4-7, 2004

General Chair: Prof. Josef Schicho

ISSAC is the yearly premier international symposium in Symbolic and Algebraic Computation that provides an opportunity to learn of new developments and to present original research results in all areas of symbolic mathematical computation.

As mentioned in the original proposal and again in the mission statement, Special Semester will be an important part of the plans of the Institute.

The first such Special Semester will be held in the fall of 2005 on Computational Mechanics, planning is well advanced and is led by Prof. Ulrich Langer. For the fall of 2006, we plan a Special Semester on Gröbner bases; plans for Special Semester for the following years include

- Mathematical Modelling of Cell Motion and Cell Movement
- Inverse Problems.

The planning of such Special Semesters takes at least two years, and agreements with many of the long-term participants have to be concluded about one year before the start of the semester. This requires that at least the order of magnitude of the Institute budget is known about two years in advance. So far, this is not the case at RICAM, although there are indications that more long-term planning will be possible in the future, which is an absolute prerequisite for hosting Special Semesters, which we consider quite important not only for furthering the development of the specific field to be treated, but also for the international standing and visibility. The success of the first Special Semesters will be quite important for establishing our international position in this “market”.

2.) The Scientific Achievements and Plans of the Institute

Group "Computational Methods for Direct Field Problems"

Group Leader:
O.Univ.-Prof. Dr. Ulrich Langer

Researchers funded via ÖAW/Upper Austrian government funds:
Dr. Sven Beuchler
Dr. Johannes Kraus
Dr. Joachim Schöberl

Researchers funded via the FWF START project Y192 led by Dr. Joachim Schöberl:
Dipl.-Ing. Almedin Becirovic
Dipl.-Ing. Robert Gaisbauer
Dipl.-Ing. Sabine Zaglmayr

Introduction

The "Computational Mathematics Group" (CMG) has focused on the development, analysis and implementation of novel fast computational methods for direct field problems. The first group of methods, developed by S. Beuchler and J. Schöberl, 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). It is worth to mention that these DD solvers are highly parallel. In October 2004 three PhD students, supported by the FWF START project Y192 *"hp-FEM"*, joined the CMG. The START price was awarded to Joachim Schöberl by the FWF in 2002. The second group of solvers, developed by J. Kraus, 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 2004. The publications [3, 4, 7] are devoted to DD techniques, whereas the papers [5, 6] deal with AMG methods for large scale data-sparse boundary element equations. The contribution [3] provides an overview on DD methods and their theoretical fundamentals. The papers [1,2] are devoted to the analysis of non-linear eddy current problems with harmonic excitations and their numerical solution via some multiharmonic technique. The results on multiharmonic techniques and other results obtained in Computational Electromagnetics were presented in a plenary talk at the 4th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS) held in Jyväakylä, Finland [9]. The results on DD methods were also presented in a plenary talk at the annual GAMM conference in Dresden, Germany [8].

1. Bachinger F., Langer U., Schöberl J.: Numerical Analysis of Nonlinear Multi- harmonic Eddy Current Problems. Johannes Kepler University of Linz, SFB "*Numerical and Symbolic Scientific Computing*", SFB Report Nr. 2004-01, Linz 2004, and submitted . (http://www.sfb013.uni-linz.ac.at)
2. Bachinger F., Langer U., Schöberl J.: Efficient Solvers for Nonlinear Time-Periodic Eddy Current Problems. Johannes Kepler University of Linz, SFB "*Numerical and Sym-*

bolic Scientific Computing", SFB Report Nr. 2004-16, Linz 2004, and submitted (http://www.sfb013.uni-linz.ac.at).
3. Korneev V.G., Langer U.: Domain decomposition methods and preconditioning, Chapter 19 in Part I of the "*Encyclopedia of Computational Mechanics*", 44 pages, John Wiley & Sons, 2004.
4. Langer U., Pohoata A., Steinbach O.: Application of preconditioned coupled FETI/BETI solvers to 2D magnetic field problems. Johannes Kepler University of Linz, SFB "*Numerical and Symbolic Scientific Computing*", SFB Report Nr. 2004-23, Linz 2004 (http://www.sfb013.uni-linz.ac.at).
5. Langer U., Pusch D.: Data-Sparse Algebraic Multigrid Methods for Large Scale Boundary Element Equation. *Applied Numerical Mathematics*, 2004 (accepted for publication).
6. Langer U., Pusch D.: Comparison of Geometrical and Algebraic Multigrid Preconditioners for Data-Sparse Boundary Element Matrices. Johannes Kepler University of Linz, SFB "*Numerical and Symbolic Scientific Computing*", SFB Report Nr. 2004-24, Linz 2004 (http://www.sfb013.uni-linz.ac.at).
7. Langer U., Steinbach O.: Coupled Boundary and Finite Element Tearing and Interconnecting Methods. In: *Domain Decomposition Methods in Sciences and Engineering* (ed. by R. Kornhuber, R. Hoppe, J. Periaux, O. Pironneau, O. Widlund, J. Xu), Lecture Notes in Computational Sciences and Engineering, vol. 40, Springer, Heidelberg, pp. 83-97, 2004.
8. Langer U.: Finite and Boundary Element Domain Decomposition Methods. Plenary talk at the Annual GAMM Conference, Dresden, Germany, March 2004 (joint talk with O. Steinbach).
9. Langer U.: Efficient Solvers in Computational Electromagnetics. Plenary talk at the ECOMMAS 2004, Jyväskylä, Finland, July 2004 (joint talk with F. Bachinger, D. Lukas, J. Schöberl, S. Zaglmayr).
10. Langer U., Steinbach O., Wendland W.L.: Adaptive Fast Boundary Element Methods in Industrial Applications. Book of Abstracts, Berichte aus dem Institut für Angewandte Analysis und Numerische Simulation, 2004/015, Stuttgart 2004.

The CMG primarily has internal cooperations with the Inverse Problem Group (IPG) and the Symbolic Computation Group (SCG). 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 V.G. Korneev (St. Petersburg) and O. Steinbach (Graz) on DD methods (see publications [3, 4, 7]). The group leader was one of the co-organizers of the workshop *"Adaptive Fast Boundary Element Methods in Industrial Applications"* held at Hirschegg, September 29 – October 2, 2004 [10]. 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. The group leader is the main organizer of the Special RICAM Semester on *"Computational Mechanics"*, that is planned for fall 2005, and the 17^{th} International Conference on Domain Decomposition, that is planned for July 3 – 7, 2006.

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 high-order finite element solvers. 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. Together with the IPP and other European partners we have recently submitted a **RTN proposal** on "*Advanced large-scale **EN**vironmental computing: **T**raining **R**ese**A**rch **N**etwork **C**onnecting **E**urope*" (***ENTRANCE***) to the European Commission within the 6^{th} Framework Programme.

Dr. Sven Beuchler

Introduction

The research area of Dr. Sven Beuchler is the field of solution methods for systems of linear algebraic equations arising from discretizations of elliptic boundary value problems. One of these methods is the finite element method (FEM).
On the one hand, the polynomial degree p can be increased and the mesh-size h is kept constant, on the other hand the polynomial degree p is kept small and the mesh-size h is decreased. The first method is called p-version of the FEM, and the second one h-version of the FEM. For uniformly elliptic problems, Dr. Beuchler has investigated several preconditioning techniques in order to solve systems of linear algebraic equations efficiently. All of these preconditioners base on Domain Decomposition methods (DD-methods) of Dirichlet-Dirichlet-type. Such a pre-conditioner has several ingredients, the solver related to the problem of the subdomains (interior solver), the Schur-complement pre-conditioner and the extension operator.

Scientific Achievements 2004

Research 2004 at RICAM

From October 2003 to August 2004, Dr. Beuchler has worked at RICAM. In this time, he has investigated the problem of the discrete harmonic extension of a polynomial function from the boundary to the interior of the hexahedron or quadrilateral.
Using methods of multi-resolution analysis, [1], he has proposed two techniques for an optimal discrete harmonic extension, [4], [5]. The corresponding DD pre-conditioner has been investigated in the paper [6]. In these papers, the finite elements are hexahedrons and quadrilaterals. In the paper [7], the case of triangular elements is considered and new shape functions for the reference triangle are developed. With the help of these functions, the element stiffness matrices are sparse in the case of piecewise polynomial coefficients on the elements. In order to compute the nonzero entries of the stiffness matrix, a cooperation with the Symbolic group at RISC is planned.

Scientific Visits and Talks

Visits:

- 28/02/04-03/03/04: Visit at the Sandia National Lab, Livermore, California (invited)

Talks:

- 26/02/04 San Francisco, SIAM Conference PP04: Parallel Multi-level solvers for degenerate problems
- 01/03/04 Livermore, USA, Sandia National Labs: A parallel multi-level pre-conditioner for the p-Version of the Finite Element Method
- 26/03/04 Dresden, GAMM Jahrestagung 2004: A DD-pre-conditioner for p-fem
- 28/05/04 Prague, Iterative Methods 2004: A DD-pre-conditioner for p-fem
- 05/06/04 Berlin, 2nd European Finite Element Fear 2004: A DD-pre-conditioner for p-fem

Scientific Cooperations

Internal Cooperations with

- with the Symbolic Group at RISC and SFB F013 (Burkhard Zimmermann)
- with the SFB project groups F1301 and F1306 at SFB F013
- with the FWF-Start project group led by Joachim Schoeberl

External Cooperations with
- Prof. Dr. V.G. Korneev, Russian State University, St. Petersburg, Russia,
- Prof. Dr. R. Schneider, Mathematisches Seminar, University of Kiel, Germany,
- Prof. Dr. C. Schwab, Seminar for Applied Mathematics ETH Zürich, Switzerland,
- Prof. Dr. L. Demkowicz, University of Texas, Austin, USA,
- Prof.. Dr. M. Jung,, HTW Dresden, Germany,
- Dipl-Math. techn. Tino Eibner, SFB 393, TU Chemnitz.

Participation at conferences

- 24/02/04-27/02/04: SIAM Conference PP04 in San Francisco
- 22/03/04-26/03/04: GAMM-Jahrestagung 2004, Dresden
- 25/05/04-28/05/04: IMET Conference in Prague
- 04/06/04-05/06/04: 2nd European Finite Element Fear in Berlin (TU Berlin)

Publications

Appeared

1. Sven Beuchler, Reinhold Schneider, Christoph Schwab: Multiresolution weighted norm equivalenes and applications. Numerische Mathematik, 98(1), 67-97, 2004.
2. Sven Beuchler: Multi-grid solver for the p-version of the fem. PAMM, 3(1), 2003, 529-530.

Accepted

3. Sven Beuchler: Multilevel solvers for a finite element discretization of a degenerate problem. accepted for publication in SIAM Journal on Numerical Analysis. revised version of SFB393 Preprint 03-04 (TU Chemnitz).
4. Sven Beuchler, Joachim Schöberl: Optimal extensions on tensor product meshes. accepted for publication in Applied Numerical Mathematics.
5. Sven Beuchler: Extension operators on tensor product structures in 2D and 3D. accepted for publication in SIAM Journal Scientific Computing.
6. Sven Beuchler: A domain decomposition pre-conditioner for p-FEM discretizations of two dimensional elliptic problems. accepted for publication in Computing.

In Preparation:

7. Sven Beuchler, Joachim Schoeberl: Internal Shape Functions for the Reference triangle.

Dr. Johannes Kraus

Introduction

Algebraic MultiGrid (AMG) and Algebraic MultiLevel (AML) methods provide powerful and state of the art solvers for large classes of sparse matrix problems in industrial applications. However, there are problems of practical interest, e.g., in the area of Computational Fluid Dynamics (CFD), Solid and Structural Mechanics (SSM), and Computational Electro Dynamics (CED), for which presently known linear solvers show a lack of robustness. In general, these problems are extremely large, making direct solvers infeasible, and highly ill-conditioned, demanding very efficient preconditioning when using iterative solvers.
We concentrate on the iterative solution of systems of linear algebraic equations arising from finite element (FE) discretization of (systems of) partial differential equation (PDEs). In particu-

lar, we address differential operators with complicated characteristics and high-dimensional kernels, respectively.
Our general objectives are the design, analysis and implementation of new robust AMG and AML algorithms that enable an efficient preconditioning of direct field problems in SSM, CED, and CFD.

Scientific Achievements 2004

Research 2004 at RICAM

Scientific achievements in 2004 have been made in the following areas:

1. Agglomeration techniques in three-dimensional space:
   This work provides a basis for various element-based AMG (and AML) methods. Its focus is on generating hierarchies of topological relations for unstructured three-dimensional (3D) finite element (FE) meshes. The related topological elements are agglomerates, faces, edges, and vertices. We provide practical definitions and propose efficient procedures, in particular for the setup of coarse faces and coarse edges. Moreover, we examine the agglomeration algorithm of Jones and Vassilevski and suggest a proper generalization for 3D meshes. This setting allows for a recursive construction of a sequence of nested coarse topologies, which can be used in different areas of finite element computations, e.g., load balancing for parallel processing, domain decomposition methods, algebraic multigrid or multilevel preconditioning methods based on incomplete factorization.
   Technical Report [KrausSynka:2004a] (see Section Publications). Full paper [KrausSynka:2004b] submitted to Computing and Visualization in Science, Springer.

2. Multilevel preconditioning using local Schur complements:
   We consider an algebraic multilevel preconditioning technique for symmetric positive definite (SPD) matrices arising from FE discretization of elliptic PDEs. The case of non-M matrices deserves closer attention. The method is based on element agglomeration and assumes access to the individual element stiffness matrices. The left upper block of the considered multiplicative two-level preconditioner is approximated by means of a new incomplete factorization procedure. The coarse-grid element matrices are simply Schur complements computed from local neighborhood matrices, i.e., small collections of element matrices. Assembling these local Schur complements results in a global Schur complement approximation that can be analyzed by regarding (local) macro elements. These components, when combined in the framework of an algebraic multilevel iteration (AMLI), yield a robust and efficient linear solver. Our numerical experiments include also the Lamé differntial equations for the displacements in the 2D plane-stress elasticity problem.
   Technical Report [Kraus:2004c]. Extended abstract [Kraus:2004b] in Proceedings of the IMET 2004, Conference on Iterative Methods, Preconditioning & Numerical PDEs.
   Paper [Kraus:2004d] submitted to Numerical Linear Algebra with Applications, John Wiley & Sons, Ltd.

3. Algebraic multigrid based on computational molecules:
   We consider the problem of splitting a symmetric positive definite (SPD) stiffness matrix A arising from FE discretization into the sum of edge matrices thereby assuming that A is given as the sum of symmetric positive semidefinite (SPSD) element matrices. We give necessary and sufficient conditions for the existence of a decomposition into SPSD edge matrices and provide a feasible algorithm for the computation of edge matrices in case of general SPSD element matrices. Based on the knowledge of edge matrices, we discuss how to alter the concept of *strong* and *weak* connections, as it is used for coarse-grid selection in classical AMG. We further derive interpolation from an energy minimization principle: The *computational molecules* involved in this process are assembled from edge matrices each of which represents the connection of two nodes in the global (algebraic) grid. The

molecules are small-sized irreducible (local) matrices with inherent kernel preservation. However, they are not necessarily SPSD. Numerical tests have shown the robustness of the new method, which we refer to as AMGm (Algebraic MultiGrid based on computational molecules). Technical Report [KrausSchicho:2004] in preparation.

Scientific Visits and Talks

1.Invited talk:

"Element-based Interpolation and Coarse-Grid Selection in Algebraic Multigrid",
ETH Zuerich, January 14th, 2004.
This talk was given in the run-up of a cooperation with Prof. Dr. R. Hiptmair on Edge-Element AMG for problems in H(**curl**).

2.Conference talk:

"Multilevel Preconditioning Based on Element Agglomeration",
presented at the IMET Conference on "Iterative Methods, Preconditioning & Numerical PDEs", held in Prague, May 25th-28th, 2004.

3.RICAM seminar talk:

"Algebraic MultiGrid Based on Computational Molecules",
RICAM Linz, December 6th, 2004.
This was a joint talk with Prof. Dr. J. Schicho (RICAM) where first results of a specific cooperation between the "Symbolic Computation Group" (SCG) and the "Computational Mathematics Group" (CMG) were presented.

Scientific Cooperations

Internal Cooperations with:

1. Prof. Dr. J. Schicho, SCG, RICAM:
   The topic of this cooperation is closely related to the third area of scientific achievements in 2004, mentioned above. We aim at the construction of edge matrices with particular properties (kernel preservation, SPSD, etc.) that provide the foundation of a new class of algebraic multigrid and multilevel methods. Thereby symbolic techniques can be utilized for a reduction of the setup costs. In a first working phase scalar elliptic self-adjoint boundary-value problems have been investigated and a robust solver has been implemented. Further cooperative work will be spent on the case of systems of PDEs, e.g., linear elasticity and Maxwell's equations.

2. Dr. J. Synka, Industrial Mathematics Institute (IndMath), University of Linz:
   In this cooperation we work on discretization techniques, in particular, variants of the finite element method (FEM) that allow for a direct computation of edge matrices (also in the case of systems of PDEs).
   Another cooperation with Dr. Synka was on 3D multilevel topology concepts (see Section Publications).

External Cooperations with:

1. Prof. Dr. P. Vassilevski, Lawrence Livermore National Laboratory (LLNL), CA, USA:
   This year, from June 1st to 3rd, Prof. Vassilevski visited RICAM and gave a lecture on "A General Framework for Algebraic Multigrid". His contributions on the convergence theory (a sharp two-grid convergence result), compatible relaxation, and null-space preserving preconditioners for saddle-point matrices greatly influence the work on AMG related topics at RICAM. For next year it is planned that Dr. Kraus visits LLNL in order to intensify the coop-

eration with the research group around Prof. Vassilevski.

2. Prof. Dr. R. Hiptmair, ETH Zuerich, Switzerland:
   The cooperation on AMG for edge element discretizations of Maxwell's equations will continue in 2005.

3. Prof. Dr. S. Margenov, Institute for Parallel Processing, BAS, Sofia, Bulgaria:
   There is an ongoing cooperation with Prof. Margenov on Algebraic Multilevel Preconditioners that is based on a contract between RICAM and the Bulgarian Academy of Sciences concerning a joint research program. The CMG, RICAM is a partner in the EU RTN Project "Advanced Environmental Computing".

4. Dr. Dalibor Lucas, University of Ostrava, Czech Republic:
   The new generation algebraic multigrid and multilevel solvers developed at RICAM are tested in different applications. Problems of optimal shape design can be solved in a nested way. In an outer optimization loop we modify shapes in order to minimize an optimization criterion. Then, for each shape a discretized state problem, here the Maxwell's equations, e.g., their magnetostatic case, are solved. Typically, tens of solutions of state systems are necessarry during the optimization, while there are only slight perturbations in the system matrix. Algebraic multigrid seems to be just the right choice, since we can map perturbations of the design interface onto the material coefficients with jumps across elements, while the discretization grid is fixed. On the development and usage of an algebraic multigrid method in shape optimization we want to cooperate with Dalibor Lukas from the Technical University of Ostrava, Czech Republic.

Participation at conferences

- IMET 2004, Conference on
  "Iterative Methods, Preconditioning & Numerical PDEs",
  held in Prague, May 25th to 28th, 2004 (see Section **Scientific Visits and Talks**).

- 21st GAMM-Seminar on
  "Robust Fast Solvers"
  held at the Max-Planck-Institute for Mathematics in the Sciences, Leipzig,
  January 26th to 28th, 2005.

Publications

Appeared:

Kraus:2004a
J.K. Kraus: "Computing interpolation weights in AMG based on multilevel Schur complements", accepted for publication in Computing, 2004.
Online published under http://www.springerlink.com/index/10.1007/s00607-004-0101-3

Kraus:2004b
J.K. Kraus: "Multilevel preconditioning based on element agglomeration",
in Proceedings of the IMET 2004, Conference on Iterative Methods, Preconditioning & Numerical PDEs, held in Prague, May 25th to 28th, 2004, pp. 93-96.

Kraus:2004c
J.K. Kraus: "Algebraic multilevel preconditioning of finite element matrices based on element agglomeration", RICAM Report No. 2004-01.

KrausSynka:2004a
J.K. Kraus and J. Synka: “An agglomeration-based multilevel topology concept with application to 3D-FE meshes”, RICAM Report No. 2004-08.
Submitted:

Kraus:2004d
J.K. Kraus: “Algebraic multilevel preconditioning of finite element matrices using local Schur complements”, submitted to Num. Lin. Alg. Appl., October 2004.

KrausSynka:2004b
J.K. Kraus and J. Synka: “An agglomeration-based multilevel topology concept with application to 3D-FE meshes”, submitted to Computing and Visualization in Science, August 2004.

In Preparation:

KrausSchicho:2004
J.K. Kraus and J. Schicho: “Algebraic construction of edge matrices and their utilization in algebraic multigrid”, RICAM Report in preparation.

Dr. Joachim Schöberl and his doctoral students: Almedin Becirovic, Robert Gaisbauer, and Sabine Zaglmayr

Introduction

J. Schöberl is working on the development of theory and software for the numerical approximation of partial differential equations. He is leading the FWF-Start project “High Order Finite Elements: Solvers and Adaptivity”, where the 3 PhD students A. Becirovic, R. Gaisbauer, and S. Zaglmayr are employed. The main research topics are the construction of high order finite elements for vector valued problems such as Maxwell equations, the design of Schwarz-preconditioners for matrices arising from high order elements, primal-dual error estimators, and mesh generation and adaptive mesh refinement.

Scientific Achievements 2004

Research 2004 before RICAM

1. J. Schöberl and S. Zaglmayr have constructed new basis functions for the Nedelec finite element spaces as needed for the approximation of Maxwell equations. This basis has the 'local complete sequence property', which allows variable order elements, and enables simple Schwarz preconditioning, publication in COMPEL.
2. A. Becirovic and J. Schöberl work with Prof. Paule and his team (RISC, Linz) on utilizing hypergeometric summation algorithms to allow simple and efficient evaluation of high order finite element basis functions as well as fast direct evaluation of the finite element matrices.
3. A. Becirovic and J. Schöberl work on primal-dual error estimators for high order finite elements. The principle is to compute the fluxes in an H(div) finite element space by a cheap postprocessing method. Publication in preparation.
4. R. Gaisbauer and J. Schöberl work on mesh generation and mesh refinement. The open source mesh generator Netgen (by J. Schöberl) was extended to handle standard CAD geometry files (IGES, Step) by including the open source geometry kernel OpenCascade. Template-based mesh refinement for geometric and anisotropic refinement for the

approximation of edge and corner singularities was implemented.

Research 2004 at RICAM

1. J. Schöberl could prove the efficiency of residual-based a posteriori error estimators for Maxwell equations, which was a conjecture so far. This was achieved by new error estimates for the Clement-operator for H(curl) proposed by J. Schöberl. Publication in preparation.

Scientific Visits and Talks

1. Visited Prof. D. Boffi, Dipartimento di Matematica, Università di Pavia, March 26-28 Talk: "Preconditioning for Maxwell equations",
2. Visited Jun. Prof. Dr. T. Hohage, Inst. f. Numerische und Angewandte Mathematik, Göttingen, April 26-28, Talk: "Preconditioning for high order finite elements",
3. Invited to Oxford Study group at Cambridge, May 12-14,
4. Visited PD Dr. B. Kaltenbacher, and PD Dr. M. Kaltenbacher, Lehrstuhl für Sensorik, Erlangen, Talk: "High Order Finite Elements", May 24-26
5. Visited Prof. C. Carstensen, Humboldt Universtiy Berlin, Aug 23-25, Work on Paper
6. Visited Dr. Ostrovski, ABB, Zürich, Sept 27,
   Talk: "High Order Finite Elements for Maxwell Equations"
7. Visited Prof. Weiland, Inst. für Theorie Elektromagnetischer Felder, TU Darmstadt, Nov 22-23, Talk: "High Order Finite Elements for Maxwell Equations"
8. Visited Prof. Biro, Inst. Grundlagen und Theorie der Elektrotechnik, TU Graz, Dec 13-15 Talk: "High Order Finite Elements"

Scientific Cooperations

Internal Cooperations with

1. SFB F013 "Numerical and Symbolic Scientific Computing", in particular Prof. Paule: Work on special function techniques for finite elements.
2. Prof. H. Irschik, Dr. J. Gerstmayr, Inst. Techn. Mechanik, JKU Linz: Work on multibody systems, publications available.

External Cooperations with

1. Prof. L. Demkowicz, UT Austin. Work on hp-error estimates for Maxwell equations.
2. PD Dr. J. M. Melenk, Reading, UK. Work on Schwarz methods for tetrahedral elements.
3. Prof. C. Carstensen, Humbold University Berlin. Work on a posteriori error estimates for Reissner Mindlin plates (paper submitted)
4. Prof. D. Boffi, Pavia. Work on approximation of Maxwell eigenvalue problems (paper submitted)
5. Junior Prof. Dr. Th. Hohage, Göttingen. Work on approximation of open resonance problems.
6. A.-Prof. O. Biro, TU Graz, Electrical Engineering. Cooperation on FEM in electrical engineering.
7. A.-Prof. Dr. Böhm, TU Vienna. Cooperation on FEM in material sciences.

Participation at conferences

1. Oberwolfach Seminar on Computational Electromagnetics, Germany, Feb 22-27
2. Progress in Electromagnetics Research Symposium (PIERS04), Pisa, Italy, March 28-31

3. International Conference on Spectral And High Order Methods (ICOSAHOM), Providence RI, Juni 21-25
4. European congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS), Jyväskylä, Finland, July 24-28
5. Scientific Computing in Electrial Engineering (SCEE), Sicilia, Sept 5-8
6. IGTE Symposium (Electrical engineering workshop), near Graz, Austria, Sept 13-15
7. Chemnitzer FEM Symposium, near Chemnitz, Germany, Sept 20-22

Publications

Appeared

1. Z. Dostal and J. Schöberl: "Minimizing Quadratic Functions Subject to Bound Constraints With the Rate of Convergence and Finite Termination", Computational Optimization and Applications, 30:23-44, 2005
2. S. Beuchler and J. Schöberl: "Extension operators on tensor product structures in 2D and 3D", Applied Numerical Mathematics, available online
3. J. Schöberl and S. Zaglmayr: "High Order Nedelec Elements with local complete sequence properties", to appear in Int. J. Computations and Mathematics in Electrical and Electronic Enginerring (COMPEL) 24

Submitted

1. J. Gerstmayr and J. Schöberl: "A 3D finite element method for flexible multibody systems", submitted to Multibody System Dynamics.
2. C. Carstensen and J. Schöberl: "Residual-based a posteriori error estimate for a mixed Reissner-Mindlin plate finite element method", submitted to Numerische Mathematik.
3. F. Bachinger, U. Langer, and J. Schöberl: "Numerical Analysis of Nonlinear Multi-harmonic Eddy Current Problems", submitted to Numerische Mathematik
4. F. Bachinger, U. Langer, and J. Schöberl: "Efficient Solvers for Nonlinear Time-Periodic Eddy Current Problems", submitted to Computation and Visualization in Sciences.
5. D. Boffi, F. Kikuchi and J. Schöberl: "Edge Element Computation of Maxwell's Eigenvalues on General Quadrilateral Meshes", submitted to Mathematical Models and Methods in Applied Sciences.
6. S. Zaglmayr, J. Schöberl, U. Langer: "Eigenvalue Problems in Surface Acoustic Wave Filter Simulation", submitted

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
Prof. Dr. Sergei Pereverzyev
Dr. Elena Resmerita
Dr. Arnd Rösch

Researchers externally funded:
Dr. Nicoleta Bila
DI Hui Cao
DI Herbert Egger
DI Benajamin Hackl
DI Andreas Hofinger
DI Shuai Lu

Introduction:

This year, the group expanded both as far as personnel and as far as topics are concerned. As can be seen from the list above, the majority of group members is externally funded.

Research in 2004 concerned inverse problems emphasizing the following topics:

- Regularization methods in Banach spaces
- Connections of inverse problems to optimization and optimal control
- Iterative regularization
- Statistical and stochastic aspects
- Applications in geophysics
- Level set methods
- Parameter identification with applications in finance and in molecular biology.
- Use of symmetry in regularization methods for inverse problems.

All of these topics will be continued; major emphasis will be laid on inverse problems in molecular biology, where a joint project with Peter Schuster (University of Vienna) has submitted for funding.
A mini-workshop on symmetry and inverse problems will be held in January of 2005. In June, some group members will attend a reunion workshop of the IPAM Special Semester on Inverse Problems, led by Heinz Engl, at UCLA, and the Applied Inverse Problems Conference in England. In fall, an international workshop on inverse problems and level set methods will be organized at RICAM. During the Special Semester on Computational Mechanics at RICAM, some events on inverse problems e.g. in plasticity will be organized.

Publications of the group leader connected with work at RICAM in 2004:

1. H.W. Engl, Identification of parameters in polymer crystallization, semiconductor models and elasticity via iterative regularization methods, in: V.G. Romanov, S.I. Kabanikhin, Yu.E. Anikonov and A.L. Bukhgeim (eds.), Ill-Posed and Inverse Problems, VSP, 2004, 99-126

2. M.Burger, H.W. Engl, A.Leitao, P.Markowich, On inverse problems for semiconductor equations, Milan Journal of Mathematics 72 (2004), 273-314

3. H.W. Engl, P. Kügler, Nonlinear Inverse Problems: Theoretical Aspects and Some Industrial Applications, in: V. Capasso and J. Periaux (eds.), Multidisciplinary Methods for Analysis, Optimization and Control of Complex Systems, Springer Heidelberg, Series Mathematics in Industry, The European Consortium for Mathematics in Industry, Band 6 Capasso, Vincenzo; Périaux, Jaques (Hrsg.) 2005, XV

4. H.W. Engl, A. Hofinger, S. Kindermann, Convergence rates in the Prokhorov metric for assessing uncertainty in ill-posed problems, Inverse Problems, 21,(1), 399-412, 2005

5. H.W. Engl, H. Egger, Tikhonov regularization applied to the inverse problem of option pricing: convergence analysis and rates, submitted

6. H.W. Engl, P. Fusek, S. Pereverzev, Natural linearization for the identification of nonlinear heat transfer laws, submitted

7. H. Egger, H.W. Engl, M. Klibanov, Global uniqueness and Hölder stability for recovering a nonlinear source term in a parabolic equation, Inverse Problems (to appear)

Talks by the group leader connected with work at RICAM in 2004:

- February 2004, Talk at the California State University of Northridge
- March 2004, University of Trondheim: Mathematics and Industry – a Relationship for Mutual Benefit
- June 2004, Perspectives in Inverse Problems, Helsinki, Finland, invited talk: Regularization in Fuzzy Control and Neural Networks, Stochastic Convergence Concepts for Inverse Problems
- June 2004, Conference "Modern Computational Methods in Applied Mathematics"; Bedlewo, Poland, invited talk: Iterative Regularization of Nonlinear Inverse Problems
- July 2004, London City: Identification of Model Parameters in Computational Finance Based on Inverse Problems Techniques
- September 2004, Talk at the University of Saarbrücken, Germany
- October 2004, Talk at Emory University, Atlanta, USA
- December 2004, International Workshop on Nonlinear PDE´s, IPM, Teheran, Iran, invited talk: Iterative Regularization of Nonlinear Inverse Problems for Partial Differential Equations, tutorial lectures on Inverse Problems

Dr. Stefan Müller

Introduction

Stefan Müller joined the Johann Radon Institute for Computational and Applied Mathematics in November 2004.

Stefan Müller studied physics at the Vienna University of Technology and chemistry at the University of Vienna. His research aims at bridging chemistry and biology on a formal level, using concepts from mathematics and computer science. He worked on a lambda-calculus model of chemical organizations and on a graph-rewriting model of morphogenesis.

Scientific Achievements 2004

Research 2004 before RICAM

Stefan Müller held a PostDoc position at the Institute for Theoretical Chemistry and Structural Biology, University of Vienna. He developed a generic model of a minimal cell for investigating evolutionary and developmental questions. One major part of the model is a gene regulatory network (GRN) which allows to study the dynamics of gene expression.

The model uses the following abstraction of the chemical processes within a living cell: (1) The system is closed. (2) Gene products bind to the regulatory regions of the genes and either enhance or inhibit their expression. (3) Polymers (proteins, RNAs) are built from activated monomers. (4) Transcription and translation are one-step reactions. (5) Polymers degrade into deactivated monomers. (6) The system is coupled to the environment via a photochemical reaction which transforms deactivated into activated monomers.

The topology of the GRN is defined in terms of an edge-weighted directed graph with vertices representing genes, edges representing gene-protein binding and edge weights representing binding constants and either enhancement or inhibition. This graph can be "decoded" from an artificial genome. Evolutionary operators like mutation and recombination act at the level of the artificial genome and cause changes in the GRN via an intricate decoding process, but always yield a valid GRN. Therefore evolutionary questions can be easily addressed within this framework. Alternatively, the GRN can be designed explicitly. Such rational network design may lead both to the engineering of new cellular behaviors (e.g. the “repressilator”) and to an improved understanding of naturally occurring networks.

The topology of the GRN determines the system of chemical equations in the minimal cell which is finally mapped to a system of nonlinear ODEs. Integration of the ODEs yields the gene expression pattern over time.

To explore the range of dynamical behavior possible in the model, Stefan Müller chose the “repressilator” as a canonical example of a GRN. He was able to reproduce the full range of dynamical behavior reported for the repressilator, both numerically and analytically.

Research 2004 at RICAM

As described above, gene regulatory networks and metabolic reaction networks can be mapped to a system of nonlinear ODEs. This conventional forward analysis of biologically relevant dynamical systems may be complemented by usage of existing and design of novel inverse methods.

Stefan Müller started to address this task by reconstructing unknown parameters from recorded solution curves, using the iterative regularization method of Landweber. Again he chose the “repressilator” as a canonical example of a GRN.

The solution of the inverse problem included three steps: (1) automatic linearization of the forward system using symbolic computation. (2) definition of the adjoint system. (3) implementation of an iterative algorithm using the solvers for the forward and the adjoint system.

This work is a preparation for a project planned together with the group of Prof.Peter Schuster (Univ. of Vienna) and submitted to WWTF.

Scientific Visits and Talks

"A minimal cell model for studying evo-devo", talk
Konrad Lorenz Institute for Evolution and Cognition Research, Altenberg, Austria

Scientific Cooperations

Internal Cooperations with
Dr. Philipp Kügler and Prof. Heinz Engl

External Cooperations with
Dr. Christoph Flamm and Prof. Peter Schuster, Institute for Theoretical Chemistry and Structural Biology, University of Vienna
Prof. Josef Hofbauer, Department of Mathematics, University College London

Participation at conferences

"A Minimal Model for Gene Regulatory Networks", poster
International Course & Conference on the Interfaces among Mathematics, Chemistry and Computer Sciences (Math/Chem/Comp 2004), June 21-26, 2004, Dubrovnik, Croatia

Publications

Appeared

Martin Beck, Gil Benkö, Gunther J. Eble, Christoph Flamm, Stefan Müller, and Peter F. Stadler. "Graph Grammars as Models for the Evolution of Developmental Pathways", In: H. Schaub, F. Detje, U. Brüggemann, editors, The Logic of Artificial Life - Abstracting and Synthesizing the Principles of Living Systems, pages 8-15, Berlin, 2004. IOS Press, Akademische Verlagsgesellschaft. GWAL 2004, Bamberg, Germany, 14-16 April, 2004, Proceedings.

Dr. Sergei Pereverzyev

Scientific Achievements.

In accordance with the **Scientific Plan for 2004** the research has been conducted in two directions. One of them is connected with realization of the **FWF-Project P17251-N12 “Fixed point regularization schemes for nonlinear ill-posed problems and their discretization”.** Within this project scientific supervision for **Mag. Shuai Lu** and **Mag. Cao Hui** has been provided. In August 2004 both of them have been employed within the framework of the project as doctoral students.
During the first Project year the main research activity has been aimed at regularization methods for naturally linearized parameter identification problems. A fast algorithm for numerical identification of nonlinear heat transfer laws has been developed. Its main advantages are the following: the original nonlinear inverse problem is reduced to a linear one; the resulting linear problem is always one-dimensional while the underlying process can depend on several time and space variables; only a single call of the solver for the corresponding direct problem is necessary. This result has been obtained in cooperation with Prof. Heinz Engl and Dr. Peter Fusek (Institut für Industriemathematik, Johannes-Kepler-Universität, Linz).
In “natural linearization” one has in mind the reduction of original nonlinear inverse problem to the sequence of linear ill-posed problems, where the regularization of one of them should be

related with the previous one. Usually, one of these linear problems is just a numerical differentiation, but the smoothness of the function to be differentiated is unknown. Surprisingly, we could not find any results providing us with a recipe for the optimal regularization parameter choice for numerical differentiation. Thus, there is a gap in the analysis of this important computational procedure, and the first goal of joint research with project team member Mag. Shuai Lu was to fill this gap. As a result, several numerical differentiation procedures have been proposed which adapt to unknown smoothness of the function to be differentiated. It is shown that the accuracy of such adaptive numerical differentiation is of the same order as one could achieve in the case of known smoothness.

The second direction that was also planned for year 2004, is the regularization of ill-posed problems with discretized random noisy data in the course of GOCE-data processing. This direction is motivated by the forthcoming Gravity field and steady-state Ocean Circulation Explorer (GOCE) satellite mission that will be launched by European Space Agency (ESA) in 2006. What makes the GOCE-regularization problem challenging is the combination of a huge number of observations and unknown gravity field parameters with uncontrolled observation noise. The elements of the theoretical base for GOCE-regularization have been elaborated in cooperation with Peter Mathé (WIAS-Berlin). A first accomplishment of this research is a general adaptation strategy for regularization parameter choice which allows to achieve the best order of accuracy using minimal information about observation noise. More precisely, one needs to know only the noise intensity and the Schatten index of the noise covariance operator. In principle, both these numbers can be estimated from the observations. A computational procedure based on this adaptation strategy has been proposed in joint paper with Frank Bauer (Group of Geomathematics, University of Kaiserslautern). Numerical tests with data from EGM96 (Earth Gravity Model-1996) show that the proposed adaptation strategy could be a method of choice for GOCE-data processing.

In accordance with the **Scientific Plan for 2004** the cooperation with the group headed by Prof. Dr. Hans Sünkel in the Space Research Institute (IWF-Graz) of Austrian Academy of Sciences has been established. As a result a joint research project "Regularization and Weighting strategy in the course of GOCE-data processing" has been started. The research partner from IWF-side is Dr. Kirco Arsov. This project is devoted to the development and investigation of the performance of new approaches to the GOCE-data processing based on adaptive regularization.
Membership in the Working Groups "Inverse Problems" and "Multiscale Modelling of the Gravity Field" of International Association of Geodesy (IGA) allows to coordinate the investigation of Inverse Problems of Satellite Geodesy with this association.

<u>Scientific cooperations with scientists from other institutions.</u>

During the year 2004 the research work has been conducted in cooperation with the following groups and scientists:

1. Department of Satellite Geodesy headed by Prof. Dr. Hans Sünkel in the Space Research Institute (IWF) of Austrian Academy of Sciences

A joint project proposal with Dr. Kirco Arsov (IWF) "Regularization and Weighting strategy in the course of GOCE-data processing" has been started.

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

Regularization of geopotential determination within the framework of forthcoming GOCE-mission. As a result, a joint article with Dr. Frank Bauer has been submitted to "European Journal of Applied Mathematics".

3. PD. Dr. Peter Mathé, Weierstrass-Institute, Berlin.

Adaptive strategies for regularization and discretization of linear ill-posed problems. As a result, a joint article has been submitted to "Inverse Problems".

Participation at conferences.

During the year 2004 the following conferences have been attended:

1. Oberwolfach Workshop on Geomathematics (May,23 – May,29)
   Invited talk with the title: "On adaptive inverse estimation of linear functionals from random noisy data – case study: GOCE- data processing".
2. Mathematical Research and Conference Center in Bedlewo (Poland), Conference"Modern Computational Methods in Applied Mathematics" (June,14-June,19)
   Invited talk with the title: " The choice of the weight in the penalty finite element methods from the view point of regularization theory".
3. Chemnitzer Symposium 2004 zu Inversen Problemen (September, 20 –September, 24)
   Invited talk with the title:" Regularization of Inverse Problems with discretized random noisy data".
4. Dagstuhl Seminar "Algorithms and Complexity for Continuous Problems" (September, 26 - October, 1)
   Invited talk with the title:" *Numerical Differentiation from view point of Regularization Theory".*
5. International conference "Mathematical Statistics 4" (CIRM, Marseille, France, December, 12 - December, 17).
   Invited talk with the title: "Regularization of Inverse Problems with discretized random noisy data".

Visits to other scientific institutions

There was a visit of Space Research Institute of Austrian Academy of Sciences (IWF-Graz). The goal was to establish scientific contacts with the Department of Satellite Geodesy headed by Prof. Dr. Hans Sünkel. During the visit (June, 29 – July, 29), a talk with the title "On adaptive inverse estimation of linear functionals from random noisy data – case study: GOCE- data processing" was given, and the directions of possible cooperation were discussed. As the result, joint project with Dr. Kirco Arsov (IWF) "Regularization and Weighting strategy in the course of GOCE-data processing" has been started.
There was an invitation to give a talk in the Colloquium of the Institute of Numerical Mathematics, University of Göttingen. A talk with the title "Adaptive model selection in inverse statistical estimation“ was given on July, 6, 2004.

Publications

1. S. Pereverzev, E. Schock, On the adaptive selection of the parameter in regularization of ill-posed problems, SIAM J. Numer. Analysis (accepted).
2. P. Mathe, S. Pereverzev, Regularization of some linear ill-posed problems with discretized random noisy data, submitted to Inverse Problems.
3. F. Bauer, S. Pereverzev, Regularization without preliminary knowledge of smoothness and error behaviour, submitted to European Journal of Applied Mathematics.
4. H. W. Engl, P. Fusek, S.V. Pereverzev, Natural linearization for the identification of nonlinear heat transfer laws, submitted.

Dr. Elena Resmerita

Introduction

Dr. Resmerita obtained her PhD from the University of Haifa, Israel, in July 2003 with a thesis entitled: “Fixed point and optimization methods in infinite dimensional Banach spaces”. In Fall 2003, a three-month visit at the Institute of Pure and Applied Mathematics, UCLA, facilitated her introduction to the field of Inverse Problems. She started working at RICAM in March 2004. Her general scientific goal here is to apply optimization methods and convex analysis techniques to Inverse Problems.

Scientific Achievements in 2004

Research 2004 before RICAM

The concepts of Bregman distance and Bregman projection were introduced a few decades ago, as tools for approaching optimization problems. Since then, there has been a growing interest in using them to solving problems in various other fields, including inverse problems.
Dr. Resmerita's scientific activity before coming to RICAM was focused on developing iterative methods for solving stochastic convex feasibility problems by means of Bregman projections. In parallel, she contributed to completing the interesting theoretical framework raised by Bregman distances and associated projections. Some of her recent results in this respect are presented in [1] and [2]. Discussions on Bregman distances at UCLA also stimulated joint work by Burger, Goldfarb and Osher on convex variational regularization.

Research 2004 at RICAM

- The paper [2] makes the transition from her Ph.D. thesis topic to the field of Inverse Problems, as it contains also an extension to reflexive Banach spaces of the popular Landweber iterative method for solving operator equations, known to work in Hilbert spaces.
- As mentioned above, some approaches of inverse problems include Bregman distances as main ingredients. Regularization methods for ill-posed problems in non-reflexive Banach spaces are among them, being also a topic of interest for Dr. Resmerita. Thus, in the preprint [3] - to be submitted soon - rates of convergence for ill-posed problems in Banach spaces were established by means of Bregman distances, assuming some regularity of the true solutions. As an application, convergence rates for maximum entropy regularization were derived, which are better than the ones already known. The results also apply to other regularization methods of current interest like BV-regularization.

Scientific Talks

- Generalized distances and their use in Inverse Problems, “Inverse Problems” Seminar, RICAM, Linz, May 2004.
- Error estimates for regularization of linear ill-posed problems in Banach spaces, “Inverse Problems” Seminar, RICAM, Linz, November 2004.

Scientific Cooperations

- Dr. R.S. Anderssen, CSIRO, Canberra, Australia
- Dr. Martin Burger, Institute for Industrial Mathematics, JKU Linz
- Prof. Dan Butnariu, University of Haifa, Israel

Publications

Appeared

1. E. Resmerita: On total convexity, Bregman projections and stability in Banach spaces, Journal of Convex Analysis 11 (1) (2004), 1-16.

Submitted

2. D. Butnariu and E. Resmerita: Bregman distances, totally convex functions and a method for solving operator equations in Banach spaces, 2004.

Preprint

3. E. Resmerita: Regularization of ill-posed problems in Banach spaces. Convergence rates, 2004.

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 2004

Research 2004 outside RICAM

Temporary professorship (Lehrstuhlvertretung) at the Technische Universität Chemnitz from April through September 2004.

Research 2004 at RICAM

The research in 2004 was focused on several mathematical fields:

1. Regularity of adjoint variables

Adjoint equations and the regularity of their solutions play an important role in the theories of inverse problems and optimal control. A new result for the adjoint state of the instationary Navier-Stokes equations was proved in a joint paper with D. Wachsmuth (TU Berlin): It was shown that the adjoint state is continuous in time with values in a Sobolev space with negative exponent. Moreover, this paper contain counterexamples and the correction to a result in the book of Dautray and Lions on embeddings of abstract functions.

2. Regularization of state constrained optimal control problems

State constrained optimal control problems have properties which are close to those of inverse problems. A Lavrentiev regularization technique is studied in a joint work with C. Meyer and F. Tröltzsch (both TU Berlin).

3. 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. An approximation rate of $h^{3/2}$ was proved in [5] for problems in an abstract setting. The method was adapted to parabolic problems and nonuniform grids in [3].
These are the first two results in literature where superlinear approximation was proved.
A complete new approach was developed together with C. Meyer (TU Berlin).
It was shown that superconvergence effects occur in FEM discretizations of optimal control problems. Exploiting these effects, the approximation order can be improved to h^2. A further paper with C. Meyer (TU Berlin) is submitted. It contains the proof of an approximation rate of h for piecewise linear controls.

Scientific Visits and Talks

Visits:

1. Karl-Franzens-Universität Graz from 04/06/16 to 04/06/18
2. Universität der Bundeswehr München from 04/10/13 to 04/10/15

Talks:

1. FEM bei Optimalsteueraufgaben, Seminar on PDEs, Chemnitz, 04/01/23
2. Error Estimates and Superconvergence Properties of Elliptic Optimal Control Problems, Annual meeting of the GAMM, Dresden, from 04/03/22 to 04/03/26
3. Regularization of pointwise state constrained optimal control problems, European Conference on computational Optimization, Dresden, from 04/03/29 to 04/03/31
4. Approximation Linear-Quadratischer Optimalsteueraufgaben, Southeast German Colloquium on Numerical Mathematics, Jena, 04/05/14
5. Discretization Concepts for Optimal Control Problems, SFB-Seminar, Graz, 04/06/17
6. Optimalsteuerprobleme mit gemischten Steuerungs-Zustandsbeschränkungen, Annual Meeting of the DMV, Heidelberg, from 04/09/13 to 04/09/17
7. Approximation of optimal control problems by finite dimensional problems, FGS Conference on Optimization, Avignon, from 04/09/20 to 04/09/24
8. Numerische Methoden für Optimierungsprobleme bei partiellen Differentialgleichungen, München, 04/10/14
9. Herausforderungen und Perspektiven bei der Optimalen Steuerung Partieller Differentialgleichungen, Hamburg, 04/11/27

Scientific Cooperations

Internal Cooperations with

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

External Cooperations with

1. Prof. F. Tröltzsch (TU Berlin)
2. Dipl.-Math. D. Wachsmuth (TU Berlin)
3. Dipl.-Ing. C. Meyer (TU Berlin)
4. Dipl.-Math. R. Simon (SFB 013 Linz)
5. Prof. T. Apel (Universität der Bundeswehr München)
6. Dipl.-Math. G. Winkler (Universität der Bundeswehr München)

Participation at conferences

1. Annual meeting of the GAMM, Dresden, from 04/03/22 to 04/03/26
2. European Conference on computational Optimization, Dresden, from 04/03/29 to 04/03/31
3. Southeast German Colloquium on Numerical Mathematics, Jena, 04/05/14
4. Annual Meeting of the DMV, Heidelberg, from 04/09/13 to 04/09/17
5. FGS Conference on Optimization, Avignon, from 04/09/20 to 04/09/24

Publications

Appeared

1. A. Rösch and D. Wachsmuth. Regularity of the adjoint state of the instationary Navier-Stokes equations. Accepted for publication in Zeitschrift für Analysis und ihre Anwendungen.
2. C. Meyer and A. Rösch. Superconvergence properties of optimal control problems. SIAM Journal on Control and Optimization, 43(3):970-985,2004.
3. A. Rösch. Error estimates for parabolic optimal control problems with control constraints. Zeitschrift für Analysis und ihre Anwendungen, 23(2):138-154,2004.
4. C. Meyer, A. Rösch, and F. Tröltzsch. Optimal Control of PDEs with regularized pointwise state constraints. Accepted for publication in Computational Optimization and Applications.
5. A. Rösch. Error estimates for linear-quadratic control problems with control constraints. Accepted for publication in Optimization Methods and Software.

Submitted

1. C. Meyer and A. Rösch. L8 -Estimates for approximated optimal control problems.

Dr. Nicoleta Bila

Introduction

The area of research for Nicoleta Bila is applied mathematics with an emphasis on symmetry analysis of differential equations, parameter identification problems modelled by PDEs, symbolic manipulation programs for symmetry analysis and variational symmetries and conservation laws.
She received her Ph.D. in Geometry from the University "Politehnica" of Bucharest, Romania, in 1999, her Ph.D. Thesis being "Symmetry groups and conservation laws for certain PDEs". Between 2000 and 2002, N. Bila was a postdoctoral research associate at Kent University and Cambridge University, working on the EPSRC project "Geometric Integration of Partial Differential Equations". In October 2002, she joined the Spezialforschungsbereich F013 Numerical and Symbolic Scientific Computing, Linz. From April 2004, she is one of the researchers externally funded (SFB F1308) at RICAM, working in the inverse problems group.

As a Ph.D. student and afterwards as a research associate, N. Bila has been interested in applying symmetry analysis theory to different mathematical models. Symmetry analysis theory links differential geometry to PDEs theory, symbolic computation, and, more recently, to numerical analysis theory. In the last two years, she has been working on connecting this theory to different inverse problems, especially parameter identification problems modelled by PDEs.

Scientific Achievements 2004

Research 2004 before RICAM

Under the guidance of Prof. H. W. Engl and Dr. P. Kügler, N. Bila studied a parameter identification problem arising in the car windshield design from the point of view of symmetry analysis theory [1]. For the studied mathematical model which is given by a second order mixed type PDE, she showed that there is a class of group of transformations, so called equivalence transformations which relate the direct problem and the inverse problem. As a consequence, the order of the model can be reduced and, for particular domains, special classes of data and parameter can be studied [1]. In this context, together with Dr. A. Leitao, she was interested in applying the Landweber method to the reduced equations associated a parameter identification problem [4].

Research 2004 at RICAM

Together with Dr. P. Kügler, N. Bila continued her work on applying the Landweber method and the derivative free Landweber method on the reduced similarity spaces associated with a parameter identification problem modeled by a PDE; a new case was studied, namely, when the mathematical model is invariant with respect to scaling transformations [4]. On the other hand, based on a recent work with Dr. J. Niesen [2], she has focused on finding new classes of symmetry reductions related to a parameter identification problem. By extending the notion of nonclassical symmetries (which is a common approach in the theory of symmetry groups) she was interested in finding nonclassical equivalence transformations [5]. Recently, together with Dr. E. Hillgarter and Dr. M. Burger, she has started working on the application of Lie groups of transformations to image processing.

Scientific Visits and Talks

- "Symmetry reductions and regularization methods"
  20.03.2004, Internal RICAM Seminar, Inverse Problems Group
- "Application of Symmetry Analysis to a PDE Arising in the Car Windshield Design"
  28.06 -1.07.2004, Edinburgh, UK - Workshop on Lie group methods and control theory
- "Nonclassical equivalence transformations"
  22.11.2004, Internal RICAM Seminar, Inverse Problems Group

Scientific Cooperations

Internal Cooperations with
Dr. Philipp Kügler, Institute for Industrial Mathematics, University of Linz
Dr. Martin Burger, Institute for Industrial Mathematics, University of Linz
Dr. Erik Hillgarter – Research Institute for Symbolic Computation (RISC), University of Linz

External Cooperations with
Dr. Jitse Niesen, Herriot-Watt University, Edinburgh, UK
Dr. Antonio Leitao, Federal University of Santa Catarina, Florianopolis, Brazil

Participation at conferences

28.06 -1.07.2004, Edinburgh, UK - Workshop on Lie group methods and control theory

Publications

Appeared

[1] N. Bila - Application of Symmetry Analysis to a PDE Arising in the Car Windshield Design, SIAM Journal of Applied Mathematics, 65 (1), 113 – 130, 2004.

[2] N. Bila, J. Niesen - On a new procedure for finding nonclassical symmetries, Journal of Symbolic Computation, 38 (6), 1523-1533, 2004.

Submitted

[3] N. Bila, E. L. Mansfield, P. Clarkson – Symmetry Group Analysis of the Shallow Water and Semi-Geostrophic Equations, submitted to the Quarterly Journal of Mathematics, 2004.

In preparation

[4] Symmetry reductions and regularization methods, with H. W.Engl,P.Kügler, A. Leitao
[5] On nonclassical equivalence transformations, with J. Niesen

For personal reasons, Dr. Bila will leave RICAM in 2005 and move to the United States.

DI Hui Cao

Scientific Achievements

Since coming to Johann Radon Institute for Computational and Applied Mathematics (RICAM) at August 2004, Cao Hui has joined the Inverse Problem Group as a team member of **FWF-ProjectP17271-N12** "Fixed point regularization schemes for nonlinear ill-posed problems and their discretization" which is held by **Professor Sergei V. Pereverzyev**.

The main topic of his research is **Regularization for naturally linearized parameter identification problems** which can be considered as a part of the project mentioned above. The general idea can be described as follows: reduce the original nonlinear problem to a finite sequence of linear ones, and regularize them subsequently.

Cao Hui has started his research with the identification of diffusion coefficients in PDE of elliptic type. This problem is extensively discussed in the literature as a model for parameter identification. On the other hand, from a paper by Kaltenbacher and Schöberl (2002), it follows that it can be naturally linearized. But these authors proposed to apply the regularization by projection to linear problem in a weaker form, and obtained error bounds only under a priori assumption concerning smoothness of the coefficient. In fact, such method can be considered as a modification of the equation error method. Our approach is different: discretized Tikhonov-Phillips regularization is applied to the linearized problem. Using recent results from regularization theory (Mathé and Pereverzev(2003)), a strategy for the choice of regularization and discretization parameters is proposed which automatically adapts to unknown smoothness of the coefficient. Estimates for the accuracy have been given and various numerical tests supporting the theoretical results have been performed.

Cao Hui will present his results in the workshop "Inverse problem" organized by the Department of Computer Science, University of Innsbruck in April 2005.

DI Herbert Egger

Introduction

DI Herbert Egger is working in the Subproject F1308, “Computational Inverse Problems and Applications” of the SFB013, “Numerical and Symbolic Scientific Computing” and since April 2004 as a Ph.D Student in the Group "Inverse Problems" at RICAM. His main research interests are in stability analysis and numerical algorithms for inverse and ill-posed problems.

Scientific Achievements 2004

Research 2004 before RICAM

In early 2004, DI Egger focused on

1. Inverse problems in mathematical finance,

in particular on stable volatility identification from option prices in a Black-Scholes framework. A second activity was concerned with

2. Stability analysis of nonlinear inverse parabolic problems

via the method of Carleman estimates. Both activities were continued in the research at RICAM starting in April 2004.

Research 2004 at RICAM

As a first activity, the research on

1. Stability of inverse parabolic problems,

was continued: Parameter identification in nonlinear parabolic problems, in particular the identification of nonlinearities, is of great interest in many technical application, e.g., related to heat transfer at high temperatures. From a practical point of view, identification from a single set of boundary measurements is especially attractive. The stable identifiability of nonlinear source terms in 1-D nonlinear parabolic equations has been shown, using Carleman estimates, in a joint work [1] with Heinz Engl and M. Klibanov (Univ. of North Carolina at Charlotte).

2. The inverse problem of option pricing,

namely the identification of local volatility surfaces from (noisy, incomplete) option prices has been analyzed in a second activity, and new convergence rate results could be proven [2].

In summer 2004, a cooperation on

3. Preconditioning iterative regularization in Hilbert scales,

has been started with A. Neubauer (University of Linz). As for well-posed problems, preconditioning can (with different limitations) also be used for ill-posed problems and may substantially decrease the number of iterations necessary to reach a prescribed stopping criterion [3,4].

In late 2004, a new cooperation on

4. Polynomial identities in the convergence rate analysis of iterative

regularization methods

has been started together with M. Rosenkranz and G. Regensburger (RICAM Symbolic Computation Group).

Scientific Visits and Talks

June 2004, “Stabilität in nichtlinearen parabolischen inversen Quellproblemen”, TU Chemnitz

Scientific Cooperations

Internal Cooperations with

- G. Regensburger, M. Rosenkranz: Polynomial identities in the convergence rate analysis of iterative regularization methods

External Cooperations with

- Neubauer (University of Linz): Preconditioning iterative regularization in Hilbert scales
- M. Klibanov (Univ. of North Carolina at Charlotte): Stability in nonlinear inverse parabolic problems

Publications

Appeared

[1] H. Egger, H.W. Engl, M.V. Klibanov: Global Uniqueness and Hölder Stability for Recovering a Nonlinear Source Term in a Parabolic Equation, Inverse Problems 21 (2005), 271-290.

Submitted

[2] H. Egger, A. Neubauer: Preconditioning Landweber Iteration in Hilbert Scales, Ricam-Report 2004-11, submitted.

[3] H. Egger: Semiiterative Regularization in Hilbert Scales, Ricam-Report 2004-12, submitted.

[4] H. Egger, H.W. Engl: Tikhonov Regularization Applied to the Inverse Problem of Option Pricing: Convergence Analysis and Rates, Ricam-Report 2004-10, submitted.

DI Benjamin Hackl

Introduction

Geometric inverse problems governed by partial differential equations are the main research area of Mr. Hackl. Especially the development of level set methods incorporating topological derivatives as well as the theoretical and numerical application of the phase field method to these type of problems are in his main focus. Besides this his research is also concerned with the identification of material parameters (like the yield surface) in visco-plastic materials, in a theoretical and practical manner.

Both research areas allow close cooperation to the research groups on inverse problems, optimal control and numerics at RICAM as well as cooperations to the projects F1306, F1309 at the SFB F013.

Scientific Achievements 2004

Research 2004 before RICAM

Before and during his civil service (June 2003 – May 2004) Mr. Hackl mainly worked in the field of geometric inverse problems, governed by partial differential equations, in close cooperation with Dr. H. Ben Ameur (Tunis), Dr. M. Burger (Linz) and Dr. W. Ring (Graz). In one research topic a new algorithm, incorporating topological derivatives into the level set method was introduced in [1], whereas a theory based regularization for geometric inverse problems in linear elasticity was considered in [2].

Furthermore he considered, in close cooperation with Dr. N. Petrinic and D. Phil. B. Elliott (both Oxford), the identification of material parameters, especially the yield surface, in visco-plastic materials, currently still on a very heuristic level.

Research 2004 at RICAM

During the last 3 months at RICAM, Mr. Hackl was concerned with incorporating topological asymptotic information into level set methods where the original problem might not be topologically differentiable. For this sake he started to implement the level set method into a femlab-matlab environment to get a more flexible testing environment and allow more advanced numerical calculations of geometric inverse problems. This research is performed together with Dr. M. Burger (Univ. of Linz).

Scientific Cooperations

Internal Cooperations with

Dr. Martin Burger, Industrial Mathematics Institute, JK University Linz, Austria. Level set methods and topological derivatives for geometric inverse problems [1, 2], ongoing project. Level set methods in linear plasticity, hrp-FEM, a-posteriori error estimators, ongoing project. Phasefield methods in inverse problems, ongoing project.

Dr. Jan Valdman, DI Johanna Kienesberger, SFB F013 Project F1306, JK University Linz, Austria. Level set methods in plasticity, hrp-FEM, “heuristic” a-posteriori error estimators, ongoing project.

External Cooperations with

Dr. Hend Ben Ameur, Laboratoire de Modelisation Mathematique et Numerique, Ecole Nationale d'Ingenieurs de Tunis. Level set methods for geometric inverse problems [2].

Dr. Wolfgang Ring, Institute of Mathematics, University of Graz, Austria.

Incorporating topological derivatives into level sets methods [1].

Dr. Nikica Petrinic, D.Phil. Benjamin Elliott, Department of Engineering Science, University of Oxford, England. Parameter identification, especially identification of the yield surface, in visco-plastic materials, ongoing project.

Participation at conferences

Publications

Appeared

[1] Martin Burger, Benjamin Hackl, Wolfgang Ring, Incorporating topological derivatives into level sets methods, J. Comp. Phys., 194(1) 2004, 334-362.

[2] Hend Ben Ameur, Martin Burger, Benjamin Hackl, Level set methods for geometric inverser problems in linear elasticity, Inv. Prob., 20(3) 2004, 673-696.

DI Andreas Hofinger

Scientific Achievements 2004

The main topic of my research is inverse problems and is subdivided into three areas:

i. Stochastic Inverse Problems
Here the goal is the extension of results of the deterministic theory for inverse problems to a stochastic setting. The approach we have chosen utilizes the Prokhorov-metric to measure convergence (rates) in the new setup.

ii. Inverse Problem of Electrocardiology
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.

iii. Neural Networks
The training of a neural network is an ill-posed problem, and has to be regularized. Although standard regularization techniques yield optimal convergence rate results, they do not take into account the underlying structure of the networks. Therefore, more appropriate, in particular, iterative and adaptive algorithms are being developed.

Participation at conferences

I have participated in two "Industrial Problem Solving Workshops" at the Universities of Victoria and British Columbia (cf. [2]), respectively (May 10th - 14th and May 17th - 21st 2004).

Scientific Visits and Talks

Related to (ii) I was invited to the University of Zaragoza for two weeks (June 14th - June 25th, 2004).

i. "Assessing Uncertainty in Ill-posed Problems", Seminar "Inverse Problems", Linz, May 4th, 2004.

ii. "Inverse Problems: Deterministic vs. Stochastic Point of View", Seminario Matemático García de Galdeano, University of Zaragoza, Spain, June 23rd, 2004.

Scientific Cooperations

Internal Cooperations

On topic (iii) there is permanent exchange of ideas with Martin Burger from the Industrial Mathematics Institute.
On topic (i) there is a cooperation with Heinz W. Engl.

External Cooperations
There is a cooperation with Stefan Kindermann (UCLA, Los Angeles) related to (i)
There is an ongoing cooperation with Ricardo Celorrio (Universidad de Zaragoza, Spain) related to (ii)

Publications

Appeared
[1] Burger M. and Hofinger A., "Regularized Greedy Algorithms for Network Training with Data Noise", Computing, (2004).
[2] Akers B., Bohun S., Gibson P., Hofinger A., Lamoureux M., Lobb J., Roberts M., "General Statistical Design of an Experimental Problem for Harmonics", Proceedings of the Eighth PIMS MITACS Industrial Problem Solving Workshop, 2004.

Submitted
[3] Engl H. W., Hofinger A., Kindermann S., "Convergence rates in the prokhorov metric for assessing uncertainty in ill-posed problems", Inverse Problems, to appear.
[4] Hofinger A., "Nonlinear function approximation: computing smooth solutions with an adaptive greedy algorithm", submitted.

DI Shuai Lu

Member of Inverse Problems Group of RICAM - graduated from Fudan University, P. R. China in July 2004; joined the RICAM in August 2004 as a Ph.D. candidate under the **FWF-Project P17251-N12 "Fixed point regularization schemes for nonlinear ill-posed problems and their discretization"**

Scientific Achievements

Optimal regularization parameter choice for numerical differentiation (Joint work with Prof. Perverzyev).
In our work, we have studied a classical ill-posed problem - numerical differentiation, assuming that the smoothness of the function to be differentiated is unknown. Using recent results on adaptive regularization of general ill-posed problems we have proposed new rules for the choice of the stepsize in the finite-difference methods, and for the regularization parameter choice in numerical differentiation regularized by iterated Tikhonov regularization. These methods are shown to be effective for the differentiation of noisy functions, and order-optional convergence results for them can be proven. A presentation with the title "Numerical Differentiation from a view point of Regularization Theory" was given in group seminar.

Participation at the conferences

1. The 2nd International Conference on Inverse Problems, Fudan University, June 2004
   20 Minutes presentation with the title of "Dimension reconstruction of fractal surface with periodic boundary condition".
2. Innsbruck Inverse Problems Workshop, University of Innsbruck, April 2005

Intention to give a presentation with the title of “Regularization by discretization for some severely ill-posed problems”.

Publications

1. S. Lu, Y. B. Wang, First and Second Order Numerical Differentiation with Tikhonov Regularization, Selected Publications of Chinese Universities: Mathematics.
2. S. Lu, S. Pereverzev, Numerical Differentiation from a view point of Regularization Theory, submitted to Mathematics of Computation.

Group "Symbolic Computation"

Group Leaders:
O.Univ.-Prof. Dr.phil. DDr.h.c. Bruno Buchberger
Ao.Univ.-Prof. Dr. Josef Schicho

Researchers funded via ÖAW/Upper Austrian government funds:
Dr. Willem De Graaf
Dr. Mircea Marin
Dr. Markus Rosenkranz
Dr. Florina Piroi
DI Alexander Zapletal

Researchers externally funded:
Dipl.-Math. Tobias Beck
Mag.Janka Pilnikoa
Dr. Georg Regensburger
Mag. Ibolya Szilagyi

Introduction

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 in the Computational Logic Group

Group leader: Professor Bruno Buchberger
Dr. Mircea Marin (employment at RICAM until September 2004)
Dr. Markus Rosenkranz (employment at RICAM since July 2004)
Dr. Florina Piroi (employment at RICAM since October 2004)
Dr. Georg Regensburger (paid by SFB 1322 since November 2004)
Mag. Alexander Zapletal (PhD student, employment at RICAM since October 2004)

The Computational Logic Group of RICAM works in close interaction with projects SFB 1302 (Project Leaders: Profs. T. Jebelean and B. Buchberger) and SFB 1322 (Project Leaders: Profs. B. Buchberger and H. Engl) of the SFB (Sonderforschungsbereich SFB F013 on "Scientific Computing" at the Johannes Kepler University) and the Theorema Group of RISC (Research Institute for Symbolic Computation, Johannes Kepler University of Linz) led by B. Buchberger. The project SFB 1322 is administered by RICAM, the project SFB 1302 by RISC. For more details about these cooperations, see the section "Cooperations of the Computational Logic Group of RICAM" below.

Researchers in the Computational Algebra Group

Group leader: Dr. Josef Schicho (employed at RICAM)
Dr. Willem de Graaf (employed at RICAM since October 2004)
Dr. Pavel Chalmoviansky (paid by SFB 1315 since April 2004)
Dr. Johannes Gahleitner (paid by SFB from April 2004 until August 2004)
Dipl.-Inf. Tobias Beck (paid by SFB 1303 since April 2004)
Mag. Jana Pilnikova (paid by SFB 1303 since April 2004)
Mag. Ibolya Szilagyi (paid by SFB 1303 since April 2004)

The Computational Algebra Group of RICAM works in close interaction with projects SFB 1303 (Project Leader Prof. J. Schicho) and SFB 1315 (Project Leaders Profs. B. Jüttler and J. Schicho) of the SFB, both administered by RICAM. For more details about these cooperations, see the section "Cooperations of the Computational Algebra Group of RICAM" below

Overview on the Work of the Symbolic Computation Area in 2004

In accordance with the initial proposal for the area "Symbolic Computation" within RICAM, the area pursues the following strategic long-term research lines:

I. Research on **Gröbner bases and related algorithmic algebraic theories** 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.

Research line I was pursued both in the WG Computational Logic (group leader B. Buchberger; with an emphasis on the Gröbner bases method, which was initiated by B. Buchberger many years ago) and in the Working Group Computational Algebra (group leader Schicho; with an emphasis on other algebraic techniques, notably constraint solving techniques for real algebraic geometry). In the WG Computational Algebra, in 2004, in research line I the main achievements were various improvements in exact and numerical constraint solving over the reals. In the WG Computational Logic the main achievement in research line I was the application of automated theory exploration methods to the computer-supported synthesis of non-trivial algorithms in Gröbner bases theory (see report of B. Buchberger below), and research on non-commutative Gröbner bases (see report of M. Rosenkranz below). Also, in this WG, work on a special semester on Gröbner bases and related theories (planned for 2006) was started (see reports of B. Buchberger and A. Zapletal below).

Research line II was pursued in the WG Computational Logic (in close interaction with the Theorema Group at RISC). The main achievements 2004 were various improved reasoners for equational logic with sequence variables, various tools for the management of mathematical knowledge (see report of F. Piroi), a new method for automated algorithm synthesis (see report of B. Buchberger below), and a methodology for rule-based programming (see report of M. Marin below).

Research line III was pursued in both Working Groups. The main achievements were a new solution method for linear boundary value problems from the perspective of algorithmic operator theory (see report of M. Rosenkranz below), the initialization of research on symbolic methods in wavelet theory (see report of G. Regensburger below), and the initialization of research of symbolic methods in algebraic multigrid methods (see the report of J. Schicho below).

Overview on the Work of the Computational Logic Group in 2004

Research Line I (Gröbner Bases Theory and Related Subjects)

The main achievements in 2004 were:

The **automated synthesis of a Gröbner bases algorithm**, see [Buchberger 6] by the synthesis method developed in [Buchberger 5]. The Gröbner bases algorithm is considered to be a non-trivial algorithm and has never been synthesized automatically before.

The theoretical foundation and implementation, with the Theorema system, of **non-commutative reduction as a basis for non-commutative Gröbner bases** in the frame of the algebraic approach to boundary value problems for differential equations, see [Rosenkranz 1-5].

Further studies **on equational theorem proving and unification**, which is a natural frame for reduction algorithms in algebraic domains. New results were achieved in equational theorem proving and unification involving so-called "sequence variables", see [Marin 3, 7] and [Buchberger 3].

The preparation of the scientific concept, by B. Buchberger, of a **RICAM special semester on Gröbner Bases** in the year 2006 and the start of the organizational preparation of the special semester (web site with Gröbner bases paper data base); the PhD student A. Zapletal is in charge of this web site.

Start of the design, by B. Buchberger, of a **formal knowledge base (definitions, theorems, and algorithms) of Gröbner bases theory** in the logic frame of Theorema (predicate logic), which will be web-accessible. This will be the first formal knowledge base for Gröbner bases theory worldwide. The implementation of this knowledge base will be the main topic for the PhD thesis of A. 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:

Further elaboration of the "lazy thinking" method for automated algorithm synthesis initiated by B. Buchberger in 2003, see [Buchberger-Craciun 1, 5].

New design of **the interaction of the invention and the verification phase** in mathematical theory exploration, see [Buchberger 2].

Software tools for the organization of mathematical theory exploration: label management, the focus windows technique for proof presentation, user interaction with theorem provers, see [Piroi-Buchberger 1, 4]

High-level combination of automated inference rules by **rule-based programming**, see [Marin-Piroi 1, 4]

Research on **constraint solving** as part of theorem proving, see [Marin-Middeldorp 6].

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

The main application of our research for other RICAM areas results exactly from the interplay between research lines I and II: The application of **algebraic techniques (in particular Gröbner bases techniques in various domains) for computer support in the exploration of functional analysis**. This research line was initiated within SFB 1302 and 1308 in 2002 by the observation that the reduction and solving power of Gröbner bases theory could be applied to the symbolic solution of boundary value problems when algebraized on the operator level, see [Rosenkranz 1]. The new project SFB 1322 (administered by RICAM) is now devoted exclusively to this direction. The new achievements along these lines are described in [Rosenkranz 3, Rosenkranz-Buchberger-Engl 4].

Gröbner bases play also a role in **the study and automated generation of wavelet systems.** A more intensive study of this new approach was initiated towards the end of 2004 and will be the main research activity of the new PostDoc G. Regensburger. Since wavelet theory is an important recent topic in numerics, with this research direction also a new interaction within RICAM to the numerics groups of Langer and Engl is emerging.

Details of the research in the RICAM Computational Logic Working Group in 2004 are described in the reports of the group members B. Buchberger (group leader), Marin (PostDoc until September 2004), Rosenkranz (PostDoc since July 2004), Piroi (PostDoc since October 2004), Regensburger (PostDoc SFB 1322), Zapletal (PhD student).

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 succeedings individual reports we will only mention specific cooperations beyond those mentioned here. Furthermore, we will not mention explicitly the cooperations within the Computational Logic Group itself – this cooperation is clear from its group structure (weekly seminar meeting, joint software venture etc), and it becomes even more apparent in the individual reports below.

Internal Cooperations

- Group of H.W. Engl: Studying the use of noncommutative Gröbner bases on the level of operator theory for the symbolic solution of linear boundary value problems.
- Group of P. Markowich: Discussion of possibible applications of the symbolic operator simplification methods for special classes of partial differential equations.
- Group of J. Schicho: Gröbner bases theory and other methods for non-linear algebra.
- Group of U. Langer: Use of generalized Gröbner bases thechniques in wavelet theory.

External Cooperations

- Project F1302 "THEOREMA: Proving, Solving, and Computing in the Theory of Hilbert Spaces" in SFB F013 of the FWF (Principal investigators: T. Jebelean, B. Buchberger. This project plays a crucial role both for research line 1 (e.g. for the noncommutative Gröbner bases used in [Rosenkranz 1] for solving boundary value problems) and for research line 2 (the proving machinery of *Theorema* is linked with the automated theory exploration).

- Project F1303 “Proving and Solving over the Reals” in SFB F013 of the FWF (Principal investigator: J. Schicho). This project focuses on computational methods in algebraic geometry and is therefore intimately linked with (commutative) Gröbner bases.

- Project F1308 “Computational Inverse Problems and Applications” in SFB F013 of the FWF (Principal investigator: H.W. Engl). The work of [Rosenkranz 1] has grown out of a fruitful combination of the symbolic tools considered in F1302 and the functional analysis tools applied in F1308; this interplay is still crucial for the further unfolding of symbolic functional analysis (research lines 1 and 3).

- Project F1322 „Computer Algebra for Pure and Applied Functional Analysis“, in SFB F013 of the FWF. Principal investigators: B. Buchberger, H.W. Engl. This project is intimate relation with research line 3 of the Computational Logic group; its concern is the systematic buildup of symbolic functional analysis as described in the individual report of M. Rosenkranz.

- *Theorema* project of the Research Institute for Symbolic Computation, Johannes Kepler University of Linz (group leader B. Buchberger). The *Theorema* group has a large overlap with the above-mentioned F1302 but extends beyond it. The aim of this project is supporting the working mathematician in all phases proving, programming, computing, and building conjectures.

- EU Calculems Network of Excellence (until November 2004): The *Theorema* group was an initiating member of the consortium. This network investigated the combined power of automated theorem provers and computer algebra systems – a combination incarnated in the *Theorema* system, which is a proving system implemented in the computer algebra package *Mathematica* (and letting the provers have full but controlled access to the powerful libraries of *Mathematica*).

- EU MKM (Mathematical Knowledge Management) Thematic Network (ongoing): The *Theorema* group is an initiating member of the consortium. This network is now the center of activity in the new field of MKM, which was initiated by B. Buchberger through the First International MKM Workshop, held in RISC, Hagenberg, in September 2001. Automated theory exploration (research line 2) can be seen as one particular MKM methodology.

- Symbolic Computation groups at the following Japanese universitites: Tsukuba (Prof. T. Ida), Kyoto (Prof. M. Sato), Kyushu (Prof. K. Yokoyama).

<u>Overview on the Work of the Computational Algebra Group</u>

In the computational algebra group, research line I was pursued in three contexts: the theory of parametrizations and the theory of algebraic power series, which are both related to Gröbner bases theory. The research on the theory of parametrizations has led to an algorithm for local parametrization of cubic surfaces and to the discovery of a connection of parametrizations in algebraic geometry and convex lattice polygons in discrete geometry. The main challenge in the investigation of algebraic power series was to come up with a convenient representation of such power series. The representation should be exact and at the same time suitable for developing algorithms for the performance of arithmetic of power series, in particular of solving algebraic equations. In order to meet this challenge, we organized a visit of Tobias Beck at the Ontario Research Centre of Computer Algebra (ORCCA) and a visit of J. Van der Hoeven (University of Paris Sud) at RICAM. The third context is the classification of solvable Lie algebras of dimension 4 over arbitrary fields, for which Groebner bases play a crucial role.

Research Line II was pursued in a cooperation of de Graaf, Pilnikova, Schicho, and M. Harrison (University of Sydney) in their investigation of a diophantine problem, namely rational parametrization of Severi-Brauer surfaces. By bringing in knowledge from the theory of Lie algebras, it was possible to come up with a quite efficient algorithm to solve this problem. Other examples are the use of topological methods (homotopy classes) in the question of deciding whether a given function on a matrix group is polynomial, or the use of the theory of cylindric algebraic decomposition which was explored to detect topological properties of level curves of real algebraic surfaces.

The special scientific atmosphere at RICAM with leading experts from numeric *and* symbolic computation made the exploration of available numerical theories in the context of classical computer algebra problems useful. This has lead to the study of the numerical error of the implicitization problem; numerical studies of the parametrization problem and of algorithms for singularities have also been initialized.

For the progress of research line III, frequent discussions of scientists between scientists in different groups at RICAM have been very important. In particular, there were several trials to solve algebraic sub-problems in numerical algorithms or convergency/correctness proofs of numerical algorithms by symbolic methods. Sometimes, these trials were not pursued because the gain of efficiency was not satisfactory, but in other cases the symbolic approach seemed promining. A concrete example is the decomposition into edge matrices in the Algebraic Multigrid Method by Molecules, where the exact solution found by symbolic means is used in the implementation of the numeric solver.

Prof. Bruno Buchberger

Introduction

B. Buchberger focuses on the following topics:

- Reasoning algorithms for supporting mathematical theory exploration
- Formal Gröbner bases theory
- Applications of Gröbner bases in functional analysis and numerics
- Design and planning of a special semester on Gröbner bases

Scientific Achievements 2004

Automated synthesis of the critical-pair-completion algorithm for constructing Gröbner bases, see [6]. This is the first time an algorithm of this logical complexity has been synthesized and proved correct automatically. Meanwhile this result has been recognized internationally as a major breakthrough in this area (see the list of invited talks below). Moreover, the synthesis method has been worked out in greater detail, see [1, 5].

Furthermore, the extension of predicate logic by sequence variables, which is an important ingredient to the logical basis of *Theorema*, was completely worked out for the first time in the literature, see [3].

Finally, the Gröbner bases methodology has found a new application area for automated proofs of origami constructions, see [4, 7, 8].

In research management, B. Buchberger made a major contribution by organizing the Seventh International Conference on Artificial Intelligence and Symbolic Computation and co-editing the proceedings [9].

Publications

Papers appeared

1. B. Buchberger, A. Craciun. Algorithm Synthesis by Lazy Thinking: Examples and Implementation in Theorema. in: Fairouz Kamareddine (ed.), Proc. of the Mathematical Knowledge Management Workshop, Edinburgh, Nov. 25, 2003, Electronic Notes on Theoretical Computer Science, Vol.93, 18 Feb. 2004, pp.24-59, www. elsevier. com/ locate/ entcs, Elsevier, ISBN 044451290X.

2. B. Buchberger. Algorithm-Supported Mathematical Theory Exploration: A Personal View and Stragegy. In: B. Buchberger, John Campbell (eds.), Proceedings of AISC 2004 (Artificial Intelligence and Symbolic Computation, September 22-24, 2004, RISC, Johannes Kepler University, Austria), Springer Lecture Notes in Artificial Intelligence, Vol. 3249, 2004, pp. 236-250.

3. T. Kutsia, B. Buchberger. Predicate Logic with Sequence Variables and Sequence Function Symbols. In: A.Asperti, G.Bancerek, A.Trybulec (eds.): Proceedings of the Third International Conference on Mathematical Knowledge Management, MKM 2004, Bialowieza, POLAND, September 19-21, 2004, Vol. 3119 of Springer Lecture Notes in Computer Science, 2004, pp. 205-219.

4. T. Ida, D. Tepeneu, B. Buchberger, J. Robu. Proving and Constraint Solving in Computational Origami. In: B. Buchberger, John Campbell (eds.) Proceedings of AISC 2004 (7 th International Conference on Artificial Intelligence and Symbolic Computation, September 22-24, 2004, RISC, Johannes Kepler University, Austria), Springer Lecture Notes in Artificial Intelligence, Vol. 3249, pp. 236-250, Springer, Berlin, Heidelberg, 2004.

5. B. Buchberger, A. Craciun. Algorithm Synthesis by Lazy Thinking: Using Problem Schemes. In: D.Petcu, V.Negru, D.Zaharie, T.Jebelean (eds), Proceedings of SYNASC 2004, 6th International Symposium on Symbolic and Numeric Algorithms for Scientific Computing Timisoara, Romania, September 26-30, Mirton Publisher. pp. 90-106.

Papers accepted

6. B. Buchberger. Towards the Automated Synthesis of a Gröbner Bases Algorithm. RICSAM (Reviews of the Spanish Royal Academy of Science), Vol. 98/1 to appear , 10 pages.

7. B. Buchberger, T. Ida. Computational Origami: Interaction of Solving, Proving and Computing. In: Proceedings of World Conference on 21st Century Mathematics, March 18 - 20, 2004, Lahore, Pakistan, accepted.

8. Judit Robu, Dorin Tepeneu, Tetsuo Ida, Hidekazu Takahashi, Bruno Buchberger. Computational Origami Construction of a Regular Heptagon with Automated Proof of its Correctness. In: Proceedings of ADG 2004 (The Fifth International Workshop on Automated Deduction in Geometry, September 16-18, 2004, University of Florida, Gainesville, FL, USA), accepted.

Editor of Proceedings

9. B. Buchberger, J. Campbell (eds.). Artificial Intelligence and Symbolic Computation. Proceedings of AISC 2004 (7 th International Conference on Artificial Intelligence and Symbolic Computation, September 22-24, 2004, RISC, Johannes Kepler University, Austria), Springer Lecture Notes in Artificial Intelligence, Vol. 3249, Springer, Berlin, Heidelberg, 2004, 285 pages.

Technical Reports

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

11. B. Buchberger, K. Nakagawa. Mathematical Knowledge Editor: A Research Plan. SFB Report, 2004, Johannes Kepler University Linz, Spezialforschungsbereich SF013 "Scientific Computing", FWF (Austrian National Science Foundation), 17 pages.

Invited Keynotes at Conferences

12. B. Buchberger. Computer-Supported Mathematical Theory Exploration: A Shift of Paradigm in Mathematical Software. Mathematica Gulf Conference 2004, Sultan Qaboos University, Department of Mathematics and Statistics, January 26 - 28, 2004.

13. B. Buchberger. How I Managed to Automate Myself. Conference "The Future of Scientific Computing", The City College of New York, April 30, 2004.

14. B. Buchberger. The Algorithmic Invention of a Gröbner Basis Algorithm. Computer Algebra Workshop at Joint Institute for Nuclear Research (Dedicated to the Memory of G. Mescsheriakov), Dubna (Moscow), May 25-26, 2004.

15. B. Buchberger. Gröbner Bases: An Overview. Invited talk at Workshop on Computer Algebra, RIMS (Research Institute of Mathematical Sciences), Kyoto University, Japan, August 2-4, 2004.

16. B. Buchberger. The Importance of Formal Methods in Mathematics. Invited talk at Workshop on Computer Algebra, RIMS (Research Institute of Mathematical Sciences), Kyoto University, Japan, August 2-4, 2004.

17. B. Buchberger. A Formal Knowledge Base for Gröbner Bases Theory. Invited talk at Annual Conference of the Japanese Society for Symbolic and Algebraic Computation (JSSAC), Atsugi, Japan, September 1-4, 2004.

18. B. Buchberger. The Theorema Project: An Overview. Workshop “Verification and Rewriting”, Institute AIST, Amagasaki, Oct. 21, 2004.

19. B. Buchberger. Proving by First and Intermediate Principles. Invited talk at Workshop on Types for “Mathematics / Libraries of Formal Mathematics”, Univ. of Nijmegen, the Netherlands.

20. B. Buchberger. Algorithmic Invention of Algorithms: Case Study Gröbner Bases. Symposium Polynomial Systems Solving, University Paris VI, November 24-26, 2004.

Invited Talks at Universities and Research Institutes

21. B. Buchberger. Gröbner Bases: Theory and Applications. Sultan Qaboos Universiy, Department of Mathematics and Statistics, January 25, 2004.

22. B. Buchberger. Algorithmic Algorithm Synthesis: Case Study Gröbner Bases. International Algebra Conference, Moscow State University, May 26 - June 2, 2004.

23. B. Buchberger. Theorema: An Overview. Kyoto University, Graduate School of Computer Science, July 22-23, 2004.

24. B. Buchberger. Algorithmic Algorithm Synthesis: Case Study Gröbner Bases. Kuyshu University, Mathematical Department, Fukuoka, Japan, August 25, 2004.

25. B. Buchberger. How to Work With the Literature. Lecture for Graduate Students, Kyoto University, Graduate School for Computer Science, October 4, 2004.

26. B. Buchberger How to Give Talks and Write Papers. Lecture for Graduate Students, Kyoto University, Graduate School for Computer Science, October 13, 2004.

27. B. Buchberger. Gröbner Bases and Automated Theorem Proving. Toho University, Mathematical Institute, Tokyo – Tsudanuma, October 9, 2004

28. B. Buchberger. Didactic Principles for Using Computer Algebra in Class. Waseda Gakuin High School, Lecture for High-school Teachers, Oct. 16, 2004.

29. B. Buchberger. Let's Solve! Waseda Gakuin High School, Teaching Experiment on Computer Algebra with High School Students, Oct. 16, 2004.

30. B. Buchberger. Computer Algebra: A Key to the Future of Mathematics, Science, and Engineering. KIAS (Korean Institute of Advanced Studies, Seoul), Oct. 28, 2004.

31. B. Buchberger. Algorithmic Algorithm Synthesis: Case Study Gröbner Bases. KAIST (University, Daejon), Oct. 29, 2004.

32. B. Buchberger. Elimination and Self-Elimination. University of Bochum, Mathematical Institute, Dec. 15, 2004.

Scientific Cooperations

See the cooperations listed in the section “Overview on the Work of the Computational Logic Group in 2004”.

Dr. Mircea Marin

Introduction

The main topics of research of Mircea Marin are: automated deduction in rule-based programming style; proof presentation styles; calculi for E-unification; distributed constraint solving; and DNA sequence analysis.

His earlier achievements include the design and implementation of a scheme which integrates higher-order functional logic programming with collaborative constraint solving, where constraint solvers can be accessed on demand as services deployed in an open environment (such as the internet). More recently, M. Marin contributed to the development of a full-fledged system for rule-based programming.

Scientific Achievements 2004

In 2004, M. Marin made progress in the implementation of the rule-based system ?Log designed during his research activity in 2003 at RICAM. In addition, he brought to a good end the joint research with Prof. A. Middeldorp, by identifying an efficient calculus for functional logic programming [5]. He started a fruitful cooperation with the members Graduate School of Life and Environmental Sciences, which turned out to be valuable in DNA-analysis.
The main contributions of M. Marin in 2004 are:

- Development of the ?Log system for rule based programming. The system provides two main features. First, it enables natural and concise implementations of many interesting deduction systems (e.g., sequent calculi for various fragments of logic), methods for E-unification (narrowing calculi and unification procedures for many relevant theories), evaluation strategies, etc. See [4],[7] for details. Second, it allows to generate certificates (called *proof objects*) for the given answers. The proof objects can be used to generate human-readable proofs. See [1] for a detailed description.

- Design of sound and complete methods for E-unification in special theories. The two main achievements here are the following: First, a sound and complete calculus for theories presented by deterministic conditional term rewriting systems. This is the result of a cooperation with Prof. A. Middeldorp of University of Innsbruck, which started in December 2003. See [6] for details. Second, a sound and complete unification procedure for terms with sequence variables and sequence functions. This is the result of a cooperation with T. Kutsia of RISC. See the related publication [3].

- Concrete implementation of a distributed system for collaborative constraint solving. This system is a realization with Jini middleware of the generic scheme for constraint functional logic programming proposed by M. Marin during his postdoc research in Japan (2000-2002). Related publication [2].

- Design of a distributed system for the analysis of upstream sequences of *Dictyostelium Discoideum*. This is the result of a very short but successful cooperation with Dr. N. Kobayashi of Graduate School of Life and Environmental Sciences, University of Tsukuba, Japan. Related publication [5].

Publications

1. Mircea Marin and Florina Piroi. Deduction and presentation in ?Log. In F. Kamareddine, editor, *Proceedings of the Mathematical Knowledge Management Symposium*, volume 93 of *ENTCS*, pages 161-182, Heriot-Watt University, Edinburgh, Scotland, February 2004. Elsevier.

2. Mircea Marin and Mircea Dragan. A Jini service for collaborative constraint solving. In *Proceedings of International Conference on Computers and Communications* (ICCC 2004), pages 235-240. Oradea, Romania, May 27-29 2004.

3. Temur Kutsia and Mircea Marin. Unification Procedure for Terms with Sequence Variables and Sequence Functions. In *Proceedings of the 18th International Workshop on Unification* (UNIF'04). Cork, Ireland, July 4-5 2004.

4. Mircea Marin and Florina Piroi. Rule-based Programming with *Mathematica*. In *6th International Mathematica Symposium* (IMS 2004). Banff, Alberta, Canada, August 1-6 2004.

5. Norio Kobayashi, Mircea Marin, Takahiro Morio, Yoshimasa Tanaka and Hideko Urushihara. In analysis of upstream sequences of Dictyostelium discoideum using a distributed computer system. In *International Dictyostelium Conference (Dicty'04).* Sainte-Adele, Quebec, Canada, August 15-20 2004.

6. Mircea Marin and Aart Middeldorp. New Completeness Results for Lazy Conditional Narrowing. In *Proceedings of the 6th ACM-SIGPLAN Conference on Principles and Practice of Declarative Programming* (PPDP'04), pages 120-131. Verona, Italy, August 24-26 2004. ACM Press.

7. Mircea Marin and Temur Kutsia. A Rule-based Approach to the Implementation of Evaluation Strategies. In *Proceedings of the 6th International Symposium on Symbolic and Numeric Algorithms for Scientific Computing* (SYNASC 2004), pages 227-241. Timisoara , Romania, September 2004. ISBN 973-661-441-7, Mirton Publishing.

8. N. Kobayashi, M. Marin, Y. Tanaka, and H. Urushihara. On the Development of an Analysis System for Upstream Sequences in Dictyostelium discoideum Genome. Computer Software, Japan Society for Software Science and Technology. 2005. To appear.

Scientific Visits and Talks

January 2004: 1-week visit of the Symbolic Computation Research Group of University of Tsukuba, Japan. The visit was devoted to discussions related to the Origami system, in the frame of cooperation started in 2003 with Prof. B. Buchberger (RISC), Prof. T. Ida (University of Tsukuba), and Dr. J. Robu (Cluj University).

Participation at Conferences

- Sixth International Mathematica Symposium (IMS 2004).
- Sixth ACM-SIGPLAN Conference on Principles and Practice of Declarative Programming (PPDP'04).
- Sixth International Symposium on Symbolic and Numeric Algorithms for Scientific Computing (SYNASC 2004).

Scientific Cooperations

In addition to the cooperations listed in the section “Overview on the Work of the Computational Logic Group in 2004”, M. Marin has worked in the following cooperations:

- With A. Middeldorp (University of Innsbruck) on narrowing [6].
- With T. Kutsia (RISC) on E-unification [3] and evaluation strategies [7].

- With M. Dragan (Software Competence Center Hagenberg) on collaborative constraint functinal logic programming [2].
- With F. Piroi (at that time, RISC-Linz) on proof presentation [1] and rule-based programming [4].
- With N. Kobayashi (Graduate School of Life and Environmental Sciences of Tsukuba) on DNA analysis [5].

Dr. Markus Rosenkranz

Introduction

Starting with his dissertation [1], Markus Rosenkranz has set forth Symbolic Functional Analysis as a new discipline of research at the borderline between computer algebra and functional analysis. It has been characterized as that part of Symbolic Computation which studies operators through algebraic datastructures (e.g. noncommutative polynomials, formal power series). In this context, relevant questions for operators include: inversion, mapping properties, eigenvalues, smoothness. The main focus is on operators arising in analysis: differential operators, integral operators, multiplication operators, and boundary operators.

Scientific Achievements 2004

Research 2004 before employment at RICAM

In [1], M. Rosenkranz has investigated well-posed boundary value problems (BVPs) for linear differential operators with constant coefficients from the perspective of Symbolic Functional Analysis, thus making the heuristic treatment of [2] precise: The Green's operator associated with the given BVP is regarded as a noncommutative polynomial whose indeterminates denote the main operators of analysis: differentiation, integration, pointwise multiplication by funtions, and boundary evaluation. The computation of the Green's operator proceeds by constructing a suitable oblique Moore-Penrose inverse of the differential operator in the BVP. A sketchy overview is presented in [5].
In the succeeding time after his thesis until employment by RICAM, M. Rosenkranz was on leave for finishing his degree in High-School Pedagogics of Mathematics/Physics ("Unterrichtspraktikum für das Lehramtsstudium Mathematik/Physik").

Research 2004 at RICAM

In his employment from July to December 2004, M. Rosenkranz has refined and generalized the results of his thesis [1]. The journal article [3] contains the essential ideas of the thesis in a condensed form, plus two important extensions: (1) An example illustrates how to treat ill-posed problems; (2) the Sturm problem is treated in a generic fashion, having symbolic parameters both in the differential operator and in the boundary conditions. A generalization in another direction is described in [4], where linear differential operators with variable coefficients are brought into the scope of the method proposed in [1].

Publications

1. M. Rosenkranz, The Green's Algebra: A Polynomial Approach to Boundary Value Problems, PhD Thesis, Johannes Kepler University, Research Institute for Symbolic Computation, Hagenberg, 2003. Available as RISC Technical Report 2003-05.

2. M. Rosenkranz, B. Buchberger, H.W. Engl, Solving Linear Boundary Value Problems via Non Commutative Gröbner Bases, Applicable Analysis, 82(7), 655-675, July 2003.

3. M. Rosenkranz, New Symbolic Method for Solving Linear Two-Point Boundary Value Problems on the Level of Operators, Journal of Symbolic Computation, accepted "Vol. 39(2)." - Pagination is not yet avalailable.

4. M. Rosenkranz, B. Buchberger, H.W. Engl, A Symbolic Algorithm for Solving Two-Point BVPs on the Operator Level, SFB Technical Report 2003-41, Johannes Kepler University Linz, October 2003.

5. M. Rosenkranz, Symbolic Solution of Simple BVPs on the Operator Level: A New Approach, SIGSAM Bulletin, 37(3), 84-87, September 2003. Extended abstract from a poster presentation at ISSAC'03.

Scientific Visits and Talks

M. Rosenkranz, The Algorithmization of Physics: Math Between Science and Engineering. Invited talk at the AISC'04 (Seventh International Conference on Artificial Intelligence and Symbolic Computation), Research Institute for Symbolic Computation, Castle of Hagenberg, Austria, September 2004. Proceedings: Springer, Lecture Notes in Artificial Intelligence (LNAI), 3249, pages 1-7.

Participation at Conferences

- International Symposium on Symbolic and Algebraic Computation (ISSAC), Drexel University, Philadelphia, Pennsylvania, August 2003. Proceedings: ACM, ISBN 1-58113-641-2. Presented the poster [5].

- Conference on Artificial Intelligence and Symbolic Computation (AISC), Castle of Hagenberg, September 2004. Proceedings: Springer, Lecture Notes in Artificial Intelligence (LNAI), 3249.

Scientific Cooperations

See the cooperations listed in the section "Overview on the Work of the Computational Logic Group in 2004".

Dr. Florina Piroi

Introduction

Florina Piroi's main research area is automated reasoning, i.e. using computers to obtain proofs of mathematical conjectures. In particular, her main topics of research are:

- Proof presentation. A frequent activity in the work of any person doing mathematics is reading and understanding proofs. Therefore, presenting computer generated proofs such that human readers are able to understand all the subtleties of such a proof is important for any automated reasoning system.

- Interactive reasoning. Ongoing research in automated reasoning has resulted in more and more developed automated proving systems. It is whished that proofs are obtained with as little interaction as possible. This is generally not possible, not because the computer programs are not capable enough, but because, also for powerful provers, user guidance during proof development is needed in order to complete proofs. This is possible in certain areas but not in all areas. In any case, user interaction helps to make automated proving more efficient and is essential for the practical relevance of automated proving.

- Mathematical knowledge management. Extensive mathematical theory explorations usually involve a large amount of (mathematical) knowledge. There is an increased need to manage the mathematical knowledge a user develops during a theory exploration session.

Scientific Achievements 2004

Research 2004 before RICAM

F. Piroi started working for RICAM with October 1st, 2004. Before this date, the central point of F. Piroi's work has been writing her PhD thesis, which was finished in August, 2004 [3]. The thesis describes the implementation and usage of several tools that assist humans in their mathematical theory exploration using computers. The first tool responds to the need of managing the mathematical knowledge developed by users of an automated reasoning system. It implements facilities to preserve the hierarchic structure of mathematical theories by management of composite, hierarchical labels. Additionally, based on the generated composite labels, the tools give the user means to address, reference and select mathematical knowledge for later use. The next tool described in [3] allows users to interact with the provers of an automated reasoning system, at certain situations during the proof generation process. The proof presentation tools in [3] are proof post-processing routines for transformation (shortening proofs by removing unnecessary proof steps, re-arranging proofs, etc) and presentation of proofs.
In a cooperation with M. Marin, F. Piroi has developed datastructures for storing and routines for presentation of justifications (also known as certificates, or proof objects) given by the ?Log system [1, 6].

Research 2004 at RICAM

Since her employement in RICAM, F. Piroi has worked on extending and improving the label management tool for mathematical knowledge management [5].

Publications

1. M. Marin, F. Piroi. Deduction and Presentation in ?Log. In F. Kamareddine, editor, Proceedings of the Mathematical Knowledge Management Symposium, volume 93 of ENTCS, pages 161-182, Heriot-Watt University, Edinburgh, Scotland, February 2004. Elsevier.

2. F. Piroi, B. Buchberger "An Environment for Building Mathematical Knowledge Libraries". In C. Benzmueller, W. Windsteiger, editors, Computer-Supported Mathematical Theory Development, Proceedings of the first "Workshop on Computer-Supported Mathematical Theory Development" held in the frame of IJCAR'04 in Cork, Ireland, July 5, 2004. ISBN 3-902276-04-5.

3. F. Piroi, "Tools for Using Automated Provers in Mathematical Theory Exploration". PhD Thesis, RISC Report Series, 04-12, August 2004

4. F. Piroi, "User Interface Features in Theorema: A Summary", In Proceedings of "Mathematical User-Interfaces Workshop". At the Third Mathematical Knowledge Management Conference, Bialowieza, Poland, September 2004.

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

6. M. Marin, F. Piroi "Rule-Based Programming with Mathematica", RICAM Report Series, 2004-03. (In Proceedings of the Sixth International Mathematica Conference, Alberta, Canada, 2004).

Participation at Conferences

F. Piroi has participated in and was a member of the organization team of the Seventh Conference on Artificial Intelligence and Symbolic Computation (AISC), RISC, Castle of Hagenberg, Austria, September 2004.
She has participated as a speaker at the following conferences:

- First Workshop on Computer-Supported Mathematical Theory Development, in the frame of the International Joint Conference on Automated Reasoning, in Cork, Ireland, July 2004.

- Third Conference on Mathematical Knowledge Management, Bialowieza, Poland, September 2004.

- Mathematical User-Interfaces Workshop, at the Third Conference on Mathematical Knowledge Management, Bialowieza, Poland, September 2004.

Scientific Cooperations

See the cooperations listed in the section “Overview on the Work of the Computational Logic Group in 2004”.

Dr. Georg Regensburger

Introduction

G. Regensburger's fields of research are Reinforcement Learning and the application of Computer Algebra to Functional Analysis, in particular wavelets.
Reinforcement Learning addresses problems of sequential decision making and stochastic control and is strongly connected to dynamic programming and Markov decision processes. A new model for Reinforcement Learning for several environments, solution methods and applications ranging from symbolic and exact computation to robotics are discussed in his joint PhD thesis with Andreas Matt [3].
Wavelets and the related filter coefficients are used in many areas of applications for instance data compression and image analysis. In a joint work with Prof. O. Scherzer [6] Symbolic Computation and combinatorial methods are used to construct parametrized wavelets.

Scientific Achievements 2004

Research 2004 before RICAM

G. Regensburger completed his PhD studies in April 2004. With Andreas Matt he continued his research on Reinforcement Learning [1]. He completed an article with Prof. H. Hauser on the resolution of singularities of algebraic curves [2] and a publication with Prof. O. Scherzer on scaling functions and wavelets [6].

Research 2004 at RICAM

Since November 2004 G. Regensburger works together with M. Rosenkranz in the SFB project F1322 "Computer Algebra for Pure and Applied Functional Analysis". In addition to the central issues of this project (as formulated in the respective SFB proposal), he pursues the investigation of wavelets in this context. In December he received the "Würdigungspreis" from the Bundesministerium für Bildung, Wissenschaft und Kultur.

Publications

1. A. Matt and G. Regensburger, An adaptive clustering method for model-free reinforcement learning. In Proceedings of the 8th International Multitopic Conference (IEEE-INMIC 2004), 362–367, Lahore, Pakistan, 2004.
2. H. Hauser and G. Regensburger, Explizite Auflösung von ebenen Kurvensingularitäten in beliebiger Charakteristik, to appear in L'Enseignement Mathématique, December 2004, 49 pages.
3. A. Matt and G. Regensburger, Reinforcement Learning for Several Environments: Theory and Applications, PhD thesis, University of Innsbruck, 2004.
4. A. Matt and G. Regensburger, Generalization over environments in reinforcement learning. IberoAmerican Journal of Artificial Intelligence, 21:47–53, 2003.
5. A. Matt and G. Regensburger. Approximate policy iteration for several environments and reinforcement functions. In Proceedings of the 6th European Workshop on Reinforcement Learning (EWRL-6), 15–17, Nancy, France, 2003.
6. G. Regensburger and O. Scherzer, Symbolic computation for moments and filter coefficients of scaling functions, to appear in Annals of Combinatorics, March 2005, 21 pages.

Participation at Conferences

Conference on Artificial Intelligence and Symbolic Computation (AISC), RISC, Castle of Hagenberg, Austria, 22–24 September 2004.

Scientific Cooperations

In addition to the cooperations listed in the section "Overview on the Work of the Computational Logic Group in 2004", G. Regensburger has worked in the following cooperations:

- With Dr. Andreas Matt (Univ. of Innsbruck) on reinforcement learning [1, 3, 4, 5].
- With Prof. H. Hauser (dto.) on singularities [2].
- With Prof. O. Scherzer (dto.) on wavelets and symbolic computation [6].

Dipl.-Ing. Alexander Zapletal

Introduction

A. Zapletal completed his diploma in Computer Science in April. The topic of his diploma thesis was "Algorithmen in der Computeralgebra für Polynomideale und –moduln." Since October 2004, A. Zapletal is a PhD student of the Johannes Kepler University Linz, specializing in Symbolic Computation, advised by B. Buchberger. Since October 2004 A. Zapletal is also employed by RICAM.
The main topic of his PhD thesis will be the build-up of a formal knowledge base for Gröbner bases theory within the Theorema system.
Additionally, A.Zapletal will assist B. Buchberger in organizing a special semester on Gröbner Bases and related methods in 2006 at RICAM.

Scientific Achievements 2004

No research so far except for the Diploma thesis.

Scientific Cooperations

See the cooperations listed in the section "Overview on the Work of the Computational Logic Group in 2004".

Prof. Josef Schicho

Introduction

The main focus of Schicho's research is to solve algebraic constraints. In particular, he studied parametrizations, as the most explicit finite description of infinite solution sets. He gave algorithms for parametrizing various classes of algebraic varieties, and for simplifying a given parametrization (as one variety may have many parametrizations, and some are simpler than others).

The traditional approach towards equation solving in computer algebra is an exact one, working with long integers/rationals and/or with finite representations of real algebraic numbers (e.g. Thom's code). The existence of rational solutions, which is a diophantine problem, is essential in Schicho's research. On the other hand, Schicho also studies symbolic-numeric algorithms, which work with flooating point numbers. Here the main challenge is to control the numerical instabilities.

Scientific Achievements 2004

An essential step in Schicho's algorithm for surface parametrization can be understood better if one studies it from the viewpoint of combinatorics/discrete geometry. This relation has been exploited in order to prove a purely combinatorial result by methods from algebraic geometry.
It has been observed recently that the class of Del Pezzo surfaces can be conveniently used in certain applications in geometric modeling. Schicho gave a parametrization algorithm and a constructive classification for this class.
Using the theory of cylindric algebraic decomposition, a new algorithm for the computation of the level curve of a real algebraic surface was constructed.
For a classical problem in computer algebra, the implizitization problem for rational surfaces, requirements in CAD applications have pushed the development of numerical methods. Schicho and Szilagyi did a first analysis of the numerical error.
A parametrization for local parametrization of cubic surfaces has been developed.
In science management, Schicho contributed by being the main organizer of the International Symposium of Symbolic and Algebraic Computation in Santander, July 2004. He is currently also co-editing a special issue of the journal "Algorithmic Algebra and Error-Correcting Codes" on algebraic curves.

Talks at Conferences and Workshops

1. J. Schicho. Dediding Rational Rationality of Algebraic Surfaces. Magma Workshop on Effective Algebraic and Arithmetic Geometry, Paris, October 2004

2. B. Jüttler, J. Schicho, M. Shalaby. Applications of Spline Implicitization. Poster at the International Symposium of Symbolic and Algebraic Computation, Santander, July 2004.

3. J. Schicho, I. Szilagyi. Numerical Stability of Surface Implicitization. Poster at the International Symposium of Symbolic and Algebraic Computation, Santander, July 2004

4. J. Schicho. Blowing Up of Flat Varieties. Workshop on Singularities, Schwaz, March 2004.

5. J. Schicho. Sparse Representation of Algebraic Power Series. Workshop on Singularities, Schwaz, March 2004.

6. J. Schicho. Numerical Study of Singularities of Plane Curves. Workshop on Singularities, Gmunden, September 2004.

Invited Talks

7. J. Schicho. Real Rational Surfaces. MSRI Workshop on Real Algebraic Geometry and Applications in Computer Aided Design, Berkeley, April 2004.

Talks in the Radon Seminar

8. J. Kraus and J. Schicho. Algebraic Construction of Edge Matrices with Applications to AMG. December 2004.

Publications

Accepted Papers

1. J. Schicho. Elementary Theory of Del Pezzo Surfaces. In: B. Jüttler, T. Dokken (eds), Computational Methods for Algebraic Spline Surfaces, Proc. ESF Workshop, Springer, 2004, pp 77-94.

Submitted Papers

2. C. Haase, J. Schicho. Lattice Polygons and the Number 2i+7.

3. G. Bodnar, S. Encinas, J. Schicho. A Local Presentation of Varieties.

4. J. Alcazar, J. Schicho, J. Sendra. Computation of the Topological Types of the Level Curves of Real Algebraic Surfaces.

5. B. Jüttler, J. Schicho, I. Szilagyi. Local Parametrization of Cubic Surfaces.

6. J. Schicho, I. Szilagyi. Numerical Stability of Surface Implicitization.

7. G. Landsmann, P. Mayr, J. Schicho. A Topological Criterion for Polynomiality.

Scientific Cooperations

Internal Cooperations

Schicho is the PhD supervisor of Beck, Pilnikova, and Szilagyi, all from the group of Symbolic Computation at RICAM. In addition to cooperations with them, he did cooperations with the following people at RICAM.

1. J. Kraus (Computational Matematics for Direct Field Problems). Schicho could solve an algebraic subproblem arising in the context of a new method for algebraic multigrid developed by Kraus.

2. W. de Graaf (Symbolic Computation). De Graaf, Schicho, Pilnikova and M. Harrison from the University of Sydney developed a new method for solving certain diophantine problems using Lie algebras.

External Cooperations

Schicho did cooperations with the following people outside RICAM.

3. B. Jüttler (University of Linz). Together with I. Szilagyi, they developed an algorithm for local parametrization of cubic surfaces. Jüttler is also the co-investigator in the project SFB 1315.

4. G. Landsmann, P. Mayr (University of Linz). This is a joint work that started during a visit of A. Kisielewicz (University of Warszawa) at RICAM in July 2004. In order to explore the purely algebraic problem of polynomiality of given functions on a linear group, topological

methods were introduced, which lead to the answer of a problem which could not be answered by algebraic means.

5. G. Bodnar (University of Linz). He and Schicho continued their cooperation on algorithms for the resolution of singularities. In particular, they developed a technique for representing local pieces of varieties together with S. Encinas (University of Valladolid).

6. H. Hauser (University of Innsbruck). Schicho and Hauser lead together the FWF project P15551 (Effective Resolution of Singularities and Related Problems). They organized two joint workshops, one in Schwaz and one in Gmunden.

7. S. Encinas (University of Valladolid). See cooperation with Bodnar above.

8. J. Alcazar, J. R. Sendra (University of Alcala, Madrid). In this cooperation a method for computing the topology of level curves of algebraic surfaces was developed.

9. M. Harrison (University of Sydney). See cooperation with de Graaf above.

Dr. Willem De Graaf

Introduction

The reasearch area of de Graaf is computational Lie theory. This topic is concerned with finding algorithms for working with objects that occur in Lie theory. Specifically de Graaf has worked on algorithms for Lie algebras, and quantum groups. Recently he also started working on Lie rings, a topic that occurs in group theory.

Scientific Achievements 2004

Research 2004 before RICAM

Before de Graaf came to RICAM he has worked on the classification of small-dimensional solvable Lie algebras. Roughly the method he used for this works as follows. One obtains all solvable Lie algebras of dimension n by extending solvable Lie algebras of dimension n-1 by a derivation. Then one gets rid of the isomorphic ones and obtains a classification of the solvable Lie algebras of dimension n.
De Graaf has carried out this procedure for n up to 4, using a technique based on Gröbner bases for finding explicit isomorphisms between Lie algebras.

Research 2004 at RICAM

At RICAM de Graaf has worked on two topics, namely Lie algebras associated to Severi-Brauer surfaces, and Lie rings.
The first topic (i.e., Lie algebras associated to Brauer-Severi surfaces) is in collaboration with M. Harison, J. Pilnikova and J. Schicho. They have developed a technique for asssociating a Lie algebra to a given Severi-Brauer surface.
Secondly, they have devised a method for checking whether the Lie algebras corresponding to two different Severi-Brauer surfaces are isomorphic. Finally, they have shown that an isomorphism between the Lie algebras leads to an isomorphism of the surfaces. Furthermore, this proof yields an algorithm for explicitly finding this isomorphism.

Concerning the topic of Lie rings de Graaf has developed and implemented an algorithm for finding a basis of a Lie ring given by generators and relations. This builds on earlier work on finitely-presented Lie algebras. The implementation is in the computer algebra system Magma, and it is expected that the implementation will become part of the core system in the near future.

Talks

1. Classification of solvable Lie algebras, at the conference: Lie Algebras, their Classification and Applications, TU Braunschweig, 20 - 22 May 2004

2. Computing with Quantum Groups, Computational Algebra Seminar, School of Mathematics and Statistics, University of Sydney, 12 August 2004

3. Constructing finitely-presented Lie rings, Nikolaus Conference 2004, RWTH Aachen, 10-11 December 2004.

Scientific Cooperations

Internal Cooperations

With J. Pilnikova and J . Schicho on the topic of Lie algebras associated to Severi-Brauer surfaces.

Participation at conferences

- Lie Algebras, their Classification and Applications, TU Braunschweig, 20 - 22 May 2004

- Nikolaus Conference 2004, RWTH Aachen, 10-11 December 2004.

Publications

Accepted

1. Classification of solvable Lie algebras, Experimental Mathematics (to appear)

2. Constructing homomorphisms between Verma modules, Journal of Lie Theory (to appear)

Dr. Pavel Chalmoviansky

Introduction

Pavel Chalmoviansky joined RICAM in April 2004. The area of his research is covered by geometric modeling and techniques in computer aided geometry. It uses both differential and algebraic geometry together with optimization methods for designing new and/or improving of existing algorithms in this area. The research is focused on the integration of numerical and symbolic methods for algebraic splines.

Scientific Achievements 2004

Research 2004 before RICAM

Approximate Parameterization of Planar Implicitly Defined Curves
He studied methods of approximate parameterizations of curves. The approximation starts with G^1 data at two points of a fixed algebraic curve. The best fitting rational Bezier curve for these data is computed as a minimum of the objective function which is composed from the first order approximation of Euclidean distance to the given curve and regularizing terms for weight of the rational Bezier segment and lengths of the control polygon. Finally, optimized curve is extrapolated at the endpoints. This gives a new starting curve for urther optimization. Iterating these steps, we get an approximation of a segment of the given algebraic curve also in case, where the curve does not have an exact parameterization or has a singularity in the area of interest.
A Circle-preserving Subdivision Scheme Based on Local Algebraic Fits
The method of local algebraic fits was applied to a given sequence of points and associated normals. The refined sequence contains also newly generated points sampled from fitted circles to original adjacent points and the corresponding normals. Iterating this approach we get a G^1 limit curve reproducing circles. The method is invariant under the group of Euclidean similarities. The experimental setup for G^2 construction and possible extensions of the method were discussed.

Research 2004 at RICAM

Approximate Parameterization of Intersection Curves: The methods of approximate arameterization can be extended to curves formed as intersection of two algebraic surfaces in E^3. The focus is directed toward an approximation of distance of a point in E^3 to the intersection curve. We use local approximation based on the modification of the surfaces so that the intersection is fixed and the new gradients along the intersection curve form an orthogonal frame for each point. The distance function can then be approximated locally by cylindrical coordinates associated with the tangent line of the curve. We are about to finish a paper on this topic.
Evolution of Approximate Parameterization of Curves: The approximation of the curve is formulated as a coupled system of ODE. One of these is a tracing of the given implicitly defined curve. The other is the evolution of the approximate parameterization. Using Runge-Kutta methods for approximation of the solution of the ODE, we expect faster and better evolution of the approximation for regular parts of the algebraic curve. This is an ongoing work.

External Cooperations

Dalibor Lukas, SFB013, Project 1309 (until September 2004 then TU Ostrava)

Talks at Conferences and Workshops

Pavel Chalmoviansky, Bert Juettler. Algebraic Subdivision of Curves. Talk at the conference DMV Tagung, Heidelberg, Germany. September 2004.

Publications

Accepted Papers

1. Pavel Chalmoviansky, Bert Juettler. Fairness Criteria for Algebraic Curves. Computing. Vol. 72, pp. 41-51. 2004.

2. Bert Juettler, Pavel Chalmoviansky. Approximate Parameterization by Planar Rational Curves. Proceedings of SCCG2004, (ed) A. Pasko. pp. 27-35, Comenius University Bratislava, 2004. ISBN 80-223-1918-X.

3. Bert Juettler and Pavel Chalmoviansky. Approximate Parameterization by Planar Rational Curves. Technical report 04-14. July 2004. Johannes Kepler University Linz, Spezialforschungsbereich SFB013.

4. Pavel Chalmoviansky and Bert Juettler. Fairness Criteria for Algebraic Curves. Geometric Modelling Dagstuhl 2002. Eds. Hahmann, S. and Brunnett, G. and Farin, G. and Goldman, R. 2004. ISBN 3-211-20818-6.

Submitted Papers

5. Pavel Chalmoviansky, Bert Juettler. A Circle-preserving Subdivision Scheme Based on Local Algebraic Fits.

Dr. Johannes Gahleitner

Introduction

Gahleitner has been working in the SFB project 1315 until August 2004. In September 2004, he finished his PhD study under the supervision of Prof. Bert Jüttler. The topic of his thesis are monois spline curves and surfaces. Since September 2004, he has started to work as a teacher for mathematics and physics in the high school Petrinum.

Scientific Achievements 2004

In his thesis, Gahleitner used monoid curves and surfaces in order to compute approximate parametrizations of curves. The curve may be given either by an implicit equation – in this case, the problem can be seen as an approximate/numerical variant of a classical problem in computer algebra – or by a finite set of support points.

Publications

Monoid Curves and Surfaces. Dissertation at the University of Linz, 2004.

Dipl.-Inf. Tobias Beck

Introduction

T. Beck is working on the global parameterization of algebraic surfaces of arbitrary degree. In the simplest case an algebraic surface is a subset of affine three-space given as the zero-set of a polynomial equation. Besides this implicit representation it is in some cases possible to give a birational map from the affine plane onto the surface, i.e. a map that is defined and invertible almost everywhere and can be represented by rational functions in both directions. Such a map is called a parameterization.

J. Schicho (Beck's thesis advisor) gave an algorithm for deciding existence of such parameterizations and computing them. This algorithm is very complex as it uses deep results from algebraic geometry. It has not been implemented yet. An implementation is the final goal of Beck's PhD research.
The main tool for the computation of parameterizations are surfaces that are "adjoint" to the given surface. They may be computed e.g. via a global "resolution" of the implicitly given surface. But there is known almost nothing about the complexity of computing such resolutions. Therefore in our approach we will first compute local analytic parameterizations of surfaces by bivariate power series, use these power series to determine systems of adjoint surfaces and finally construct a global parameterization.

Scientific Achievements 2004

There is an algorithm by Luengo at al for computing power series solutions to certain polynomial equations. It relies on a representation of algebraic power series by so called "locally smooth systems" and works by normal form computations. We have implemented this algorithm in Aldor/Algebra and experimentally studied its practical usability. Results were presented in a talk at CATLAN 2004. In this context we also tried to find systems that are as small as possible.
The main achievement this year is a generalization of the classical Newton-Puiseux algorithm for curves that results into a new algorithm for computing multivariate power series roots to polynomial equations. A paper is in preparation.

Scientific Visits and Talks

- From 1st of April to 13th of April T. Beck was invited to the workshop "Real Algebraic Geometry and Geometric Modeling" at MSRI at the University of California in Berkeley, California.

- From 1st of November to 16th of November T. Beck was invited by Marc Moreno Maza to ORCCA at the University of Western Ontario in London, Ontario. There he gave several introductory talks on the computation of algebraic power series in order to start cooperation.

Scientific Cooperations

Internal Cooperations

T. Beck is working intensively with his thesis advisor J. Schicho. Here the connection between power series solution to polynomial equations and the classical problem of resolution of algebraic varieties is of special importance. First ideas have been presented in the "Workshop on Singularities" in Gmunden.

External Cooperations

- We have started cooperation with Marc Moreno Maza from ORCCA, University of Western Ontario in London, Ontario. Together we are working on a new computational model for algebraic power series that only uses computations of greatest common divisors.

- We invited Joris van der Hoeven from the Université Paris-Sud in Orsay Cedex, France, for a short stay at RICAM. Together we have developed some technical improvements of Luengo's algorithm and started to analyze its asymptotic complexity.

- For Jan Valdman, employed at the "SFB F013 Numerical and Symbolic Scientific Computing" at Johannes Kepler Univarsität Linz, T. Beck implemented a symbolic solver for polynomial equations arising in the numerical analysis of elastoplastic material. Unfortunately we couldn't improve the performance and didn't pursue this direction further.

Participation at conferences

- T. Beck. Standard Bases and Algebraic Power Series Computations. Workshop on Singularities, Schwaz, March 2004

- T. Beck. Multivariate Algebraic Power Series for Aldor/Algebra. Workshop on Categorical Programming Languages CATLAN 2004, Santander, July 2004

- T. Beck, J. Schicho. Local Analytic Resolution of Singularities. Workshop on Singularities, Gmunden, September 2004

Mag. Janka Pilnikova

Introduction

Janka Pilnikova joined RICAM in April 2004 as a PhD student under supervision of Prof. Dr. Josef Schicho. Her research interest is algebraic and arithmetic geometry, in particular finding rational points on surfaces and consequently finding a rational parametrization.
She is working on her PhD thesis on rational parametrization of Del Pezzo surfaces.

Scientific Achievements 2004

Research 2004 before RICAM

Rational Quadratic Forms.
The Hasse principle can be used for deciding whether the rational form in any number of variables has a rational solution, and in the affirmative case also for finding such a solution. The algorithm for solving quadratic forms over rationals has been implemented in Magma.

Research 2004 at RICAM

Arithmetics of Severi-Brauer surfaces (Del Pezzo of degree 9).
Severi-Brauer surfaces can be understood as visualizations of central simple algebras of degree 3 over rational numbers, namely the surface is the set of 3-dimensional left ideals of the corresponding algebra.
1. Galois descent
Galois descent is a very efficient method based on Galois cohomology for constructing Severi-Brauer surfaces. The algorithm is implemented in Magma.
2. Parametrization of Severi-Brauer surfaces

To find a parametrization of a Severi-Brauer surface, one first reduces the problem to Del Pezzo surfaces of degree 9. Afterwards the Lie algebra of the group of automorphisms of the surface is found. Then one finds an isomorphism of the algebra and the algebra corresponding to the group of automorphisms of projective plane, and uses this isomorphism for finding a parametrization of the given Severi-Brauer surface. In case the given Severi-Brauer surface has a rational parametrization, the constructed Lie algebra is the algebra associated to the central simple algebra of the surfaces.
The algorithm for rational parametrization of Severi-Brauer surfaces is implemented in Magma. A paper on algorithms for Severi-Brauer surfaces is in preparation.

Scientific Visits and Talks

- September 2004, visiting scholar at Magma group in School of Mathematics and Statistics, University of Sydney
- a talk "Finding Rational Points on Severi-Brauer Surface", Computational Algebra Seminar, September 9, 2004, University of Sydney

Scientific Cooperations

Internal Cooperations

- Prof. Dr. Josef Schicho
- Dr. Willem A. de Graaf

External Cooperations

Dr. Michael Harrison, University of Sydney

Participation at conferences

- a lecture "Quaternary Rational Quadratic Forms", Workshop on singularities, Schwaz, March 10-13, 2004
- a talk "Hasse Principle for Rational Quadratic Forms", SFB Statusseminar, April 5-7, 2004, Strobl
- a talk "Finding Rational Points on Severi-Brauer Surface", Algebraic Geometry and Number Theory with Magma, October 4-8, 2004, Institute Henri Poincaré, Paris
- a talk "Rational parametrization of del Pezzo surfaces of degree 9", Nikolaus conference, December 10-11, 2004, Aachen

Mag. Ibolya Szilagyi

Introduction

The research interest of Ibolya Szilágyi is symbolic algebra. In particular, her main topic is symbolic-numeric techniques for cubic surfaces. Algebraic surfaces - which are frequently used in geometric modelling - are represented either in implicit or parametric form. These two representations are appropriate to solve different classes of problems. Hence, the automatic transition between these two representation is of fundamental importance. The two conversion problems are called parametrization and implicitization. General cubic surfaces admit both implicit and rational parametric form. The main focus of this research is to use symbolic and numeric tools to solve problems related to the mentioned conversion problems in the case of cubic surfaces.

Scientific Achievements 2004

Research 2004 at RICAM

Local parametrization of non-singular cubic surfaces
Several techniques for parameterizing a rational algebraic surface as a whole exist. However, in many applications, it suffices to parameterize a small portion of the surface. This motivates the analysis of local parametrizations, i.e., parametrizations of a small neighborhood of a given point of a surface. In [2] I. Szilágyi together with Prof. Dr. Josef Schicho and Prof. Dr. Bert Jüttler introduced several techniques for generating such parameterizations for nonsingular cubic surfaces. For this class of surfaces, it is shown that the local parametrization problem can be solved for all points, and any such surface can be covered completely. The methods are symbolic-numeric. Symbolic objects are manipulated, on the other hand it is assumed that the coefficients of the polynomials and the coordinates of the points are floating point numbers. The reason for the decision to work with floating point numbers comes from the applications.
Condition number of the implicitization problem
For a numerically given parametrization we cannot compute an exact implicit equation, just an approximate one. In [1] together with J. Schicho a condition number was introduced to measure the worst effect on the solution (implicit representation) when the input data is perturbed by a small amount. The condition number depends not only on the input (parametric form), but also on the estimation of the degree of the implicit form. It can be used to give an upper bound for the error in the computed implicit representation. This condition number allows to give a stability test of various implicitization techniques.

Scientific Visits and Talks

- Local parametrization of cubic surfaces. Invited talk at University of Debrecen, Hungary, April 16, 2004.
- Numerical stability of surface implicitization, Radon seminar, November 15, 2004.

Scientific Cooperations

Internal Cooperations

Name	Institution	Topic	Publication
J. Schicho	RICAM	Symbolic/numerics	[1, 2]
B. Jüttler	University of Linz	Parametrization	[2]
M. Aigner	University of Linz	Robustness	in progress

Participation at conferences

- Implicitization and Parametrization Using Symbolic-Numeric Techniques. International Conference in Applied Informatics, Eger, Hungary, January 28-30, 2004
- Workshop on algebraic geometry and singularities, Tirol, Austria, February 25-27, 2004
- SFB workshop on numerical and symbolic scientific computation, Strobl, Austria
- Local parametrization of cubic surfaces. Geometri Tagung, Vorau, Austria, June 7-11, 2004
- Numerical Stability of Surface Implicitization (poster presentation). ISSAC-International Symposium on Symbolic and Algebraic Computation, Santander, Spain, July 4-7, 2004
- Workshop on algebraic geometry and singularities, Gmunden, Austria, September 16-18, 2004
- Local parametrization of cubic surfaces. Workshop on Algebraic Geometry and Geometric Modelling, Nice, France, September 27-29, 2004
- Numerical Stability of Surface Implicitization. RICAM Seminar, Linz, November 15, 2004

Publications

Appeared Papers

1. J. Schicho, I. Szilágyi, Numerical Stability of Surface Implicitization. SFB-Report 2004-27, J. Kepler University, Linz.

2. Szilágyi and B. Jüttler and J. Schicho, Local Parametrization of Cubic Surfaces. SFB-Report 2004-31, J. Kepler University, Linz.

Submitted Papers

3. J. Schicho, I. Szilágyi, Numerical Stability of Surface Implicitization. Submitted to Journal of Symbolic Computation, 2004

4. I. Szilágyi and B. Jüttler and J. Schicho, Local Parametrization of Cubic Surfaces. Submitted to Journal of Symbolic Computation, 2004.

Group "Financial Mathematics"

Group Leaders:
Univ.-Prof. Dr. Gerhard Larcher
o.Univ.-Prof. Dr. Walter Schachermayer

Researchers funded via ÖAW/Upper Austrian government funds:
Dr. Karel Janecek
Dr. Gottlieb Pirsic
Dr. Jörn Saß
Dr. Klaus Scheicher
Univ.-Doz. Dr. Arne Winterhof

Researchers externally funded:
DI Nina Brandstätter FWF
Dr. Wilfried Meidl FWF

Introduction

On the concrete scientific achievements will be reported in the following short description and in the reports of the single ÖAW-researchers.
The main organisatorial and further activities and achievements in the year 2004 were:

1) We were able to employ the new ÖAW researcher Karel Janecek from the Carnegie Mellon University, Pittsburgh. He is co-author of Steven Shreve, who is a first-class expert in mathematical finance.
2) We organized a workshop on "Complexity and Discrepancy" at the Radon Institute in October 2004, with talks of the leading international experts in this field (e.g. Ian Sloan or Greg Wasilkowski)
3) G. Pirsic became co-leader of a FWF-research project (together with F.Pillichshammer (Linz) and W. Schmid (Salzburg))
4) J. Saß became leader of a FWF-research project (start in February 2005)
5) A. Winterhof received the renowned Edmund-and-Rosa-Hlawka Award of the Austrian Academy of Sciences.

We repeat from former reports that it is the aim of this group to combine two quite different approaches to mathematical finance namely the approach via MC-simulation techniques and the approach via stochastic finance. On some details about these two approaches see below. The collaboration between these two groups is managed via a long-running joint project on "Markov-Monte Carlo and Markov-Quasi-Monte Carlo simulation in Utility Maximisation with Transaction Costs". This work now is also supported by a FWF-project led J. Saß and is carried out in collaboration with the Institute for Statistics at the Faculty of Economics at the University Linz.
The main collaboration within the Radon Institute at the moment is a joint project with the Group of Kunisch. In this project we try to apply a concept of Kunisch to the valuation of american options.

The first of the two approaches to mathematical finance of our group (especially represented by the group leader Gerhard Larcher and the ÖAW researchers Pirsic, Scheicher and Winterhof) is concerned with simulation with special emphasis to its application in mathematical finance. We are especially interested in simulation based on Monte Carlo and on quasi-Monte Carlo methods. We investigate fundamental questions arising in this context (complexity estimates, construction and analysis of well distributed point sets, analysis of simulation schemes, …) and the possibilities of the applications of these techniques to problems in finance. These investigations frequently lead to questions and problems of a number-theortical nature. Recent papers of the group leader dealing with this aspect of research are:

1. G. Larcher, F. Pillichshammer (2004) Walsh Series Analysis of the Star-Discrepancy of Digital Nets and Sequences. In H. Niederreiter (Editor) "Monte Carlo and Quasi-Monte Carlo Methods 2002" Springer-Verlag, (2004), 315 – 328
2. M. Drmota, G. Larcher, F. Pillichshammer (2004) Precise Distribution Properties of Hammersley and Related Point Sets. To appear in: Manuscripta Mathematica (2005)
3. P. Kritzer, G. Larcher, F. Pillichshammer (2004) On the Distribution of Shifted Digital Nets. Submitted (2004)
4. G. Larcher, F. Pillichshammer (2004) Properties of Sums of Digital Sums. Submitted (2004)

The other approach (especially represented by the group leader Walter Schachermayer and the ÖAW researchers Saß and Janecek) is concerned with stochastic finance. In the center of the investigations in this direction at the moment is the "utility maximisation in incomplete financial markets" and "utility maximisation under transaction costs". Recent papers of the group leader dealing with this aspect of research for example are:

1) M. Drmota, W. Schachermayer, J. Teichmann (2004) A hyper-geometric approach to the BMV-conjecture. Preprint (30 pages), submitted (2004).
2) W. Schachermayer (2004) Utility Maximisation in Incomplete Markets. In: Stochastic Methods in Finance, Lectures given at the CIME-EMS Summer School in Bressanone/Brixen, Italy, July 6-12, 2003 (M. Fritelli, W. Runggaldier, eds.), ISBN 3540229531, Springer Lecture Notes in Mathematics, Vol. 1856 (2004), pp. 225-288.
3) F. Delbaen, W. Schachermayer (2004) What is a Free Lunch? Notices of the AMS, Vol. 51 (2004), No. 5, pp. 526-528.
4) P. Guasoni, W. Schachermayer (2004) Necessary Conditions for the Existence of Utility Maximizing Strategies under Transaction Costs. Statistics and Decisions, Vol. 22 (2004), No. 2, pp. 153-170.
5) W. Schachermayer (2005) Portfolio Optimization in Incomplete Financial Markets. In: Interest Rate Models - Theory and Practice (D. Brigo, F. Mercurio, eds.), Notes of the Cattedra Galileiana lectures, June 2001, Springer Finance, ISBN 3540221492 (2005).
6) F. Hubalek, W. Schachermayer (2004) Optimizing Expected Utility of Dividend Payments for a Brownian Risk Process and a Peculiar Nonlinear ODE. Insurance: Mathematics and Economics, Vol. 34 (2004), No. 2, pp. 193-225.
7) W. Schachermayer (2005) A Note on Arbitrage and Closed Convex Cones. Mathematical Finance, Vol. 15 (2005), No. 1, pp. 183-189.
8) M. Davis, W. Schachermayer, R. Tompkins (2004) The Evaluation of Venture Capital as an Instalment Option: Valuing Real Options Using Real Options. Zeitschrift für Betriebswirtschaft, Vol. 3 (2004).
10) W. Schachermayer (2004) The Fundamental Theorem of Asset Pricing under Proportional Transaction Costs in Finite Discrete Time. Mathematical Finance, Vol. 14 (2004), No. 1, pp. 19-48.

Dr. Karel Janecek

Introduction

The main topic of research is optimal control under transaction costs. This is an on-going research from Dr. Janecek's Ph.D. studies at Carnegie Mellon Univeriesty, Pittsburgh. Another line of Dr. Janecek's research includes the analysis of the risk aversion coefficient used in financial markets for practical trading and investments.

Scientific Achievements 2004

Research 2004 before RICAM

Optimal control under transaction costs: The first part of the research was finalized in "Asymptotic analysis for optimal investment and consumption with transaction costs", Janecek, K., Shreve, S., *Finance and Stochastics* 8, 181-206 {2004).

Research 2004 at RICAM

A completely new probabilistic approach for solving the problem of optimal control under transaction costs has been finished recently, and the work is currently in the process of finalizing a draft for submission. The new approach includes modeling of futures contracts trading rather than stock trading, which appears to be an original concept.

Scientific Visits and Talks

1. Till Oct 15: Carnegie Mellon University, Ph.D. studies
2. TU Wien, April 2004
   Talk: *Comparison of futures model trading vs. stock trading under transaction costs*

Scientific Cooperations

Internal Cooperations with

Karl Kunish (RICAM), **Joern Sass** (RICAM):
Numerical analysis of optimal control under transaction costs.

Walter Schachermeyer
Topics concerning no-arbitrage and replicability analysis under transaction costs.

External Cooperations with

Steven E. Shreve, Carnegie Mellon University:
The asymptotic analysis of optimal control under transaction costs, futures trading

Participation at conferences

1. IMA Workshop, May 3 – May 7, 2004, University of Minnesota, MN 55455
2. Bachelier Finance Society, Third World Congress, July 21-24, 2004, Intercontinental Hotel, Chicago, IL

Talk: *Futures trading model with transaction costs*

Publications

Appeared
"Asymptotic analysis for optimal investment and consumption with transaction costs", Janecek, 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

The main topic of research of Dr. Pirsic are quasi-Monte Carlo methods of numerical integration. This entails mainly the investigation of so-called low-discrepancy point sets, in particular digital point sets such as (t,m,s)-nets and (t,s)-sequences. It has been observed that these are particularly apt for application in numerical Mathematical Finance. The reason for this is suspected in the nature of the considered integrands in this area, which often lie in weighted Sobolev spaces, which in turn are shown to be very well suited to quasi-Monte Carlo methods.

Scientific Achievements 2004

Research 2004 at RICAM

The main focus of research in this year lay on the exploration of cyclic digital nets. These are digital low-discrepancy point sets given by a construction defined by Niederreiter and modelled to translate the concept of cyclic codes to digital nets.

Dr. Pirsic implemented this new construction and carried out extensive computer searches for point sets with good net quality parameter t. Later, cooperation with Dick and Pillichshammer lead also to exhaustive computations of the mean square worst case error with respect to a weighted Sobolev space. There, a so-called component-by-component construction algorithm was employed. The theoretic background for this lead to the paper [3].

The computational results quickly lead to the suspicion of a close relation to polynomial lattice rules, another established and well-investigated digital net construction. This, as well as a similar relation to Schmid's constacyclic Shift-nets could be established and is also mentioned in [3].

Still in the same paper, also the Walsh-analysis of digital nets over finite fields of arbitrary prime power order could be laid out explicitly for the first time.

Another topic this year was the construction of digital point sets on non-unit cube regions. This was done specifically for two-dimensional ellipsoids, the three-dimensional sphere- and torus surfaces and n-dimensional simplices. There the transformations involved in the curvilinear models proved at a first attempt to be too complex to be computationally feasible in practice. However, due to interest in the community in a character group other than spherical harmonics on the sphere, which would be a by-product of the analysis of the corresponding point set, research in this direction may be continued at a future point.

As simplices often appear in various practical numerical computation situations, results pertaining to these are particularly interesting. Apart from rediscovery of transformations already considered by Cools and his group, another construction was found that builds essentially on an IFS-representation of the simplex. Techniques developed in [2] could also be applied, but as of yet not be brought to a result of the desired quality. Also this may be pursued further later.

Scientific Visits and Talks

1. 16 April, University Salzburg, cooperation with Schmid's group
2. 18 November, University Salzburg, Talk: "Darstellung von Shift-Netzen als zyklische digitale Netze"

Scientific Cooperations

External Cooperations with

Name	Institution	Topic	Publication
F. Pillichshammer	Univ. Linz	Low-discrepancy seq.s (LDS)	[2],[3]
J. Dick	Univ. New South Wales	LDS	[3]
R. Schuerer	Univ. Salzburg	Computational mathematics	
W. Schmid	Univ. Salzburg	LDS	

Participation at conferences

1. 7 Jun - 11 Jun, MC2QMC 2004, Juan-les-Pins
2. 27 Sept - 1 Oct, Number Theoretic Algorithms and Related Topics 2004, Strobl
   4 Oct - 5 Oct, Workshop on Complexity and Discrepancy, Linz

Publications

Submitted

1. H. Maharaj, G. L. Matthews, and G. Pirsic, Riemann-Roch spaces of the Hermitian function field with applications to algebraic geometry codes and low-discrepancy sequences, accepted by Journal of Pure and Applied Math.
2. L. L. Cristea, F. Pillichshammer, K. Scheicher and G. Pirsic, Discrepancy estimates for point sets on the s-dimensional Sierpinski carpet, accepted by Quaestiones Mathematicae.
3. J. Dick, G. Pirsic, F. Pillichshammer, Cyclic digital nets, hyperplane nets and multivariate integration in weighted Sobolev spaces, submitted to Transactions of the AMS.

Dr. Jörn Saß

Introduction

In 1969/71 Merton derived in the continuous time Black-Scholes model optimal dynamic portfolio policies using stochastic control theory. For a utility maximization criterion using utility func-

tions with constant relative risk aversion it is optimal to keep a constant fraction of the wealth (portfolio value) invested in each stock. But the performance of the Merton strategy applied to market data is quite poor and practitioners still prefer the static Markowitz model.
So it is still an important problem of financial mathematics to derive in continuous time optimal trading policies in more realistic models which allow e.g. for transaction costs or for non-constant coefficients. The computation of these strategies is numerically difficult. As in 2003, when he joined the RICAM, in 2004 the research of Dr Sass was focused on finding explicit trading strategies for different optimization problems to make the modern portfolio theory better applicable.

Scientific Achievements 2004

In 2004 Dr Sass continued his work on models under transaction costs. 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 [2] 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 continuous time [5] 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 methods. Afterwards the resulting strategy can be shown to be optimal in the class of impulse control strategies.
The work of Dr Sass and Prof Haussmann on portfolio optimization under partial information lead to the final versions of [1, 3, 4]. These papers consider a model where the appreciation rates of the stocks (drift of the stock returns) are given as a continuous time Markov chain. But the stock prices are the only information an investor has. Hence these rates cannot be observed, so a hidden Markov model (HMM) results. In [3] an explicit trading strategy is derived using extended HMM filtering results and Malliavin calculus, the involved parameter is dealt with, and these strategies are applied to market data. In [1] the model is generalized to cover non-constant volatilities and stochastic interest rates, and in [4] a quite successful volatility model (dependence on the filter for the rates) is proposed.
The work in [1,3,4] inspired the submission of an FWF proposal on 'Computing Optimal Portfolio Policies under Partial Information'. Besides some extensions of the models the emphasis of the project is placed on the efficient computation and implementation of theses strategies, including parameter estimation. This proposal (project P 17947) was approved in the FWF meeting on November 29/30 with a volume of € 184 491.09. So it allows for two co-workers on the level of doctoral students for about 34 months. One co-worker will be DI Hahn who is currently working in the FWF project S 8305 (project leader Prof Larcher) on the corresponding parameter estimation using Markov chain Monte Carlo (MCMC) methods and who is already supervised by Dr Sass.

Scientific Visits and Talks

1. Mathematisches Seminar, Universität Kiel, Germany, May 10-14
   Talk: Portfoliooptimierung bei partieller Beobachtung, May 14
2. Abteilung Optimierung und Operations Research, Universität Ulm, Germany, May 24/25
   Talk: Portfolio Optimization for HMM Stock Returns: From Constant to Stochastic Volatility, May 24
3. Department of Mathematics, UBC, Vancouver, Canada, June 6-26
   Talk: Portfolio Optimization under Transaction Costs in the CRR model, June 16
4. Institut für angewandte Mathematik, Universität Bonn, Germany, December 6-10
   Talk: Portfolio Optimization under Partial Information, December 9

Talks held at conference are listed below.

Scientific Cooperations

Internal Cooperations

Name	Topic	Publication
M. Hahn G. Larcher	Computation of optimal portfolio strategies under partial information	in progress
K. Janecek K. Kunisch	Numerical solution of free boundary problems arising in finance	in progress

It should be emphasized at this point that there were also a lot of discussions with colleagues from the Optimization Group and the Inverse Problems Group which were very helpful for the ongoing projects. They may lead to further collaborations in the future.

External Cooperations

Name	Institution	Topic	Publication
S. Frühwirth-Schnatter	Institut für Angewandte Statistik , JKU Linz	MCMC methods for hidden Markov models	in progress
U. G. Haussmann	UBC, Vancouver	Portfolio optimization under partial information	[1,2,3]
A. Irle	Universität Kiel	Portfolio optimization under transaction costs	[5]
M. Schäl	Universität Bonn	Numeraire portfolio under transaction costs	in progress

Furthermore, there are ongoing discussions with Prof V. Krishnamurthy, UBC, Vancouver, on problems of parameter estimation in Markov switching models which may lead to a cooperation.

Guests

From December 8 to December 12 Prof A. Irle, University of Kiel, stayed at RICAM for joint work. He gave a talk in the RICAM Kolloquium on Optimal Stopping Problems in Mathematical Finance

Participation at conferences

1. Stochastik Tage 2004, Karlsruhe, Germany, March 23-26
   Talk: Portfolio Optimization under Transaction Costs in the CRR model,March 23
2. PIMS-MITACS Minicourse in Mathematical Finance, June 14-18 (cf. visits, 3.)
   Talk: Portfolio Optimization under Transaction Costs in the CRR model, June 16
3. Stochastic Finance 2004, Lisbon, Portugal, September 26-30
   Talk: Good Portfolio Strategies under Transactions Costs: A renewal Theoretic Approach, September 27

Publications

Appeared

1. U. G. Haussmann and J. Sass (2004): Optimal terminal wealth under partial information for HMM stock returns. In: G. Yin and Q. Zhang (eds.): Mathematics of Finance: Proceedings of an AMS-IMS-SIAM Summer Conference June 22-26, 2003, Utah, AMS Contemporary Mathematics 351, 171-185.
2. J. Sass: Portfolio optimization under transaction costs in the CRR model. To appear in: Mathematical Methods of Operations Research.
3. J. Sass, U.G. Haussmann (2004): Optimizing the terminal wealth under partial information: The drift process as a continuous time Markov chain. Finance and Stochastics 8, 553–578.
4. J. Sass and U.G. Haussmann (2004): Portfolio optimization under partial information: Stochastic volatility in a hidden Markov model. In: Ahr, D., Fahrion, R., Oswald, M., Reinelt, G. (eds.): Operations Research Proceedings 2003, Springer, Berlin, 387-394.

Submitted

5. A. Irle, J. Sass: Good portfolio strategies under transaction costs: A renewal theoretic approach.

Dr. Klaus Scheicher

Introduction

Dr. Scheicher joined RICAM in September 2003 coming from Johannes Kepler University. His main research area is number theory, especially number systems.

Number systems are intimately connected with the construction of pseudo and quasi random numbers. Both of these concepts yield applications for high dimensional numerical integration problems. Especially, it turned out that quasi random numbers can be used to evaluate financial derivatives. Pseudo random numbers have applications in mathematical finance as well as cryptology.

Scientific Achievements 2004

The main topic of research was the analysis of canonical number systems in polynomial rings over the integers and beta-expansions of real numbers. Both concepts are strongly connected with special dynamical systems, so called shift radix systems (for short SRS) over lattices.

It is an important problem for number systems to determine the set of numbers which can be represented. For example, in decimal base, negative integers do not admit finite representations.

In general, the classification of systems with this property is a complicated problem and, at the moment, a complete solution of this problem seems to be out of reach. However, for special cases, several partial results have been achieved.

In [2], Dr. Scheicher considered an analogue of so called beta-expansions in the field of formal Laurent series over a finite field. There are striking analogies of these expansions to the classical beta-expansions defined in the real numbers. Results corresponding to classical theorems as well as open problems have been proved. Especially, the above mentioned finiteness problem could be completely solved in this case. In contrast, such a result is hardly expected in the classical case. Furthermore, the counterparts of a theorem of K. Schmidt on the expansions of rational elements by Pisot numbers and a conjecture on expansions by Salem numbers could be established.

All these problems have been solved in the notion of SRS. The analogues of SRS over formal Laurent series can be considered as special kinds of linear feed back shift registers which are widely used for the generation pseudo random number sequences. Therefore, the new algorithm provides a promising candidate as random number generator. This would yield several applications for Monte Carlo Methods in mathematical finance. Since the underlying dynamical system has good mixing properties, there probably exist also applications in cryptology.

In [3], the cooperation with Prof. S. Akiyama from Nigata/Japan has been continued. In contrast to the above mentioned paper [1], SRS in algebraic number fields have been considered. In [3], a symmetric variant of the SRS concept has been studied. It turned out to be easier than the original version, and all SRS corresponding to finite expansions could be classified in dimension two. However, symmetric SRS give rise to changes in the set of digits of the corresponding number systems. They are the symmetric canonical number systems and symmetric beta-expansions.

The cooperation together with Dr. W. Steiner from T.U. Vienna has been continued. The main object of research is to study certain low discrepancy sequences (for short LDS) which are strongly connected with beta-expansions and Pisot numbers. These sequences have been defined by S. Ninomiya from Tokyo and successfully applied for numerical integration problems. It is the aim of this project to study the so called bounded remainder set of this sequence. This concept was firstly studied by H. Kesten and W.M. Schmidt.

A further cooperation is actually running with Prof. A. Pethö from Debrecen and Prof. J.M. Thuswaldner from Leoben. This project will focus on so called matrix radix systems which can be viewed as a generalization of the SRS setting.

Scientific Visits and Talks

1. 28. Feb. M.U. Leoben.
2. 20. Sept.-26.Sept. Univ. Debrecen, Department of Mathematics.

Scientific Cooperations

Internal Cooperations

Name	Institution	Topic	Publ.
G. Pirsic	RICAM	LDS	[4]

External Cooperations

Name	Institution	Topic	Publ.
S. Akiyama	Univ. Niigata/Japan	NS	[3]
L. L. Cristea	Univ. Linz	LDS	[4]

F. Pillichshammer	Univ. Linz	LDS	[4]
W.Steiner	TU. Vienna	NS, LDS	In progress
J.M.Thuswaldner	MU. Leoben	NS	[1]
A.Pethö	Univ. Debrecen	NS	In progress

Participation at conferences

1. 27 Sept - 1 Oct, Number Theoretic Algorithms and Related Topics 2004, Strobl, Talk: “Two new kinds of digit systems”.
2. 4 Oct - 5 Oct, Workshop on Complexity and Discrepancy, Linz.

Publications

Appeared

1. K. Scheicher and J. M. Thuswaldner, On the Characterization of Canonical Number Systems. Osaka J. Math., 41:1--25, 2004.

Submitted

2. K. Scheicher beta-expansions in algebraic function fields over finite fields. Submitted to Acta Arithmetica.
3. S. Akiyama and K. Scheicher Symmetric shift radix systems and finite expansions. Submitted to Quarterly Journal of Mathematics.
4. L. L. Cristea, G. Pirsic, F. Pillichshammer and K. Scheicher, Discrepancy estimates for point sets on the s-dimensional Sierpinski carpet, accepted by Publicationes Mathematicae.

Univ.-Doz. Dr. Arne Winterhof

Introduction

Dr Winterhof joint RICAM in August 2003 coming from National University of Singapore. His main research area is the theory of finite fields including applications in cryptography, coding theory, and pseudorandom number generation including application in mathematical finance. In his field of interest are also related areas as combinatorics, (computer) algebra, (algorithmic) number theory, and theoretical computer science.
His most important achievements are the development of new exponential sum techniques, bounds on the number of solutions of equations over finite fields, and their applications in cryptography, pseudorandom number generation, coding theory, and number theory.

Scientific Achievements 2004

Dr Winterhof got the Edmund and Rosa Hlawka price of the Austrian Academy of Sciences for his achievements in discrete mathematics and theoretical computer science. He has been leading the FWF project S8313 (Number theoretic methods in cryptography and pseudorandom number generation, two employees: Dr W. Meidl and Mag N. Brandstätter) and supervised the diploma thesis of N Brandstätter. He organized two mini-workshops in international conferences on pseudorandom number generation (Number theoretic algorithms and applications (Strobl), Finite fields and applications (Oberwolfach)).

In 2004 Dr Winterhof's research focused on pseudorandom number generation including its applications in mathematical finance, cryptography and character sums with applications to coding theory and analysis of algorithm.

1. Nonlinear pseudorandom number generation
Nonlinear methods for the generation of pseudorandom numbers are attractive alternatives to linear methods. A 'good' lattice structure is a desirable feature of pseudorandom numbers for Monte-Carlo simulations (e.g. for applications in financial mathematics) and a low linear complexity profile is disastrous for applications in cryptography. In [2] Dr Winterhof and Dr Dorfer (TU Vienna) transferred several known lower bounds on the linear complexity of periodic nonlinear sequences to quality results on the lattice structure. The same authors and Dr Meidl (National University of Singapore, now RICAM) analyzed the lattice structure on average over all finite sequences over a finite field in [1].
Initially, a nonlinear pseudorandom number generator was defined as a recurrence sequence over a finite field. In the series of papers [6,7,9,14,19] Dr Winterhof, Dr Meidl and Prof. Niederreiter (National University of Singapore) introduced new explicit nonlinear generators and studied their linear complexity and distribution.

2. Cryptographic functions and sequences
The successful research on theoretical results that support the assumption that certain cryptosystems are secure have been continued. In the series of papers [3,4,13,16,17] Dr Winterhof, Mag Brandstätter (PhD-student at RICAM) and Dr Kiltz (University of California, San Diego) proved several lower bounds on functions related to cryptosystems based on the discrete logarithm problem. The papers [5,15,18] deal with complexity measures (linear complexity, autocorrelation) of sequences suitable for stream ciphers.
In [11,12,20] Prof Shparlinski (Macquarie University Sydney) 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 and the predictability, i.e. unsuitability in cryptography, of some nonlinear pseudorandom number generators.

3. Multiplicative character sums and applications
In [8] Dr Winterhof and Prof Niederreiter proved bounds on multiplicative character sums of nonlinear pseudorandom numbers in parts of the period. These results yield information on the distribution of primitive elements in finite fields and provide a first step for the derandomization of search algorithms for primitive elements.
Character sum techniques were also used in [10] to prove the existence of special permutations of finite fields, called orthomorphisms. Orthomorphisms are important for the design of character check codes (e.g. ISBN, International bank account number (IBAN), IC-No.).

Teaching

Winter term 03/04: Coding theory (University of Vienna)
Winter term 04/05: Pseudorandom number generation (Kepler University Linz)

Scientific Visits and Invited Talks

1. National University of Singapore (3 weeks): Hidden number problem and applications.
2. Technical University of Vienna: Stream ciphers and number theory: Sidelnikov sequences.
3. University of Salzburg: Linear complexity of Sidelnikov sequences.

Scientific Cooperation

Internal Cooperation with

Brandstätter:	Cryptography
Larcher:	Pseudorandom number generation
Meidl:	Cryptography, Pseudorandom number generation

External Cooperation with

C. Adelmann (Braunschweig)	Integer factoring problem
H. Aly (Kairo)	LUC cryptosystem
G. Dorfer (TU Vienna)	Lattice test and linear complexity
E. ElMahassni (Sydney)	Pseudorandom number generation
M. Garaev (Mexico)	Sidelnikov sequences
E. Kiltz (California)	Discrete logarithm problem
T. Lange (Copenhagen)	Boolean functions and discrete logarithm
F. Luca	Sidelnikov sequences
H. Niederreiter	Character sums, Pseudorandom number generation
I. Shparlinski	Cryptography
A. Topuzoglu	Higher order pseudorandom number generators

Participation at / Organization of Conferences and Contributed Talks

1. Public Key Cryptography PKC'04, Singapore: A nonuniform algorithm for the hidden number problem in subgroups.
2. Monte Carlo and Quasi Monte Carlo Methods MC2QMC'04, Juan-les-Pins: On the distribution of some new explicit inversive pseudorandom numbers and vectors.
3. Workshop on number theoretic algorithms and applications, Strobl, co-chair.
4. Sequences and Their Applications SETA'04, Seoul: On the distribution of some new explicit nonlinear congruential pseudorandom numbers.
5. Finite Fields and Applications, Oberwolfach: Linear complexity of Sidelnikov sequences.

Publications

Appeared

1. G. Dorfer, W. Meidl and A. Winterhof, Counting functions and expected values for the lattice profile at n, Finite Fields and Their Applications 10 (2004), 636—652.
2. G. Dorfer and A. Winterhof, Lattice structure of nonlinear pseudorandom number generators in parts of the period, Proceedings MCQMC 2002, Springer, 2004, 199—211.
3. E. Kiltz and A. Winterhof, Lower bounds on weight and degree of bivariate polynomials related to the Diffie-Hellman mapping, Bulletin of the Australian Mathematical Society 69 (2004), 305—315.
4. E. Kiltz and A. Winterhof, Polynomial interpolation of cryptographic functions related to Diffie-Hellman and discrete logarithm problem, Discrete Applied Mathematics, to appear.
5. W. Meidl and A. Winterhof, On the autocorrelation of cyclotomic generators, Proceedings Fq7, Lecture Notes in Computer Science 2948 (2004), 1—11.
6. W. Meidl and A. Winterhof, On the linear complexity profile of some new explicit inversive pseudorandom number generators, Journal of Complexity 20 (2004), 350—355.
7. W. Meidl and A. Winterhof, On the joint linear complexity profile of explicit inversive multisequences, Journal of Complexity, to appear.
8. H. Niederreiter and A. Winterhof, Multiplicative character sums of nonlinear recurring sequences, Acta Arithmetica 111(2004), 299—305.

9. H. Niederreiter and A. Winterhof, On the distribution of some new explicit nonlinear congruential pseudorandom numbers, (extended abstract), SETA'04 Proceedings, 94--98, Seoul, 2004.
10. H. Niederreiter and A. Winterhof, Cyclotomic R-orthomorphisms of finite fields, Discrete Mathematics, to appear.
11. I. Shparlinski and A. Winterhof, A nonuniform algorithm for the hidden number problem in subgroups and cryptographic applications, Proceedings PKC 2004, Lecture Notes in Computer Sciences 2947 (2004), 416—424.
12. I. Shparlinski and A. Winterhof, Noisy interpolation of sparse polynomials in finite fields, Applicable Algebra in Engineering, Communication and Computing, to appear.
13. A. Winterhof, A note on the linear complexity profile of the discrete logarithm in finite fields, Progress in Computer Science and Applied Logic 23 (2004), 359—367.
14. A. Winterhof, On the distribution of some new explicit inversive pseudorandom numbers and vectors, Proceedings MCQM2C, to appear.

Submitted

15. N. Brandstätter and A. Winterhof, Some notes on the two-prime generator of order 2.
16. N. Brandstätter and A. Winterhof, Approximation of the discrete logarithm in finite fields of even characteristic by real polynomials.
17. N. Brandstätter, Tanja Lange and A. Winterhof, Interpolation of the discrete logarithm in finite fields of characteristic two by Boolean functions.
18. W. Meidl and A. Winterhof, Some notes on the linear complexity of Sidelnikov-Lempel-Cohn-Eastman sequences, submitted.
19. H. Niederreiter and A. Winterhof, On the distribution of some new explicit nonlinear congruential pseudorandom numbers.
20. I. Shparlinski and A. Winterhof, Hidden number problem in small subgroups.

Mag. Nina Brandstätter

Introduction

Mag Brandstätter joint RICAM in April 2004, immediately after finishing her diploma at University of Vienna. Her main research interests are character sums and cryptographic applications.

Scientific Achievements 2004

Mag Brandstätter finished her diploma thesis [1] on complexity lower bounds of real functions approximating the discrete logarithm. Such results support the assumption that cryptosystems based on the discrete logarithm are secure. [3] is an improved result from her diploma thesis. A similar idea was used to extend results on the complexity of Boolean functions representing the discrete logarithm in finite fields of odd characteristic to characteristic two. She started writing her PhD-thesis on cryptographic suitable sequences. Results on a particular interesting sequence, the two-prime generator, were obtained in [2].

Participation at Conferences and Talks

Workshop on number theoretic algorithms and applications, Strobl.
Workshop on cryptography, Oberwolfach: Some notes on the two prime generator of order 2.

Publications

1. N. Brandstätter, diploma thesis, Approximation of the discrete logarithm by real functions,

University of Vienna, 2004.
2. N. Brandstätter and A. Winterhof, Some notes on the two-prime generator of order 2.
3. N. Brandstätter and A. Winterhof, Approximation of the discrete logarithm in finite fields of even characteristic by real polynomials.
4. N. Brandstätter, Tanja Lange and A. Winterhof, Interpolation of the discrete logarithm in finite fields of characteristic two by Boolean functions.

Dr. Wilfried Meidl

Introduction

Dr Meidl joint RICAM in September 2004 coming from National University of Singapore. His main research areas are cryptography, pseudorandom sequences and permutable functions.

Scientific Achievements 2004

For the papers [1,6,7,8,10] see Dr Winterhof.
The k-error linear complexity of periodic binary sequences is defined to be the smallest linear complexity that can be obtained by changing k or fewer elements of the sequence per period. For the period length p^n in [2,3] a relationship between the linear complexity and the minimum value k for which the k-error linear complexity is strictly less than the linear complexity was deduced. [4] focussed on the case of 2^n-periodic binary sequences. An exact formula for the expected 1-error linear complexity was given and old bounds for the expected k-error linear complexity, k>1, were improved.
Let S1, S2,..., St be t N-periodic sequences over a finite field Fq. The joint linear complexity L(S1, S2,…, St) is the least order of a linear recurrence relation that S1, S2,…, St satisfy simultaneously. Since the Fq-linear spaces $(Fq)^t$ and Fq^t are isomorphic, a multisequence can also be identified with a single sequence **S** having its terms in the extension field Fq^t. The linear complexity L(**S**) of **S**, i.e. the length of the shortest recurrence relation with coefficients in Fq^t that **S** satisfies, may be significantly smaller than L(S1, S2,…, St). In [5] relations between L(**S**) and L(S1, S2,…, St) were investigated.
The linear complexity profile and the lattice profile provide information on the local randomness of a sequence.
In [9] relationships between linear complexity profile and lattice profile were used to completely describe the lattice profile of a sequence over a finite field in terms of the continued fraction expansion of its generating function.

Teaching

Winter term 03/04: Linear algebra (National University of Singapore)
Summer term 04: Elementary coding theory (National University of Singapore)

Participation at conferences and talks

1. Workshop on number theoretic algorithms and applications: On the linear complexity profile of explicit inversive pseudorandom number generators.
2. Sequences and Their Applications SETA'04, Seoul: Discrete Fourier transform, joint linear complexity and generalized joint linear complexity of multisequences.

Publications

Appeared

- G. Dorfer, W. Meidl and A. Winterhof, Counting functions and expected values for the lattice profile at n, Finite Fields and Their Applications 10 (2004), 636—652.
- W. Meidl, How many bits have to be changed to decrease the linear complexity? Des. Codes Cryptogr. 33 (2004), 109-122.
- W. Meidl, Linear complexity and k-error linear complexity for p^n-periodic sequences, Coding, Cryptography and Combinatorics, 227-235, Progr. Comput. Sci. Appl. Logic, 23, Birkhäuser, Basel 2004.
- W. Meidl, On the stability of 2^n-periodic binary sequences, IEEE Trans. Inform Theory, to appear.
- W. Meidl, Discrete Fourier Transform, Joint Linear Complexity and Generalized Joint Linear Complexity of Multisequences, Proceedings SETA´04, Lecture Notes in Comput. Sci, to appear.
- W. Meidl and A. Winterhof, On the autocorrelation of cyclotomic generators, Proceedings Fq7, Lecture Notes in Computer Sciences 2948 (2004), 1—11.
- W. Meidl and A. Winterhof, On the linear complexity profile of some new explicit inversive pseudorandom number generators, Journal of Complexity 20 (2004), 350—355.
- W. Meidl and A. Winterhof, On the joint linear complexity profile of explicit inversive multisequences, Journal of Complexity, to appear.

Submitted

- W. Meidl, Continued fraction for formal Laurent series and the lattice structure of sequences.
- W. Meidl and A. Winterhof, Some notes on the linear complexity of Sidelnikov-Lempel-Cohn-Eastman sequences.

Group "Analysis of Partial Differential Equations"

Group Leaders:
o.Univ.-Prof. Dr. Peter Markowich
ao.Univ.-Prof. Dr. Christian Schmeiser

Researchers funded via ÖAW/Upper Austrian government funds:
Dr. Shun-Yin Chu
Dr. Yasmin Dolak
Dr. Norayr Matevosyan

Introduction

After A. Leitao left RICAM early in 2004, two new group members, S.-Y. Chu and Y. Dolak have been hired, who obtained their PhD degrees in Hongkong and Vienna, respectively. S.-Y. Chu specializes in the analysis of nonlinear partial differential equations with an emphasis on problems from fluid mechanics. Y. Dolak is mainly interested in Mathematical Biology.

Both new group members continue to work on subjects connected to their PhD theses but have also been involved in new cooperation projects with other RICAM members or members of the Univ. of Linz.

In particular, Mathematical Biology will become a common theme for several internal and external cooperations with 'hot' biological problems such as cell motility, ionic channels, and parameter identification in chemotaxis models.

In the following, the activities of the group members employed by RICAM are described in individual sections.

Dr. Shun-Yin Chu

Introduction

Some different subjects of his research works are considered. Starting from the middle of 2004 he mainly worked on oscillations, asymptotic structures and movements of spikes and bubbles of mathematical biology. In particular, he considered the non self-similar solutions of anisotropic curve shortening flow in which governed by fourth order partial differential equation in one dimension. He analyzed the solutions by ways of mathematical analysis. This work is cooperated with M. Burger in Industrial Mathematics Institute, JKU, and some colleagues in this group as P.A. Markowich and C. Schmeiser.
The second subject of his work is the formation of blowup solution of Keller-Segal models in any dimensional problems. One cannot deal with the solution, especially in higher dimensional case, because upon the formation of singularities it destroys our understanding mathematical knowledge even in weak formulation of the solution, and there is no symmetric entropy that can be realized to the solution.
Another subject worked before he came to RICAM is the regularity criterion of Prandtl's system in which governed by the incompressible fluid near on the boundary obtained by vanishing viscosity limit of incompressible Navier-Stokes equations.

Scientific Achievements 2004

Research 2004 before RICAM
He worked on weak solutions of two-dimensional strongly degenerate parabolic equation. Starting from the weak solution in the class of bounded variation, the Holder-continuous regularity of the solution can be hold from that the weak solution is of VMO.

Research 2004 at RICAM
He focused on the stability problems of one-dimensional Cahn-Hilliard equation, and properties of anisotropic curve flows. From the basic stability theory, one knows that this problem has loss of stability on one-dimensional approach. By multiple scale method, a system of partial differential equations needed to be solved and some compatibility criterions of the solutions are involved.

Scientific Visits and Talks

Wolfgang Pauli Institute for Applied Mathematics, University of Vienna, Vienna, 27-28 October
Talk: Some progress on Prandtl's system

Institute of Mathematical Sciences, The Chinese University of Hong Kong, Hong Kong, 7 December 2004 - 5 January 2005
Talk: To be announced

Scientific Cooperations

Internal Cooperations with
1. Prof. Dr. P. Markowich, Analysis of Partial Differential Equations
2. Prof. Dr. Christian Schmeiser, Analysis of Partial Differential Equations

External Cooperations with
3. Dr. M. Burger, Industrial Mathematics Institute
4. Prof. Zhouping Xin, The Institute of Mathematical Sciences, The Chinese University of Hong Kong, Hong Kong

Participation at conferences

The Third International Congress of Chinese Mathematicians, Hong Kong, 17–22 December, 2004.

Dr. Yasmin Dolak

Introduction

Yasmin Dolak's research area is the mathematical modeling of chemotaxis and cell movement. During her PhD (which she finished in November 2004), she worked on kinetic and macroscopic models for chemotaxis and the connection between the two. In particular, she was interested in cases where random motion of cells only plays a minor role, which leads to advection-dominated models for cell movement.

Scientific Achievements 2004

Research 2004 before RICAM

In 2004, she focused mainly on the analysis 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. Of special interest is the case of small diffusivity - a similar model has been derived previously by C. Schmeiser and Y. Dolak as a macroscopic limit of a kinetic equation. Convergence of solutions as the diffusion coefficient goes to zero was investigated as well as the asymptotic behavior of the system. For the latter, a system of ordinary differential equations describing the meta-stable dynamics was derived, and an efficient numerical algorithm to compute solutions over long time periods was developed.
Another field of research was the mathematical modeling of cell movement on the scale of individual cells. The aim is to develop microscopic models taking into account the internal dynamics of the cytoskeleton and then, by a limiting procedure, derive macroscopic models that will be easier to handle both analytically and numerically. First simple models have been derived together with C. Schmeiser and Dietmar Ölz from the TU Vienna.

Research 2004 at RICAM

At RICAM, the project on the modeling of cell movement together with C. Schmeiser and D. Ölz was continued. Cooperation with Prof. Vic Small, the leader of an experimental group at the Institute of Molecular Biotechnology was started. Y. Dolak was also one of the organizers of an international workshop on the "Modelling of Cell Motility and Angiogenesis" that took place from Nov. 8-11 at the Wolfgang Pauli Institute in Vienna.
Additionally, a new project was started together with Philipp Kügler from the Johannes Kepler University of Linz. The aim is to estimate parameters describing cellular behavior using methods from inverse problems.

Scientific Visits and Talks

February 2004: Talk at the Workshop on Mathematical Biology and Evolutionary Dynamics at the IMPA in Rio de Janeiro, Brazil ("An advection-dominated model for chemotaxis")

March 2004: Stay at the Université des Sciences et Technologies de Lille, France

September 2004: Participation in the Summer School on Cell Adhesion and Migration at the University of Nottingham, UK

Scientific Cooperations

External Cooperations with
1. Philipp Kügler, Johannes Kepler University, Linz

2. Dietmar Ölz, Vienna University of Technology

3. Vic Small, IMBA, Austrian Academy of Sciences

Publications

Appeared
Y. Dolak: Advection-dominated Models for Chemotaxis. PhD thesis, Vienna University of Technology 2004

Submitted
Y. Dolak and C. Schmeiser: The Keller-Segel model with small diffusivity.

Dr. Norayr Matevosyan

Introduction

Over the last 5 years Dr Matevosyan has been working mainly with Free Boundary problems, in particular with Free Boundary problems (in future F.B.p.) with contact points. Follows a list of problems he has already worked with: superconductivity phenomena in F.B.p-s with contact points, parabolic and fully nonlinear F.B.p-s with contact points, obstacle like two-phase F.B.p-s. New interests include The Level Sets Methods for Obstacle problems.

A secondary area of research of Dr Matevosyan is uniqueness theorems for harmonic functions. His research in this area started 6 years ago. As a result a paper on this subject have been published.

Scientific Achievements 2004

In 2004 Dr Matevosyan focused on the folowing problems: F.B.p-s with contact points for superconductivity problems, tangential touch between free and fixed boundaries in obstacle like two-phase problems (colaboration with J. Andersson and H. Mikayelyan),
global solutions and parabolically tangential touch of the free and fixed boundaries. New research interests that have not been mentioned in the last years report include regularity of the free boundary in obstacle like problems (colaboration with A. Hakobyan), the level sets methods for obstacle problems (cooperation with M. Burger).

In the report from year 2003 the following scientific plans for year 2004 were formulated:

1. The research of F.B.p-s for superconductivity phenomena.

2. Studies of obstacle like two-phase F.B.p-s with contact points.

3. Research on F.B.p-s with parabolic fully nonlinear operators.

   The first two points have been realized in the following publications. The third goal has been postponed to year 2005 due to expanded research interests.

Scientific Visits and Talks

Prof. Dr. Henrik Shahgholian
Department of Mathematics, Royal Institute of Technology,
Stockholm, May 2004

Dr. Aram Hakobyan
Faculty of Mathematics, Yerevan State University
Yerevan, October 2004

Summer School
Recent Trends in Partial Differential Equations, July 12-16th 2004 Santander, Spain.

Workshop
Technologial Applications of PDEs, February 2-9 2004 Florianopolis, Brazil.
Global and Geometric Aspects in Nonlinear PDE, October 6 -12, 2004 Yerevan, Armenia.

Scientific Cooperations

Name	Institution	Topic	Publications
Internal Cooperations with			
P. Markowich	Vienna University, RICAM	Free Boundaries	1
External Cooperations with			
N. Arakelian	Armenian Acad. of Sci.	Harmonic functions	1
J. Andersson	KTH (Stockholm)	Free Boundaries	1
H. Mikayelyan	Leipzig University	Free Boundaries	1
A. Hakobyan	Yerevan State University	Free Boundaries	in progress
M. Burger	University of Linz, INDMATH	Level Sets Methods	in progress

Participation at conferences

Summer Schools
Recent Trends in Partial Differential Equations, July 12-16th 2004 Santander, Spain.

Workshops
Technologial Applications of PDEs, February 2-9 2004 Florianopolis, Brazil.
Global and Geometric Aspects in Nonlinear PDE, October 6 -12, 2004 Yerevan, Armenia.

Publications

Submitted

- N. Matevosyan: Tangential touch between free and fixed boundaries in a problem from superconductivity, to appear in Communications in Partial Differential Equations.

- N. Matevosyan, J. Andersson, H. Mikayelyan, On the tangential touch between the free and the fixed boundaries for the two-phase obstacle-like problem, to appear in Arkiv för Matematik.

Prof. Dr. Christian Schmeiser

Introduction

The employment of C. Schmeiser at RICAM ended Sept. 30, 2004. However, C. Schmeiser will remain group leader together with P. Markowich

In 2004, ongoing research work on chemotaxis models for cell populations, on quantitative long time convergence results for kinetic models, and on semiconductor models was continued and/or completed. New research directions include the analysis of travelling wave solutions for kinetic transport equations, dimension reduction asymptotics for nonlinear Schrödinger equations, and numerical methods for stochastic differential equations.

An important new research field is modelling of the cytoskeleton for the description of cell movement. In 2004, this activity involved the organization of a workshop at the Wolfgang Pauli Institute Vienna (together with Y. Dolak), the production of a joint research proposal with the experimental biology group of Vic Small (IMBA, Vienna), as well as first modelling attempts together with Y. Dolak and a PhD student from Vienna.

Together with Shun-Yin Chu, a study of oscillatory solutions of the Cahn-Hilliard equation has been started.

Scientific Achievements 2004

Kinetic transport models for chemotaxis have been studied in the publications 3 and 12, below. Publ. 8 is concerned with the modelling of in vitro experiments of the chemotactic motion of leukocytes, which have been reported in the biological literature. The long time behaviour of a version of the classical Keller-Segel model for chemotaxis is studied in 11.

A recent approach by Desvillettes and Villani for quantitative long time convergence analyses of kinetic transport models has been applied to a general class of linear models and to a special nonlinear model in 1 and 4, respectively. A very challenging nonlinear model is considerd in 5. The Desvillettes-Villani approach is carried out for a linearized version in 16.

Other research directions and corresponding publications are:
Semiconductor models and macroscopic limits: 6, 13, 15, 18
Kinetic profiles for shock waves: 7, 17
Dimension reduction in NLS: 9, 10
Cubature on Wiener space: 14
Anisotropic Sobolev imbeddings: 19

Scientific Visits and Talks

March 22 – April 2 and May 17-28: visiting professor, Univ. de Lille 1
April 14-17: A-HYKE2 Conf., Paris (invited talk)
July 14-16: Workshop on 'Advances in Modelling and Simulation of Semiconductor Devices, Berlin (invited talk)
August 21 – Sept. 4: Workshop on 'Kinetic Models for Multiscale Problems, Banff
Sept. 13-17: HYP2004 Conf., Osaka (invited talk)
Sept. 19-23: MAFPD6 Conf., Kyoto (invited talk)

Scientific Cooperations

Internal Cooperations with
Shun-Yin Chu: oscillatory solutions of the Cahn-Hilliard equation
Yasmin Dolak: modelling of the cytoskeleton for the description of cell movement
P. Markowich: nonlinear Schrödinger equations, macroscopic limits of kinetic models, chemotaxis

External Cooperations with
L. Neumann, K. Fellner, D. Ölz, A. Soreff, R.M. Weishäupl, V. Miljanovic, J. Haskovec (PhD students at the WK Differential Equations, Vienna): different subjects
C. Cuesta (PostDoc, TU Wien): travelling waves in kinetic models
B. Perthame (ENS, Paris): chemotaxis

N. BenAbdallah, P. Degond, F. Mehats (MIP, Toulouse): semiconductors, nonlinear Schrödinger equations
J. Dolbeault (Dauphine, Paris): macroscopic limits of kinetic models
J. Teichmann (TU Wien): cubature methods for stochastic differential equations

Publications

Appeared

1. L. Neumann, C. Schmeiser, Convergence to global equilibrium for a kinetic model for fermions, to appear in SIAM J. Math. Anal.

2. K. Fellner, C. Schmeiser, Burgers-Poisson: a nonlinear dispersive model equation, SIAM J. Appl. Math. 64 (2004), pp. 1509-1525.

3. F. Chalub, P. Markowich, B. Perthame, C. Schmeiser, Kinetic models for chemotaxis and their drift-diffusion limits, Monatsh. Math. 142 (2004), pp. 123-141.

4. K. Fellner, L. Neumann, C. Schmeiser, Convergence to global equilibrium for spatially inhomogeneous kinetic models of non-micro-reversible processes, Monatsh. Math. 141 (2004), pp. 289-299.

5. K. Fellner, F. Poupaud, C. Schmeiser, Existence and convergence to equilibrium of a kinetic model for cometary flows, J. Stat. Phys. 114 (2004), pp. 1481-1499.

6. P. Degond, C.D. Levermore, C. Schmeiser, A note on the energy-transport limit of the semiconductor Boltzmann equation, in Transport in Transition Regimes, N. Ben Abdallah, A. Arnold, P. Degond, I. Gamba, R. Glassey, C.D. Levermore, and C. Ringhofer (eds.), IMA Vol. In Math. And its Appl. 135, Springer-Verlag, 2004.

Submitted

7. C. Cuesta, C. Schmeiser, Kinetic profiles for shock waves of scalar conservation laws.

8. D. Ölz, C. Schmeiser, A. Soreff, Multistep navigation of leukocytes: a stochastic model with memory effects.

9. W. Bao, P. Markowich, C. Schmeiser, R.M. Weishäupl, On the Gross-Pitaevskii equation with strongly anisotropic confinement: formal asymptotics and numerical experiments.

10. N. BenAbdallah, F. Mehats, C. Schmeiser, R.M. Weishäupl, The nonlinear Schrödinger equation with a strongly anisotropic harmonic potential.

11. Y. Dolak, C. Schmeiser, The Keller-Segel model with small diffusivity.

12. Y. Dolak, C. Schmeiser, Kinetic models for chemotaxis: hydrodynamic limits and the back-of-the-wave problem.

13. J. Dolbeault, P. Markowich, D. Ölz, C. Schmeiser, Nonlinear diffusion limits of kinetic equations with relaxation type collision kernels.

14. C. Schmeiser, A. Soreff, J. Teichmann, Cubature algorithms on Wiener space.

15. V. Miljanovic, C. Schmeiser, On the Shockley-Read-Hall model for semiconductors.

16. K. Fellner, V. Miljanovic, C. Schmeiser, Convergence to equilibrium for the linearized cometary flow equation.

17. C. Cuesta, C. Schmeiser, Weak shocks for a one-dimensional BGK kinetic model for conservation laws.

18. J. Haskovec, C. Schmeiser, Transport in semiconductors at saturated velocities.

19. J. Haskovec, C. Schmeiser, Anisotropic generalizations of the Sobolev and Morrey imbedding theorems

Group "Optimization and Optimal Control"

Group Leader:
O.Univ.-Prof. DI. Dr. Karl Kunisch

Researchers funded via ÖAW/Upper Austrian government funds:
Dr. Roland Griesse
Dr. Boris Vexler

Introduction

The work of the group started with Dr. Griesse joining RICAM on July 15, 04. Later, on October 1, 04, Dr. Vexler started his appointment. Thus this report covers the work of only half a year. The overall scope of this small group is the advance of numerical analysis and computational techniques for optimal control problems with partial differential equations as constraints. The solutions of such problems are characterized by large coupled systems of partial dfferential equations. Their efficient numerical solution still presents a significant challenge, especially if the underlying partial differential equations are complicated themselves and if the optimal control formulation contains contraints and the cost-functionals are highly non-linear. These features are typical for the problems which are studied in this group. Dr. Griesse took up research on optimal control of magnetohydrodynamical systems in addition to continuing his work on sensitivity analysis of optimal control problems. Dr. Vexler stared to investigate vortex reduction in non-stationary flows described by the Navier-Stokes equations. The delicate issue here is the adequate quantification of vorticity, which is still at the forefront of research also in the fluids mechanics community. In addition he continues work on adaptivity for solving discretized optimality systems for infinite – dimensional systems. – Thus one of the points which was announced as "Plans" in the annual report 2003, i.e. the numerical treatment of the HJB-equation arising in optimal control, was altered. The reasons are two-fold. First, the realization of the newest developments in the fluid-mechanics community regarding quantification of vorticity in the context of optimal control appear to be very exciting. Secondly there was a change in the decision concerning the appointment for the position which is now occupied by Dr. Vexler. - It is planned to turn to the numerical treatment of the HJB-equation at a later stage.

Scientific Cooperations

Cooperations which involve members of the group are described under their names below.

In addition joint work between the Financial Mathematics (Dr. Janecek) and the Optimization and Optimal Control group is planned in which recent results by Ito and Kunisch regarding the numerical analysis of parabolic variational inequalities should be applied to improve numerical methods to solve free boundary problems arising in problems of finance, e.g. to improve results on the shape of the trading regions arising in portfolio optimization under transaction costs. The key will be the development of semi-smooth Newton techniques which allow superlinearly convergent iterative algorithms.

Publications

[1] J.Halinger, T.Kozubek, K.Kunisch and G.Peichl:
An embedding domain approach for a class of 2-d shape optimization problems: mathematical analysis, J. Math. Anal. Appl., 290(2004), 665-685.

[2] M.Hinze and K. Kunisch:
Second order methods for boundary control of the instationary Navier-Stokes system,

Zeitschrift f\"ur Angewandte Mathematik und Mechanik, 84(2004), 171-187.

[3] M.Hintermüller, V.A.Kovtunenko and K.Kunisch:
The primal-dual active set method for a crack problem with non-penetration, IMA Journal of Applied Mathematics, 69(2004), 1-26.

[4] M.Hintermüller and K.Kunisch:
Total bounded variation regularization as bilaterally constrained optimization problems,
SIAM J. Appl. Mathematics 64(2004), 1311-1333.

[5] K.Kunisch, S.Volkwein and L.Xie:
HJB-POD based feedback design for the optimal control of evolution problems, SIAM J. on Applied Dynamical Systems, 4(2004), 701-722.

[6] K.Ito and K.Kunisch:
The primal-dual active set method for nonlinear optimal control problems with bilateral constraints, SIAM J. on Control and Optimization, 43(2004), 357-376.

[7] S.Chaabane, J.Ferchichi and K.Kunisch:
Differentiability of the L^1-tracking functional linked to the Robin inverse problem,
Inverse Problems 20(2004), 1083-1098.

[8] M.Hintermüller, K.Kunisch, Y.Spasov and S.Volkwein:
Dynamical system based optimal control of incompressible fluids, International Journal for Numerical Methods in Fluids 4(2004), 345-359.

Dr. Roland Griesse

Introduction

Dr. Roland Griesse conducts research in the field of optimal control of elliptic and parabolic partial differential equations. His interests extend from the mathematical analysis to the numerical solution of control- and state-constrained problems. One of Dr. Griesse's particular areas of expertise is the sensitivity analysis of optimal solutions under parameter perturbations. Apart from parameter studies, such variations in problem parameters may originate in data uncertainty or discretization errors.
In the recent past, Dr. Griesse has directed his attention towards the optimal control of systems of PDEs with complex phenomena which arise in chemical reactions with or without turbulence, crystal growth, and magnetohydrodynamical applications.

Scientific Achievements 2004

Research 2004 before RICAM

Before joining RICAM, Dr. Griesse held a postdoctoral position at the University of Graz. Together with Ao. Univ-Prof. Dr. Alfio Borzi, he worked on analytical and numerical aspects of the optimal control of so-called lambda-omega systems. These reaction-diffusion systems are considered representative for certain forms of chemical turbulence. Due to the turbulent behavior, solving the optimality system is numerically challenging. An efficient smoothing scheme for the nonlinear FAS multigrid method was proposed in publications [8] and [9].

In a second cooperation, Dr. Griesse and Ao. Univ-Prof. Dr. Stefan Volkwein prepared a series of papers [4] and [6] on the analysis and solution of control-constrained optimal boundary control problems for a 3D reaction-diffusion model. In particular, primal-dual active set and semismooth Newton methods were applied in order to efficiently handle the constraints.

Research 2004 at RICAM

After joining RICAM, Dr. Griesse started the investigation of optimal control problems for the magnetohydrodynamics (MHD) system. These equations describe the mutual interaction of electrically conducting fluids and magnetic fields. In particular, the Lorentz force acts as a contactless volume force in the fluid which renders the control by magnetic fields very attractive in metallurgical applications. For instance, magnetic fields are used to stir molten metals during solidification, to dampen their undesired convection-driven flow during casting, to filter out impurities, and to melt and even levitate metals. Together with the group leader Prof. Kunisch, Dr. Griesse is currently preparing a first paper concerning the mathematical aspects for optimal control of the stationary MHD system.
In addition, Dr. Griesse has written a joint paper with Michael Hintermüller and Michael Hinze on the parametric sensitivity analysis of optimal control problems for the Navier-Stokes equations [7], contributing to the presently ongoing investigation of stability properties of PDE-constrained optimal control problems.

Scientific Visits and Talks

08.03.04 – 10.03.04 “Parametric Sensitivities for Perturbed Reaction-Diffusion Optimal Control Problems”, University of Heidelberg, Germany (invited by Boris Vexler)

29.03.04 – 31.03.04 “Parametric Sensitivities for Perturbed Reaction-Diffusion Optimal Control Problems”, European Conference on Computational Optimization (EUCCO), Dresden, Germany

29.03.04 – 31.03.04 “A Nonlinear Primal-Dual Active Set Method for Optimal Boundary Control Problem of a 3D Reaction-Diffusion Model”, European Conference on Computational Optimization (EUCCO), Dresden, Germany

05.04.04. - 09.04.04 University of Technology Dresden, Germany (cooperations with Andrea Walther and Michael Hinze)

05.05.04 “Parametric Sensitivity Derivatives for Constrained Optimal Control problems”, University of Hamburg, Germany

01.06.04 – 04.06.04 “Parametric Sensitivity Derivatives of Perturbed Optimal Control Problems”, University of Technology Chemnitz, Germany (invited by Arnd Rösch)

22.06.04 – 01.07.04 “Parametric Sensitivity Analysis for a Perturbed 3D Reaction-Diffusion Problem”, Workshop on Nonlinear Large Scale Optimization, Ettore Majorana Center for Scientific Culture, Erice, Italy

13.09.04 – 17.09.04 “Parametric Sensitivity Analysis for 3D Reaction-Diffusion Control Problems”, Annual Meeting of the DMV (German Mathematical Society), Heidelberg, Germany

29.11.04 “Parametric Sensitivity Analysis for 3D Reaction-Diffusion Control Problems”, University of Technology, Vienna, Austria (visit to Prof. Christian Schmeiser)

Scientific Cooperations

Internal Cooperations with

Prof. Dr. Karl Kunisch, Research Group "Optimization and Control"
Dr. Boris Vexler, Research Group "Optimization and Control"
Dr. Arnd Rösch, Research Group "Inverse Problems"
Prof. Dr. Ulrich Langer, Research Group "Computational Methods for Direct Field Problems"
Dr. Joachim Schöberl, Research Group "Computational Methods for Direct Field Problems"

External Cooperations with

Jun.-Prof. Dr. Andrea Walther, University of Technology, Dresden, Germany
Prof. Dr. Michael Hinze, University of Technology, Dresden, Germany
Ao. Univ.-Prof. Dr. Stefan Volkwein, University of Graz, Austria
Ao. Univ.-Prof. Dr. Alfio Borzi, University of Graz, Austria
Ao. Univ.-Prof. Dr. Michael Hintermüller, University of Graz, Austria

Participation at conferences

29.03.04 – 31.03.04 European Conference on Computational Optimization (EUCCO), Dresden, Germany

01.04.04 – 02.04.04 International Workshop on Flow Control by Tailored Magnetic Fields (FLOWCOMAG), Forschungszentrum Rossendorf, Germany

22.06.04 – 01.07.04 Workshop on Nonlinear Large Scale Optimization, Ettore Majorana Center for Scientific Culture, Erice, Italy

Publications

Appeared

[1] R. Griesse
Parametric Sensitivity Analysis in Optimal Control of a Reaction-Diffusion System – Part I: Solution Differentiability
Numerical Functional Analysis and Optimization 25(1-2), pp. 93-117, 2004.

[2] R. Griesse
Parametric Sensitivity Analysis in Optimal Control of a Reaction-Diffusion System – Part II: Practical Methods and Examples
Optimization Methods and Software 19(2), pp. 217-242, 2004.

[3] R. Griesse and A. Walther
Evaluating Gradients in Optimal Control – Continuous Adjoints Versus Automatic Differentiation
Journal of Optimization Theory and Applications 122(1), pp. 63-86, 2004.

[4] R. Griesse and S. Volkwein
A Semi-Smooth Newton Method for Optimal Boundary Control of a Nonlinear Reaction-Diffusion System
Proceedings of the Sixteenth International Symposium on Mathematical Theory of Networks and Systems (MTNS), Leuven, Belgium, July 5-9, 2004.

[5] R. Griesse and A. Walther

Using AD-Generated Derivatives in Optimal Control of an Industrial Robot
Progress in Industrial Mathematics at ECMI 2002, Volume 5, pp. 127-132, 2004.

Accepted

[6] 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, to appear.

[7] A. Borzi and R. Griesse
Experiences with a Multigrid Method for the Optimal Control of a Chemical Turbulence Model, International Journal for Numerical Methods in Fluids, to appear.

Submitted

[8] R. Griesse and M. Hintermüller and M. Hinze
Differential Stability of Control Constrained Optimal Control Problems for the Navier-Stokes Equations.

[9] A. Borzi and R. Griesse
Distributed Optimal Control of Lambda-Omega Systems.

Preprints

[10] R. Griesse
Lipschitz Stability of Solutions to Some State-Constrained Elliptic Optimal Control Problems, Report No. 297 (February 2004), Special Research Center F003 “Optimization and Control”, University of Graz and University of Technology, Graz.

[11] R. Griesse and S. Volkwein
A Semi-Smooth Newton Method for Optimal Boundary Control of a Nonlinear Reaction-Diffusion System, Report No. 316 (June 2004), Special Research Center F003 “Optimization and Control”, University of Graz and University of Technology, Graz.

[12] R. Griesse and M. Hintermüller and M. Hinze
Differential Stability of Control Constrained Optimal Control Problems for the Navier-Stokes Equations, RICAM Report No. 04-14 (October 2004).

Dr. Boris Vexler

Introduction

The research area of Dr. Vexler is the development of efficient numerical algorithms for solution of optimization problems governed by partial differential equations. An important aspect of his research is the development and implementation of algorithms for finding an efficient finite element discretization by generating a sequence of adaptively refined meshes. These algorithms are based on a posteriori error estimators derived for the error with respect to a quantity of physical interest. The developed methods are applied to the optimization problems in fluid dynamics as well as for the parameter identification in multidimensional reactive flows.

Scientific Achievements 2004

Research 2004 before RICAM (Numerical Analysis Group, University of Heidelberg)

In 2004, Dr. Vexler has finished his PhD. Thesis [1], where he has investigated adaptive finite element methods for parameter identification problems. He developed a posteriori error estimators for the discretization errors in general parameter identification problems, see [2]. For this paper he was awarded a 2nd prize at the Leslie Fox Prize Meeting. Complementary to the a posteriori error estimation, he has been working on a priori error analysis for optimization problems. In paper [8], the optimal order of convergence is proven for finite element approximation of elliptic parameter identification problems with pointwise measurements.

The developed methods were applied to parameter identification problems in fluid dynamics and chemical models in multidimensional reactive flows. In [5] and [7], parameter identification problems in the context of CFD applications are considered. The parameters arise by the modeling of unknown (Dirichlet or Neumann) boundary conditions. The precise estimation of these parameters leads to calibrated models with good prediction properties. The papers [3] and [6] deal with parameter estimation for multidimensional combustion problems. Here, the Arrhenius parameters and diffusion coefficients for a hydrogen flame are calibrated. The underlying model consists of the compressible Navier-Stokes equations and nine (nonlinear) convection-diffusion-reaction equations for chemical species.

Research 2004 at RICAM

In October 2004, Dr. Vexler has started his work in RICAM. In the last months, he has worked on the problem of optimal vortex reduction by non-stationary flows described by Navier-Stokes equations. For this problem he has investigated the appropriate choice of the cost functional, which has to be directly related to a physically correct definition of a vortex. Several numerical tests based on space time finite element discretization show the importance of the right choice of the vortex description for such problems.

Moreover, in the last months, Dr. Vexler has continued his work on efficient numerical solution of optimization problems governed by parabolic partial differential equations. In the recent paper [9], precise algorithmic evaluation of the derivatives required in second order optimization algorithms is discussed based on space time finite element discretization. Additionaly, a storage reduction technique is proposed allowing for only logarithmic growth of storage with respect to the fineness of the time-discretization.

Scientific Visits and Talks

28.03.2004 - 29.03.2004 "Adaptive Finite Element Methods for Parameter Identification Problems", RICAM, Linz, Austria (invited by Prof. Dr. Heinz W. Engl)

09.05.2004 - 18.05.2004 "Adaptive Finite Element Methods for Parameter Identification Problems", University of Pau, France (invited by Prof. Dr. Roland Becker)

14.06.2004 - 18.06.2004 "Adaptive Finite Element Methods for Parameter Identification Problems", University of Graz, Austria (invited by Prof. Dr. Karl Kunisch)

30.06.2004 - 02.07.2004 "Parameter Estimation and Sensitivity Analysis with Adaptive Finite Elements", International Workshop on Parameter Estimation and Optimal Design of Experiments (PARAOPE 2004), Heidelberg, Germany

24.07.2004 – 28.07.2004 "Mesh Adaptation for Parameter Calibration in Fluid Dynamics", European Congress on Computational Methods in Applied Sciences and Engineering (ECCO-

MAS 2004), Jyväskylä, Finland

16.11.2004 - 18.11.2004 “Adaptive Finite Element Methods for Optimization Problems”, University of Graz, Austria (invited by Prof. Dr. Karl Kunisch)

Scientific Cooperations

Internal Cooperations with

Prof. Dr. Karl Kunisch, Research Group "Optimization and Control", RICAM
Dr. Roland Griesse, Research Group "Optimization and Control", RICAM
Dr. Joachim Schöberl, Research Group "Computational Mathematics for Direct Field Problems", RICAM
PD Dr. Arnd Rösch, Research Group "Inverse Problems”, RICAM

External Cooperations with

Prof. Dr. Rolf Rannacher, University of Heidelberg, Germany
Prof. Dr. Roland Becker, University of Pau, France
Dr. Malte Braack, University of Heidelberg, Germany
Dipl. Math. Dominik Meidner, University of Heidelberg, Germany

Participation at conferences

30.06.2004 - 02.07.2004 International Workshop on Parameter Estimation and Optimal Design of Experiments (PARAOPE 2004), Heidelberg, Germany

24.07.2004 - 28.07.2004 European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2004), Jyväskylä, Finland

Publications

Published

1) B. Vexler
Adaptive Finite Element Methods for Parameter Identification Problems,
PhD thesis, University of Heidelberg, 2004.

2) R. Becker and B. Vexler.
A Posteriori Error Estimation for Finite Element Discretization of Parameter Identification Problems, Numerische Mathematik, Vol. 96-3, pp. 435-459, 2004.

3) R. Becker, M. Braack and B. Vexler.
Numerical Parameter Estimation for Chemical Models in Multidimensional Reactive Flows, Combustion Theory and Modelling, Vol. 8-4, pp. 661-682, 2004.

4) R. Becker and B. Vexler.
A Posteriori Error Estimates for Parameter Identification, in Proc. of ENUMATH 2003, Prag, Aug. 18-22, pp. 131-140, 2004.

5) B. Vexler.
Mesh Adaptation for Parameter Calibration in Fluid Dynamics
in Proc. of ECCOMAS 2004, Jyväskylä, July 24-28, 2004.

Accepted

6) R. Becker, M. Braack and B. Vexler.
Parameter Identification for Chemical Models in Combustion Problems, Applied Numerical Mathematics, to appear, 2004.

7) R. Becker and B. Vexler.
Mesh Refinement and Numerical Sensitivity Analysis for Parameter Calibration of Partial Differential Equations, Journal of Computational Physics, to appear, 2004.

Submitted

8) R. Rannacher and B. Vexler.
A Priori Error Estimates for the Finite Element Discretization of Elliptic Parameter Identification Problems with Pointwise Measurements, submitted, 2004.

9) R. Becker, D. Meidner and B. Vexler.
Efficient Numerical Solution of Parabolic Optimization Problems by Finite Element Methods, submitted, 2004.

Preprints

10) R. Becker, M. Braack and B. Vexler.
Numerical Parameter Estimation for Chemical Models in Multidimensional Reactive Flows, Preprint 2004 - 20 (SFB 359), University of Heidelberg, 2004

11) R. Rannacher and B. Vexler
A Priori Error Estimates for the Finite Element Discretization of Elliptic Parameter Identification Problems with Pointwise Measurements, Preprint 2004 - 29 (SFB 359), University of Heidelberg, 2004

12) R. Becker and B. Vexler.
Mesh Refinement and Numerical Sensitivity Analysis for Parameter Calibration of Partial Differential Equations, Report 2004-15, RICAM, Linz, 2004